

DRAFT REPORT

Validation of an Androgen Receptor Binding Assay–Task 7

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Participation

The following principal staff participated in the conduct of this study:

Study Director:

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Scientists:

Lyle Sasser, Ph.D.

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Jeff Creim

Data Facilitator:

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Quality Assurance :

Mary Lynn

Janet Coultier

Study Dates and Data Retention

Study initiation date:

10 June 2005

Experimental start date:

10 July 2005

Experimental end date:

28 October 2005

Richland, Battelle will retain all supporting documentation, including raw data and written records, for a period of up to five years following submission of the final report to Environmental Protection Agency. Also, electronic data files will be provided to Data Coordination Center at Battelle, Columbus. At the end of this period, Battelle will be notified to determine whether the data (excluding proprietary information) will be transferred, retained, or destroyed.

Statement of Compliance

This study was conducted in compliance with U.S. EPA Good Laboratory Practice Regulations as set forth in Part 160 Title 40 of the Code of Federal Regulations with the exception listed below. This study was conducted under my scientific guidance and management.

Exception: The dose solutions used in the study were not analyzed; however, the stability of the stock concentrations of methyltrienolone, dexamethasone and some of the test chemicals in ethanol were evaluated and are reported separately by Battelle. As directed by EPA, the supplier's purity values was accepted and no further characterization was conducted except for those chemicals noted in the item above that were tested for stability.

James E. Morris, Ph.D.

Study Director

Signature

Date

Quality Assurance Statement

This study was inspected in accordance with Battelle, Richland standard operating procedures. Based on audits conducted, the results reported herein accurately reflect the methods used and the data collected for this study.

All findings were reported to the Study Director and Battelle, Richland Management.

Inspection/Audit Dates:	Study Phase Audited:	Date(s) reported to Study Director and Management:
September 28, 2005	Audit of assay activities	September 29, 2005

Quality Assurance

Signature

Date

Glossary of Abbreviations

$B_{\max}$	binding maximum
EPA	Environmental Protection Agency
HAP	hydroxylapatite
IC_{50}	concentration at which 50% of specific activity is inhibited
K_d	dissociation constant
K_i	inhibitory constant
TEDG + PMSF buffer	buffer with Tris, ethylene diamine tetraacetic acid, dithiothreitol, glycerol, sodium molybdate, triamcinolone acetonide and phenylmethylsulfonyl fluoride

Summary

The objective of this study was to evaluate the inhibition of androgen receptor binding of R1881 in rat ventral prostate cytosol by known chemicals. This *in vitro* test method involved combining cytosol, tracer, and test or control substances in a common reaction vessel. The inhibitory effect of the test substance on androgen receptor binding of R1881 was evaluated by measuring the amount of bound ^3H -R1881 (tracer). Battelle, Richland conducted three separate experiments to evaluate the inhibition of androgen receptor binding of ^3H -R1881 by the test substances.

The cytosol used in these experiments was prepared and characterized at Battelle Richland. A series of saturation and competitive binding experiments were conducted using the cytosol.

A total of three saturation experiments were conducted and the amount of cytosolic protein used for each incubation in the saturation binding experiments was 0.6 mg. The K_d observed across the three saturation experiments was 0.92, 0.90, and 0.92 nM and the B_{max} observed was 11.85, 11.34, and 11.11 fmoles/100 ug.

A series of competitive binding experiments were conducted using 1.0 mg of cytosolic protein for each assay tube. The IC_{50} values for R1881 were determined to be 1.76, 1.77, 1.50, 1.50, 1.47, 1.59, 1.13, 1.57, 1.64, 1.53, 1.61, 1.35, 1.67, 1.41, 1.58, 1.39, 1.21, and 1.44 nM. The IC_{50} values for dexamethasone were determined to be 40.0, 36.7, 35.1, 33.0, 41.9, 30.2, 1.91, 32.4, 32.3, 38.0, 40.4, 18.6, 34.7, 35.3, 39.2, 34.3, 29.8, and 36.69 μM . The RBA values for dexamethasone in comparison to R1881 were, 0.0044, 0.0044, 0.0043, 0.0045, 0.0035, 0.0053, 0.0059, 0.0049, 0.0051, 0.0040, 0.0040, 0.0073, 0.0048, 0.0040, 0.0040, 0.0041, 0.0041, and 0.0039 %.

For the unknown substances the following data was derived from the series of competitive assays in which each unknown was measured in three separate assay runs.

The IC_{50} values for CR42340 were determined to be 1.85, 2.00 and $2.19 \times 10^{-9}\text{M}$. The RBA values for CR42340 in comparison to R1881 were 85.21, 81.92, and 69.66 %.

The IC_{50} values for CR42341 were determined to be 5.13, 7.42 and $7.10 \times 10^{-7}\text{M}$. The RBA values for CR42341 in comparison to R1881 were 0.2713, 0.1629, and 0.2035 %.

The IC_{50} values for CR42342 were determined to be 4.84, 5.56 and $3.05 \times 10^{-8}\text{M}$. The RBA values for CR42342 in comparison to R1881 were 3.45, 2.53, and 5.16 %.

The IC_{50} values for CR42343 were determined to be 2.38, 4.62 and $2.21 \times 10^{-6}\text{M}$. The RBA values for CR42343 in comparison to R1881 were 0.0629, 0.0319, and 0.0719 %.

The IC_{50} values for CR42344 were determined to be 3.51, 4.73 and $2.29 \times 10^{-6}\text{M}$. The RBA values for CR42344 in comparison to R1881 were 0.0428, 0.0312, and 0.0696 %.

The IC_{50} values for CR42345 were determined to be 2.01, 1.82 and $1.92 \times 10^{-6}\text{M}$. The RBA values for CR42345 in comparison to R1881 were 0.0831, 0.0777, and 0.0820 %.

The IC₅₀ values for CR42346 were determined to be 9.22, 10.60 and 9.14 x10⁻⁸M. The RBA values for CR42346 in comparison to R1881 were 1.51, 1.15, and 1.58 %.

The IC₅₀ values for CR42348 were determined to be 3.15, 4.81, and 2.25 X10⁻⁵M. The RBA values for CR42348 in comparison to R1881 were 0.0048, 0.0031, and 0.0071 %.

The IC₅₀ values for CR42349 were determined to be 2.70, 2.93, and 1.62 X10⁻⁵M. The RBA values for CR42349 in comparison to R1881 were 0.0055, 0.0050, and 0.0098 %.

The IC₅₀ values for CR42350 were determined to be 5.15, 4.84, and 4.81 X10⁻⁵M. The RBA values for CR42349 in comparison to R1881 were 0.0031, 0.0034, and 0.0032 %.

The IC₅₀ values for CR42351 were determined to be 9.08, 9.70 and 8.86 x10⁻⁵M. The RBA values for CR42351 in comparison to R1881 were 0.0018, 0.0015, and 0.0018 %.

The IC₅₀ values for CR42352 were determined to be 2.71, 3.94, and 2.36 X10⁻⁹M. The RBA values for CR42352 in comparison to R1881 were 0.0042, 0.0041, and 0.0057 %.

The IC₅₀ values for CR42353 were determined to be 2.87, 4.03, and 3.06 X10⁻⁵M. The RBA values for CR42353 in comparison to R1881 were 0.0039, 0.0040, and 0.0045 %.

The IC₅₀ values for CR42355 were determined to be 5.09, 6.72 and 6.44 x10⁻⁵M. The RBA values for CR42355 in comparison to R1881 were 0.0027, 0.0018, and 0.0022 %.

The IC₅₀ values for CR42360 were determined to be 2.83, 4.16, and 3.19 X10⁻⁵ M. The RBA values for CR42360 in comparison to R1881 were 0.0040, 0.0039, and 0.0042 %.

The IC₅₀ values for CR42363 were determined to be 4.17, 4.41, and 5.05 X10⁻⁵ M. The RBA values for CR42363 in comparison to R1881 were 0.0038, 0.0037, and 0.0030%.

The IC₅₀ values for CR42365 were determined to be 4.70, 4.36, and 4.69 X10⁻⁷ M. The RBA values for CR42365 in comparison to R1881 were 0.3747, 0.4060, and 0.3203 %.

The IC₅₀ values for CR42367 were determined to be 3.15, 3.95, and 3.33 X10⁻⁴ M. The RBA values for CR42367 in comparison to R1881 were 0.0006, 0.0004, and 0.0005 %.

The IC₅₀ values for CR42368 were determined to be 1.28, 1.33, and 1.66 X10⁻⁵ M. The RBA values for CR42368 in comparison to R1881 were 0.0137, 0.0133, and 0.0090 %.

The IC₅₀ values for CR42369 were determined to be 2.96, 3.18 and 3.14 x10⁻⁵M. The RBA values for CR42369 in comparison to R1881 were 0.0047, 0.0038, and 0.0046 %.

The IC₅₀ and RBA values were calculated for the following test substances by extrapolation since activity was approaching the 50% inhibition.

The IC₅₀ values for CR42347 were determined to be 5.20, 11.80 and 7.43 x10⁻⁵M. The RBA values for CR42347 in comparison to R1881 were 0.0027, 0.0010, and 0.0019 %.

The IC₅₀ values for CR42354 were determined to be 1.76, 1.50, and 1.44 X10⁻⁴M. The RBA values for CR42354 in comparison to R1881 were 0.0009, 0.0011, and 0.0011 %.

The IC₅₀ values for CR42361 were determined to be 3.89, 3.04 and 3.07 x10⁻⁴M. The RBA values for CR42361 in comparison to R1881 were 0.0004, 0.0005, and 0.0005 %.

The IC₅₀ values for CR42362 were determined to be 6.08, 6.61, and 8.96 X10⁻⁴ M. The RBA values for CR42362 in comparison to R1881 were 0.0003, 0.0003, and 0.0002%.

The following test substance did not exhibit any significant inhibition of the binding of [³H] R1881 to the androgen receptor.

The IC₅₀ and RBA values for CR42357 were not determined because of insufficient activity.

The IC₅₀ and RBA values for CR42358 were not determined because of insufficient activity.

The IC₅₀ and RBA values for CR42359 were not determined because of insufficient activity.

Introduction

The Food Quality Protection Act of 1996 was enacted by Congress to authorize the Environmental Protection Agency (EPA) to implement a screening program on pesticides and other chemicals found in food or water sources for endocrine effects in humans. Thus, the U.S. EPA is implementing an Endocrine Disruptor Screening Program. In this program, comprehensive toxicological and ecotoxicological screens and tests are being developed for identifying and characterizing the endocrine effects of various environmental contaminants, industrial chemicals, and pesticides. The program's aim is to develop a two-tiered approach, e.g., a combination of in vitro and in vivo mammalian and ecotoxicological screens (Tier 1) and a set of in vivo tests (Tier 2) for identifying and characterizing endocrine effects of pesticides, industrial chemicals, and environmental contaminants. Validation of the individual screens and tests is required, and the Endocrine Disruptor Method Validation Committee will provide advice and counsel on the validation assays.

One potential endocrine target for environmental chemicals is the androgen receptor. The objective of this study was to evaluate the inhibition of androgen receptor (AR) binding of R1881 in rat ventral prostate cytosol by known chemicals, thus validating androgen receptor binding as a potential tool for screening environmental chemicals. Rat ventral prostate cytosol was selected because it provided a biological source of the androgen receptor. Since the assay was evaluated for its potential to serve as a screening assay, the use of rat tissue enhanced its availability.

Experimental Methods

Test Substances Information and Preparation

Battelle provided the following test materials at the necessary dilutions:

- Reference Substance: Unlabelled R1881–Methyltrienolone (CAS No. 965-93-5) (Lot# 3411228)
- Test Substance: Dexamethasone (CAS No. 50-02-2)(Lot # P4311T)

The test and reference substances were used in the androgen receptor-binding assay to determine relative binding affinities (RBAs).

The following were prepared at Battelle, Richland:

- Buffer with Tris(Tris base; Lot# 120K5444 & Tris HCl; Lot# 072K5420), ethylene diamine tetraacetic acid(EDTA; Lot# 99H0095), dithiothreitol (DTT) (Lot# 51K17412), glycerol (Lot# 10655Ka), Sodium molybdate (Lot # 30K0210) and phenylmethylsulfonyl fluoride (PMSF) (Lot# 60K0701)- (TEDG + PMSF Buffer) (pH 7.4) (lot 0677-10-01)
- Triamcinolone acetonide (TRIAM) (Sigma; Lot # 40K1266)
- Absolute ethanol (AAPER ; Lot# 03K10UA)

- Hydroxylapatite (HAP) (lot# 154014, 190682, 251603, 251604)

The following reagent was obtained from supplier as identified:

- Substrate: ^3H -R1881 (CAS No. 965-93-5) (Perkin-Elmer Cat# NET 590; Lot # 3559-507; Specific Activity = 82 Ci/mmol)

R1881 Preparation

Chemical Repository, Sequim, Washington provided the R1881 stock solutions (30 mM) prepared in absolute ethanol. Chemical Repository was responsible for the preparation and analysis of the R1881 stocks.

Dilutions of the unlabeled R1881 stock were prepared in ethanol for the saturation assays at 1.0×10^{-5} and 1.0×10^{-6} M. In the assay, 7.5 ul, 15.0 ul, 21.0 ul, 30.0 and 45.0 ul of the 1.0×10^{-5} M stock was used to generate a final unlabeled R1881 concentration in the assay tubes of 0.025, 0.05 0.07, 0.10, and 0.15 uM. To generate a final unlabeled R1881 concentration in the assay tubes of 0.25, 0.05 and 0.10 uM, 7.5, 15 or 30 ul of 1.0×10^{-6} M stock were used.

Dilutions of the R1881 stock solutions were prepared in ethanol for competitive assays. The final assay target concentrations for R1881 were 1.0×10^{-6} (NSB), 1.0×10^{-7} , 1.0×10^{-8} , 1.0×10^{-9} , 1.9×10^{-10} , and 1.0×10^{-11} M. The total volume of solvent used in each assay was no more than 3.33% of the total assay volume.

Dexamethasone Preparation

Chemical Repository (Sequim, WA) provided the dexamethasone stock solutions (30 mM) prepared in absolute ethanol. The Chemical Repository was responsible for the preparation of the dexamethasone stock.

Dilutions of the dexamethasone stock solutions were prepared in ethanol by Battelle, Richland. The final target concentrations for dexamethasone in assay tubes were 10^{-3} , 10^{-4} , 10^{-5} , 10^{-6} , 10^{-7} , 10^{-8} , 10^{-9} , and 10^{-10} M. The total volume of solvent used in each assay was no more than 3.33% of the total assay volume.

Marker/Tracer Preparation

The marker/tracer solution was prepared from the radiolabeled R1881 received from vendor and stored at- 20°C in the original container.

Dilutions of the ^3H R1881 stock were prepared in ethanol for the saturation assays at 1.0×10^{-7} and 1.0×10^{-8} M. In the saturation assay, 7.5 ul, 15.0 ul, 21.0 ul, 30.0 and 45.0 ul of the 1.0×10^{-7} M stock was used to generate a final ^3H R1881 concentration in the assay tubes of 0.25, 0.5 0.7, 1.0, and 1.5 nM. To generate a final ^3H R1881 concentration in the assay tubes of 2.5, 5.0 and 10.0 nM, 7.5, 15 or 30 ul of 1.0×10^{-7} M stock were used.

For competitive assays, the [^3H]-R1881 was diluted with ethanol to achieve a substrate solution at a concentration of 10 nM. The substrate solution (30 μL) was added to the incubation mixtures to achieve a final concentration of 1 nM [^3H]-R1881 in the 300 ul volume for the assay.

Preparation of Rat Ventral Prostate Cytosol

Rat ventral prostate cytosol was prepared by Battelle, Richland.

- The rat prostate cytosol was prepared by Battelle – Richland per Battelle SOPs # 331-ED-I-99-00 and 331-AR-I-01-01). Briefly, the ventral prostate tissues were collected from 190 Sprague-Dawley male rats (85 to 100 days of age) castrated 24 hours prior to being humanely killed. The supplier was Charles River. For the study, weighed and trimmed prostate tissues are placed in ice-cold buffer prepared with Tris, Ethylenediaminetetraacetic acid and Glycerol (TEDG) with phenylmethylsulfonyl fluoride (PMSF) with final extraction volume equaling a ratio of 0.1 g of tissue per 1.0 ml TEDG buffer with PMSF. The tissues are homogenized and the cytosol pooled, aliquoted and stored at –80 degrees centigrade.

Assays

Protein Assay:

The protein concentration of the cytosol preparation was determined for each batch of the cytosol as described in Battelle, Richland SOP (331-ER-I-02-00). In brief, a six-point curve was prepared, ranging from 0.2 to 2.0 mg protein / ml. The protein standards were made from bovine serum albumin (BSA). Protein was determined using a BioRad Protein Assay Kit purchased from BioRad (Hercules, CA). To a 1- μ l aliquot of standard or unknown, 200 μ L of dye reagent was added and mixed. The samples were placed at room temperature for at least 5 minutes and up to an hour to allow for color development. Absorbance (600 nm) was measured using a plate reader. The protein concentration of the cytosol sample was determined by extrapolation of the absorbance value using the standard curve developed using the protein standard.

Evaluation of the Cytosol for Conducting Androgen Receptor Competitive Binding Assays

Prior to conducting the androgen receptor competitive binding assays with unknown chemicals, the cytosol was characterized at Battelle, Richland. This was accomplished in two steps as follows:

- 1) A series of saturation radioligand binding assays was conducted to demonstrate androgen receptor specificity and saturation. Nonlinear regression analysis of these data and subsequent Scatchard plots document androgen receptor binding affinity (K_d) and the number of receptors (B_{max}).
- 2) A series of androgen receptor competitive binding assays were conducted using R1881 and dexamethasone, substances with known affinities for the androgen receptor. Comparison of IC_{50} values (i.e., the concentration of a substance that inhibits [^{3} H]-R1881 binding by 50%) from

these assays with reported values in the literature assisted in documenting that the cytosol was appropriate for routine use in the laboratory.

Saturation Radioligand Binding Assay

Androgen receptor saturation binding experiments measured total, non-specific, and specific binding of increasing concentrations of ^3H -R1881 under conditions of equilibrium.

The experimental setup and details of the saturation binding assay are specified in the study protocol and specific assay protocols. The saturation binding experiments were conducted as three independent replicates. The same technician conducted all three replicate experiments.

Competitive Binding Assay (Inhibition of Androgen Receptor Binding of ^3H -R1881 by Test substance)

An androgen receptor competitive binding assay measures the binding of a single concentration of ^3H -R1881 in the presence of increasing concentrations of a test substance. The experimental setup and details of the competitive binding assay are specified in the attached study protocol. These experiments tested the androgen receptor binding of ^3H -R1881 in the presence of multiple concentrations of a test substance. The inhibition experiments were conducted as three independent replicates. All three replicate experiments for a given test substance were conducted by the same technician and there were three (triplicate) repetitions for each concentration within a given replicate.

Control samples were included for each replicate experiment. These included:

- Vehicle or ethanol control (substrate, buffer, vehicle [used for preparation of test substance solutions], and cytosol)
- Non-specific background control (substrate, buffer, R1881, and cytosol).

Six repetitions of each type of control were included with each replicate experiment and were treated the same as the other samples. The control sets were split so that three tubes (of each control type) were run at the beginning and three at the end of each replicate set. Except for run 504 where 2 ethanol control samples were dropped due to spillage.

Description of Data Calculations

Battelle, Richland supplied all raw data in electronic format using Microsoft Excel[®] spreadsheets and Prism templates.

IC₅₀ Calculation

Data for the non-radiolabeled R1881 standard curve and each test substance were plotted as the percentage of ^3H -R1881 bound versus the molar concentration (log) of competitor. Estimates of IC₅₀ values were determined using appropriate nonlinear curve fitting software to fit a one-site competitive binding model. The model was constrained to fit the bottom of the curve to 0% and the top to 100%.

Relative Binding Affinity Values

The RBA value for each test article was calculated by dividing the IC_{50} value for R1881 by the IC_{50} of the test substance and expressing the value as a percent (e.g., RBA for R1881 = 100%).

Criteria for Data Acceptance

All data obtained were reported except runs 503 and 504 were dropped due to unacceptable standard curves.

Results

Rat ventral prostate cytosol was prepared by Battelle, Richland at a protein concentration of 5.532 mg/mL. A series of saturation and competitive binding experiments were conducted using the cytosol.

A total of three saturation experiments were conducted and the amount of cytosolic protein used for each incubation in the saturation binding experiments was 0.6 mg. The K_d observed across the three saturation experiments was 0.92, 0.90, and 0.92 nM and the B_{max} observed was 11.85, 11.34, and 11.11 fmoles/100 ug. Two additional assays were conducted but not used because of unacceptable standard curve and/or weak positive response.

A series of competitive binding experiments were conducted using 1.0 mg of cytosolic protein for each assay tube. The IC_{50} values for R1881 were determined to be 1.76, 1.77, 1.50, 1.50, 1.47, 1.59, 1.13, 1.57, 1.64, 1.53, 1.61, 1.35, 1.67, 1.41, 1.58, 1.39, 1.21, and 1.44 nM. The IC_{50} values for dexamethasone were determined to be 40.0, 36.7, 35.1, 33.0, 41.9, 30.2, 1.91, 32.4, 32.3, 38.0, 40.4, 18.6, 34.7, 35.3, 39.2, 34.3, 29.8, and 36.69 μ M. The RBA values for dexamethasone in comparison to R1881 were, 0.0044, 0.0044, 0.0043, 0.0045, 0.0035, 0.0053, 0.0059, 0.0049, 0.0051, 0.0040, 0.0040, 0.0073, 0.0048, 0.0040, 0.0040, 0.0041, 0.0041, and 0.0039 %.

For the unknown substances the following data was derived from the series of competitive assays in which each unknown was measured in three separate assay runs.

The IC_{50} values for CR42340 were determined to be 1.85, 2.00 and 2.19 $\times 10^{-9}$ M. The RBA values for CR42340 in comparison to R1881 were 85.21, 81.92, and 69.66 %.

The IC_{50} values for CR42341 were determined to be 5.13, 7.42 and 7.10 $\times 10^{-7}$ M. The RBA values for CR42341 in comparison to R1881 were 0.2713, 0.1629, and 0.2035 %.

The IC_{50} values for CR42342 were determined to be 4.84, 5.56 and 3.05 $\times 10^{-8}$ M. The RBA values for CR42342 in comparison to R1881 were 3.45, 2.53, and 5.16 %.

The IC₅₀ values for CR42343 were determined to be 2.38, 4.62 and 2.21 x10⁻⁶M. The RBA values for CR42343 in comparison to R1881 were 0.0629, 0.0319, and 0.0719 %.

The IC₅₀ values for CR42344 were determined to be 3.51, 4.73 and 2.29 X10⁻⁶M. The RBA values for CR42344 in comparison to R1881 were 0.0428, 0.0312, and 0.0696 %.

The IC₅₀ values for CR42345 were determined to be 2.01, 1.82 and 1.92 x10⁻⁶M. The RBA values for CR42345 in comparison to R1881 were 0.0831, 0.0777, and 0.0820 %.

The IC₅₀ values for CR42346 were determined to be 9.22, 10.60 and 9.14 x10⁻⁸M. The RBA values for CR42346 in comparison to R1881 were 1.51, 1.15, and 1.58 %.

The IC₅₀ values for CR42348 were determined to be 3.15, 4.81, and 2.25 X10⁻⁵M. The RBA values for CR42348 in comparison to R1881 were 0.0048, 0.0031, and 0.0071 %.

The IC₅₀ values for CR42349 were determined to be 2.70, 2.93, and 1.62 X10⁻⁵M. The RBA values for CR42349 in comparison to R1881 were 0.0055, 0.0050, and 0.0098 %.

The IC₅₀ values for CR42350 were determined to be 5.15, 4.84, and 4.81 X10⁻⁵M. The RBA values for CR42349 in comparison to R1881 were 0.0031, 0.0034, and 0.0032 %.

The IC₅₀ values for CR42351 were determined to be 9.08, 9.70 and 8.86 x10⁻⁵M. The RBA values for CR42351 in comparison to R1881 were 0.0018, 0.0015, and 0.0018 %.

The IC₅₀ values for CR42352 were determined to be 2.71, 3.94, and 2.36 X10⁻⁹M. The RBA values for CR42352 in comparison to R1881 were 0.0042, 0.0041, and 0.0057 %.

The IC₅₀ values for CR42353 were determined to be 2.87, 4.03, and 3.06 X10⁻⁵M. The RBA values for CR42353 in comparison to R1881 were 0.0039, 0.0040, and 0.0045 %.

The IC₅₀ values for CR42355 were determined to be 5.09, 6.72 and 6.44 x10⁻⁵M. The RBA values for CR42355 in comparison to R1881 were 0.0027, 0.0018, and 0.0022 %.

The IC₅₀ values for CR42360 were determined to be 2.83, 4.16, and 3.19 X10⁻⁵ M. The RBA values for CR42360 in comparison to R1881 were 0.0040, 0.0039, and 0.0042 %.

The IC₅₀ values for CR42363 were determined to be 4.17, 4.41, and 5.05 X10⁻⁵ M. The RBA values for CR42363 in comparison to R1881 were 0.0038, 0.0037, and 0.0030%.

The IC₅₀ values for CR42365 were determined to be 4.70, 4.36, and 4.69 X10⁻⁷ M. The RBA values for CR42365 in comparison to R1881 were 0.3747, 0.4060, and 0.3203 %.

The IC₅₀ values for CR42367 were determined to be 3.15, 3.95, and 3.33 X10⁻⁴ M. The RBA values for CR42367 in comparison to R1881 were 0.0006, 0.0004, and 0.0005 %.

The IC₅₀ values for CR42368 were determined to be 1.28, 1.33, and 1.66 X10⁻⁵ M. The RBA values for CR42368 in comparison to R1881 were 0.0137, 0.0133, and 0.0090 %.

The IC₅₀ values for CR42369 were determined to be 2.96, 3.18 and 3.14 x10⁻⁵M. The RBA values for CR42369 in comparison to R1881 were 0.0047, 0.0038, and 0.0046 %.

The IC₅₀ and RBA values were calculated for the following test substances by extrapolation since activity was approaching the 50% inhibition.

The IC₅₀ values for CR42347 were determined to be 5.20, 11.80 and 7.43 x10⁻⁵M. The RBA values for CR42347 in comparison to R1881 were 0.0027, 0.0010, and 0.0019 %.

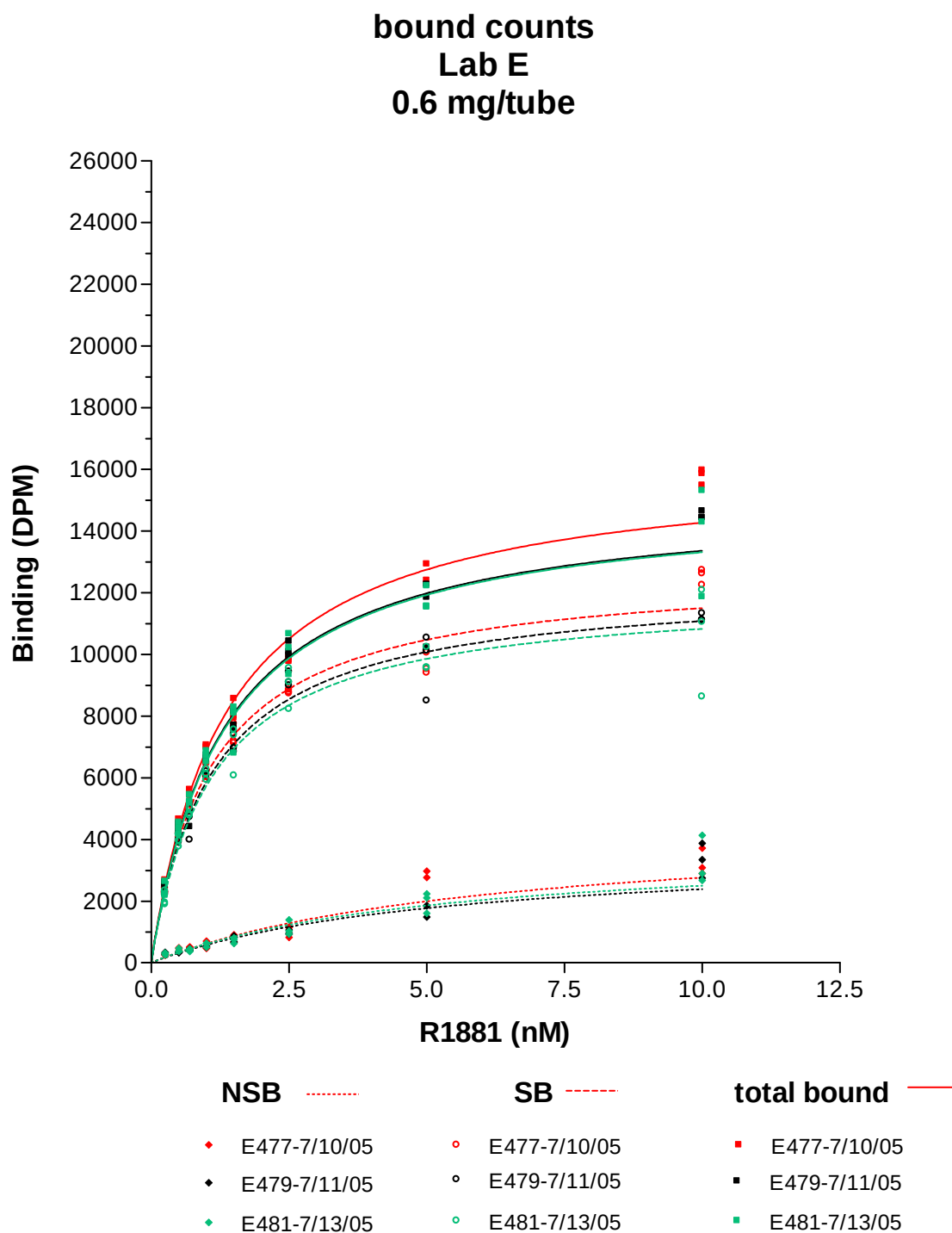
The IC₅₀ values for CR42354 were determined to be 1.76, 1.50, and 1.44 X10⁻⁴M. The RBA values for CR42354 in comparison to R1881 were 0.0009, 0.0011, and 0.0011 %.

The IC₅₀ values for CR42361 were determined to be 3.89, 3.04 and 3.07 x10⁻⁴M. The RBA values for CR42361 in comparison to R1881 were 0.0004, 0.0005, and 0.0005 %.

The IC₅₀ values for CR42362 were determined to be 6.08, 6.61, and 8.96 X10⁻⁴ M. The RBA values for CR42362 in comparison to R1881 were 0.0003, 0.0003, and 0.0002%.

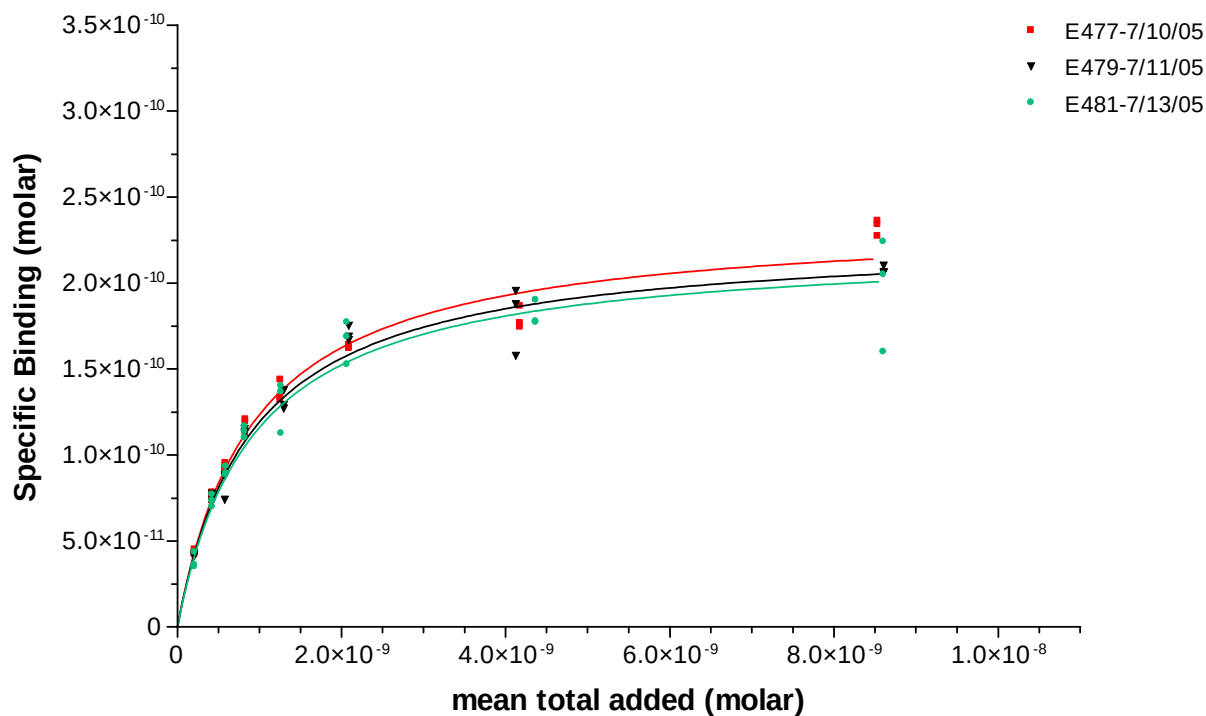
The following test substance did not exhibit any significant inhibition of the binding of [³H] R1881 to the androgen receptor.

The IC₅₀ and RBA values for CR42357 were not determined because of insufficient activity.
The IC₅₀ and RBA values for CR42358 were not determined because of insufficient activity.
The IC₅₀ and RBA values for CR42359 were not determined because of insufficient activity.

Figure 1: Saturation Binding and Scatchard Plots of ^3H -R1881 to the Androgen Receptor

Lab E

0.6 mg/tube



Specific bound	E477-7/10/05	E479-7/11/05	E481-7/13/05
BMAX	2.370e-010	2.268e-010	2.222e-010
KD	9.194e-010	9.039e-010	9.156e-010
Std. Error			
BMAX	5.754e-012	7.052e-012	9.612e-012
KD	4.358e-011	5.508e-011	7.680e-011
95% Confidence Intervals			
BMAX	2.251e-010 to 2.490e-010	2.122e-010 to 2.414e-010	2.023e-010 to 2.422e-010
KD	8.290e-010 to 1.010e-009	7.897e-010 to 1.018e-009	7.563e-010 to 1.075e-009
Goodness of Fit			
Degrees of Freedom	22	22	22
R ² (unweighted)	0.9735	0.9742	0.9417
Weighted Sum of Squares (1/Y ²)	0.06464	0.1082	0.2198
Absolute Sum of Squares	2.078e-021	1.823e-021	3.947e-021
Sy.x	9.718e-012	9.102e-012	1.339e-011
Data			
Number of X values	24	24	24
Number of Y replicates	1	1	1
Total number of values	24	24	24
Number of missing values	0	0	0

Scatchard Display
Lab E
0.6 mg/tube

- E477-7/10/05
- ▼ E479-7/11/05
- E481-7/13/05

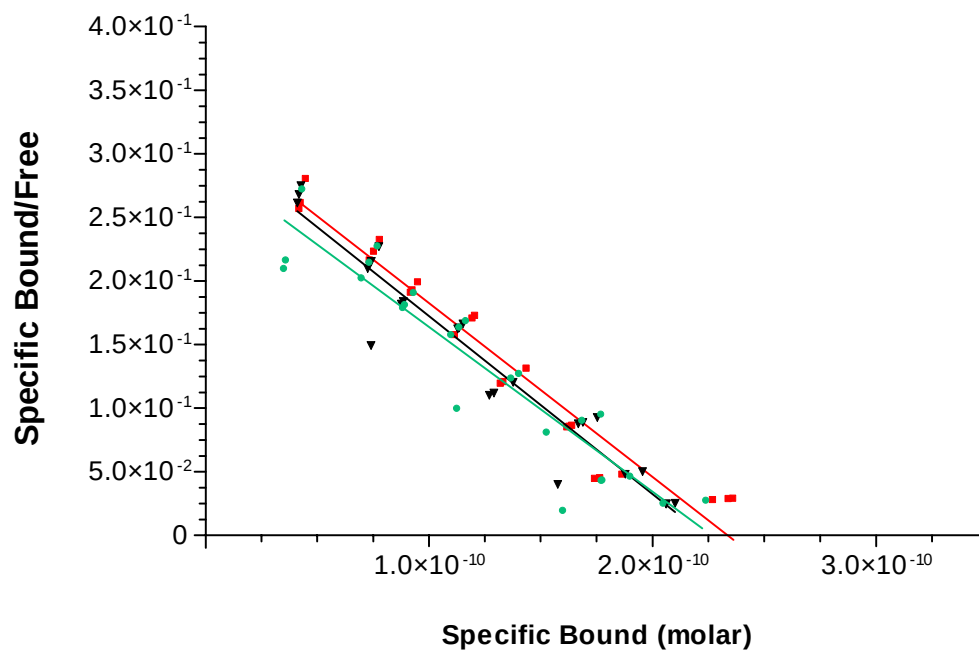
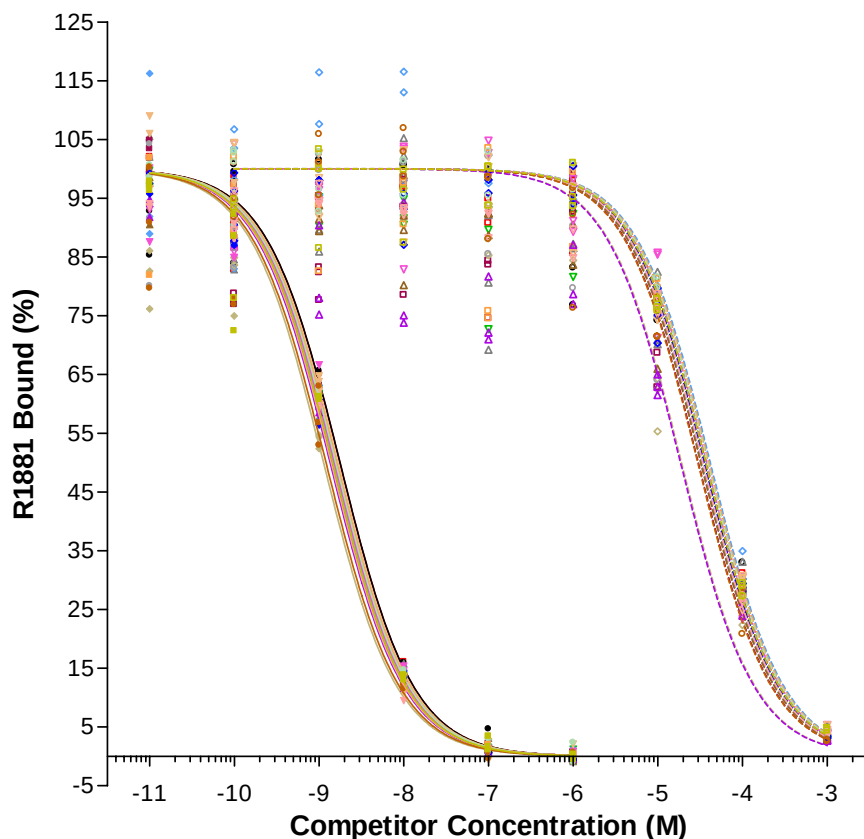


Figure 2: Competitive Binding of R1881 and Dexamethasone (Weak Positive) to the Androgen Receptor

WA 4-11-7 Competitive

**Standard Curve and 'Weak Positive'
Protein
1.0 mg per tube**



Standard Curve	Weak Positive	Standard Curve	Weak Positive
■ E-489-8/9/05	□ E-489-8/9/05	▼ E-508-9/28/05	▼ E-508-9/28/05
• E-490-8/11/05	◦ E-490-8/11/05	■ E-509-10/03/05	■ E-509-10/03/05
▼ E-491-8/15/05	▼ E-491-8/15/05	▲ E-510-10/04/05	▲ E-510-10/04/05
▲ E-499-9/12/05	▲ E-499-9/12/05	▼ E-511-10/06/05	▼ E-511-10/06/05
◆ E-501-9/13/05	◆ E-501-9/13/05	◆ E-512-10/10/05	◆ E-512-10/10/05
■ E-502-9/14/05	■ E-502-9/14/05	● E-513-10/13/05	● E-513-10/13/05
◆ E-504-9/20/05	◆ E-504-9/20/05	▼ E-514-10/18/05	▼ E-514-10/18/05
● E-506-9/26/05	● E-506-9/26/05	● E-515-10/19/05	● E-515-10/19/05
▲ E-507-9/27/05	▲ E-507-9/27/05	■ E-516-10/27/05	■ E-516-10/27/05

Table 1: Saturation Binding Experiments

Run number	Assay date	Technician	K_d (M)	B_{max} (fmol/100 ug)
477	10 July 2005	JEC	0.92×10^{-9}	11.85
479	11 July 2005	JEC	0.90×10^{-9}	11.34
481	13 July 2005	JEC	0.92×10^{-9}	11.11
Mean			0.91×10^{-9}	11.43
SD			0.01×10^{-9}	0.38

Table 2: Competitive Binding Experiments

Run number	Assay date	Technician	R1881		Dexamethasone	
			IC ₅₀ (M)	RBA	IC ₅₀ (M)	RBA(%)
489	09 August, 2005	JEC	1.76×10^{-9}	100	4.00×10^{-5}	0.0044
490	11 August, 2005	JEC	1.77×10^{-9}	100	3.67×10^{-5}	0.0048
491	15 August, 2005	JEC	1.50×10^{-9}	100	3.51×10^{-5}	0.0043
499	12 September 2005	JEC	1.50×10^{-9}	100	3.30×10^{-5}	0.0045
501	13 September 2005	JEC	1.47×10^{-9}	100	4.19×10^{-5}	0.0035
502	14 September 2005	JEC	1.59×10^{-9}	100	3.02×10^{-5}	0.0053
504	20 September 2005	JEC	1.13×10^{-9}	100	1.91×10^{-5}	0.0054
506	26 September 2005	JEC	1.57×10^{-9}	100	3.24×10^{-5}	0.0049
507	27 September 2005	JEC	1.64×10^{-9}	100	3.23×10^{-5}	0.0051
508	28 September 2005	JEC	1.53×10^{-9}	100	3.80×10^{-5}	0.0040
509	03 October 2005	JEC	1.61×10^{-9}	100	4.04×10^{-5}	0.0040
510	04 October 2005	JEC	1.35×10^{-9}	100	1.86×10^{-5}	0.0073
511	06 October 2005	JEC	1.67×10^{-9}	100	3.47×10^{-5}	0.0048
512	10 October 2005	JEC	1.41×10^{-9}	100	3.53×10^{-5}	0.0040
513	13 October 2005	JEC	1.58×10^{-9}	100	3.92×10^{-5}	0.0040
514	18 October 2005	JEC	1.39×10^{-9}	100	3.43×10^{-5}	0.0041
515	19 October 2005	JEC	1.21×10^{-9}	100	2.98×10^{-5}	0.0041
516	27 October 2005	JEC	1.44×10^{-9}	100	3.69×10^{-5}	0.0039
	Mean		1.51×10^{-9}		3.38×10^{-5}	0.0046
	SD		0.17×10^{-9}		0.64×10^{-5}	0.0009

Abbreviations: IC₅₀, concentration at which 50% of activity is inhibited; RBA, relative binding affinity,
RBA of dexamethasone = (IC₅₀ of R1881 / IC₅₀ of dexamethasone) × 100

**Summary Table
(IC50 and RBA)
Lab E**

Run identification:	499	501	502			
Assay start date:	9/12/2005	9/13/2005	9/14/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.50E-09	1.47E-09	1.59E-09	1.52E-09	6.24E-11	4.10%
Weak Positive						
IC50:	3.30E-05	4.19E-05	3.02E-05	3.50E-05	6.09E-06	17.39%
RBA:	0.0045%	0.0035%	0.0053%	0.0044%	0.0009%	19.78%
RBA of means:				0.0043%		
 CR42343						
IC50:	2.38E-06	4.62E-06	2.21E-06	3.07E-06	1.34E-06	43.73%
RBA:	0.0629%	0.0319%	0.0719%	0.0556%	0.0210%	37.81%
RBA of means:				0.0495%		
 CR42344						
IC50:	3.51E-06	4.73E-06	2.29E-06	3.51E-06	1.22E-06	34.74%
RBA:	0.0428%	0.0312%	0.0696%	0.0478%	0.0197%	41.16%
RBA of means:				0.0434%		
 CR42348						
IC50:	3.15E-05	4.81E-05	2.25E-05	3.40E-05	1.30E-05	38.07%
RBA:	0.0048%	0.0031%	0.0071%	0.0050%	0.0020%	40.48%
RBA of means:				0.0045%		
 CR42349						
IC50:	2.70E-05	2.93E-05	1.62E-05	2.42E-05	7.01E-06	28.99%
RBA:	0.0055%	0.0050%	0.0098%	0.0068%	0.0026%	38.76%
RBA of means:				0.0063%		

Run identification:	489	490	491			
Assay start date:	8/9/2005	8/11/2005	8/15/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.76E-09	1.77E-09	1.50E-09	1.68E-09	1.52E-10	9.07%
Weak Positive						
IC50:	4.00E-05	3.67E-05	3.51E-05	3.72E-05	2.51E-06	6.75%
RBA:	0.0044%	0.0048%	0.0043%	0.0045%	0.0003%	6.27%
RBA of means:				0.0045%		
CR42357						
IC50:	no activity	no activity	no activity	no activity	no activity	no activity
RBA:	no activity	no activity	no activity	no activity	no activity	no activity
RBA of means:				no activity		
CR42362						
IC50:	6.08E-04	6.61E-04	8.96E-04	7.21E-04	1.53E-04	21.21%
RBA:	0.0003%	0.0003%	0.0002%	0.0002%	0.0001%	26.91%
RBA of means:				0.0002%		
CR42365						
IC50:	4.70E-07	4.36E-07	4.69E-07	4.58E-07	1.96E-08	4.27%
RBA:	0.3747%	0.4060%	0.3203%	0.3670%	0.0434%	11.81%
RBA of means:				0.3661%		
CR42367						
IC50:	3.15E-04	3.95E-04	3.33E-04	3.47E-04	4.20E-05	12.08%
RBA:	0.0006%	0.0004%	0.0005%	0.0005%	0.0001%	13.10%
RBA of means:				0.0005%		
CR43268						
IC50:	1.28E-05	1.33E-05	1.66E-05	1.43E-05	2.05E-06	14.38%
RBA:	0.0137%	0.0133%	0.0090%	0.0120%	0.0026%	21.49%
RBA of means:				0.0118%		

Run identification:	504	509	510			
Assay start date:	9/20/2005	10/3/2005	10/4/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.13E-09	1.61E-09	1.35E-09	1.36E-09	2.39E-10	17.52%
Weak Positive						
IC50:	1.91E-05	4.04E-05	1.86E-05	2.60E-05	1.24E-05	47.65%
RBA:	0.0059%	0.0040%	0.0073%	0.0057%	0.0017%	28.89%
RBA of means:				0.0052%		
 CR42352						
IC50:	2.71E-05	3.94E-05	2.36E-05	3.00E-05	8.32E-06	27.71%
RBA:	0.0042%	0.0041%	0.0057%	0.0047%	0.0009%	20.02%
RBA of means:				0.0029%		
 CR42353						
IC50:	2.87E-05	4.03E-05	3.01E-05	3.30E-05	6.32E-06	19.15%
RBA:	0.0039%	0.0040%	0.0045%	0.0041%	0.0003%	7.35%
RBA of means:				0.0041%		
 CR42359						
IC50:	no activity	no activity	no activity	no activity	no activity	no activity
RBA:	no activity	no activity	no activity	no activity	no activity	no activity
RBA of means:				no activity		
 CR42360						
IC50:	2.83E-05	4.16E-05	3.19E-05	3.39E-05	6.85E-06	20.19%
RBA:	0.0040%	0.0039%	0.0042%	0.0040%	0.0002%	4.64%
RBA of means:				0.0040%		

Run identification:	506	507	508			
Assay start date:	9/26/2005	051905	9/28/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.57E-09	1.64E-09	1.53E-09	1.58E-09	5.68E-11	3.60%
Weak Positive						
IC50:	3.24E-05	3.23E-05	3.80E-05	3.42E-05	3.28E-06	9.57%
RBA:	0.0049%	0.0051%	0.0040%	0.0047%	0.0006%	12.03%
RBA of means:				0.0046%		
 CR42340						
IC50:	1.85E-09	2.00E-09	2.19E-09	2.01E-09	1.73E-10	8.61%
RBA:	85.2113%	81.9181%	69.6624%	78.9306%	8.1936%	10.38%
RBA of means:				0.0000%		
 CR42350						
IC50:	5.15E-05	4.84E-05	4.81E-05	4.94E-05	1.89E-06	3.83%
RBA:	0.0031%	0.0034%	0.0032%	0.0032%	0.0002%	5.32%
RBA of means:				0.0032%		
 CR42354						
IC50:	1.76E-04	1.50E-04	1.44E-04	1.57E-04	1.69E-05	10.77%
RBA:	0.0009%	0.0011%	0.0011%	0.0010%	0.0001%	10.42%
RBA of means:				0.0010%		
 CR42363						
IC50:	4.17E-05	4.41E-05	5.05E-05	4.54E-05	4.55E-06	10.03%
RBA:	0.0038%	0.0037%	0.0030%	0.0035%	0.0004%	11.94%
RBA of means:				0.0035%		

Run identification:	511	512	513			
Assay start date:	10/6/2005	10/10/2005	10/13/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.67E-09	1.41E-09	1.58E-09	1.55E-09	1.32E-10	8.51%
Weak Positive						
IC50:	3.47E-05	3.53E-05	3.92E-05	3.64E-05	2.43E-06	6.68%
RBA:	0.0048%	0.0040%	0.0040%	0.0043%	0.0005%	10.89%
RBA of means:				0.0043%		
 CR42342						
IC50:	4.84E-08	5.56E-08	3.05E-08	4.49E-08	1.29E-08	28.83%
RBA:	3.4525%	2.5341%	5.1638%	3.7168%	1.3346%	35.91%
RBA of means:				3.4609%		
 CR42345						
IC50:	2.01E-06	1.82E-06	1.92E-06	1.92E-06	9.81E-08	5.12%
RBA:	0.0831%	0.0777%	0.0820%	0.0809%	0.0029%	3.53%
RBA of means:				0.0810%		
 CR42351						
IC50:	9.08E-05	9.70E-05	8.86E-05	9.21E-05	4.35E-06	4.73%
RBA:	0.0018%	0.0015%	0.0018%	0.0017%	0.0002%	12.27%
RBA of means:				0.0017%		
 CR42358						
IC50:	no activity	no activity	no activity	no activity	no activity	no activity
RBA:	no activity	no activity	no activity	no activity	no activity	no activity
RBA of means:				no activity		
 CR43261						
IC50:	3.89E-04	3.04E-04	3.07E-04	3.33E-04	4.85E-05	14.56%
RBA:	0.0004%	0.0005%	0.0005%	0.0005%	0.0000%	9.02%
RBA of means:				0.0005%		

Run identification:	514	515	516			
Assay start date:	10/18/2005	10/19/2005	10/27/2005	average	SD	coefficient of variation
Standard Curve						
IC50:	1.39E-09	1.21E-09	1.44E-09	1.35E-09	1.24E-10	9.20%
Weak Positive						
IC50:	3.43E-05	2.98E-05	3.69E-05	3.37E-05	3.62E-06	10.77%
RBA:	0.0041%	0.0041%	0.0039%	0.0040%	0.0001%	2.12%
RBA of means:				0.0040%		
 CR42341						
IC50:	5.13E-07	7.42E-07	7.10E-07	6.55E-07	1.24E-07	18.90%
RBA:	0.2713%	0.1629%	0.2035%	0.2126%	0.0548%	25.77%
RBA of means:				0.2059%		
 CR42346						
IC50:	9.22E-08	1.06E-07	9.14E-08	9.64E-08	7.93E-09	8.23%
RBA:	1.5104%	1.1450%	1.5800%	1.4118%	0.2337%	16.55%
RBA of means:				1.3991%		
 CR42347						
IC50:	5.20E-05	1.18E-04	7.43E-05	8.15E-05	3.38E-05	41.41%
RBA:	0.0027%	0.0010%	0.0019%	0.0019%	0.0008%	44.17%
RBA of means:				0.0017%		
 CR42355						
IC50:	5.09E-05	6.72E-05	6.44E-05	6.08E-05	8.75E-06	14.38%
RBA:	0.0027%	0.0018%	0.0022%	0.0023%	0.0005%	20.81%
RBA of means:				0.0022%		
 CR42369						
IC50:	2.96E-05	3.18E-05	3.14E-05	3.09E-05	1.19E-06	3.85%
RBA:	0.0047%	0.0038%	0.0046%	0.0044%	0.0005%	11.32%
RBA of means:				0.0044%		

n/a = not active

Appendix 1: Copy of Battelle, Richland Protocol No. SR-04-WA 4-11-07 and protocol amendment

<u>Assay Protocol</u>	<u>Battelle Pacific Northwest Laboratories</u> <u>P.O. Box 999 Battelle Boulevard</u> <u>Richland, Washington 99352</u>	<u>SR-04-WA</u> <u>4-11-01</u>

PROTOCOL

1. **Title:** Validation of an Androgen Receptor Binding Assay – Task 7
2. **Sponsor:** Battelle Memorial Institute
505 King Avenue
Columbus, Ohio 43201-2693
3. **Testing Facility:** Battelle, Richland
331 Building, P7-51
Richland, WA 99352
4. **Objective:** To provide data for 30 additional test substance for building the data base on chemicals for the validation of the AR assay using rat prostate cytosol prepared in Battelle laboratory, radiolabeled R 1881, R1881 and dexamethasone (test substance) and 30 additional unknown test substances. This protocol is specific to the study to be conducted at Battelle-Richland.
5. **Duration:** approximately 76 days
6. **Proposed Study Dates:**
 - a. Initiation of *In Vitro* Studies: June 26, 2005
 - b. Completion of *In Vitro* Studies: September 9, 2005
7. **Protocol Approval:**
 - a. Study Director: James E. Morris Date: 6/10/05
James E. Morris, Ph.D.
 - b. WAL: Michael L. Blanton Date: 6/7/05
Michael L. Blanton
 - c. Sponsor: David P. Fouchens Date: 6/6/05
David P. Fouchens, Ph.D.

<u>Assay Protocol</u>	<u>Battelle Pacific Northwest Laboratories</u> <u>P.O. Box 999 Battelle Boulevard</u> <u>Richland, Washington 99352</u>	<u>SR-04-WA</u> <u>4-11-01</u>

Reviewed By:

- a. MSL QA Representative: Mary E. Lynn Date: 6/7/05
Mary E. Lynn
- b. EDSP Battelle QAM: Terri L. Pollock Date: 6-6-05
Terri L. Pollock

8. **Test, marker and reference substances:**

- a.1 **Test Substance:** Dexamethasone (CAS # 50-02-2) will be prepared by and supplied by the Chemical Repository, Battelle, Sequim, Washington. Dexamethasone is also, identified as weak positive. There are 30 additional test substances identified by the following bar codes (code numbers): CR43240, CR43241, CR43242, CR43243, CR43244, CR43245, CR43246, CR43247, CR43248, CR43249, CR43250, CR43251, CR43252, CR43253, CR43254, CR43255, CR43256, CR43257, CR43258, CR43259, CR43260, CR43261, CR43262, CR43263, CR43264, CR43265, CR43266, CR43267, CR43268 and CR43269.
- a.2 **Reference substance:** Radioinert Methyltrienolone (CAS 965-93-5, Perkin-Elmer, NEN, catalog number NLP 005005MG) will be prepared by and supplied by the Chemical Repository, Battelle, Sequim, Washington.
- a.3 **Marker:** Radiolabeled R 1881 Tracer (CAS # 965-93-5) Perkin-Elmer [17 α -methyl- ^3H]-R 1881. Specific Activity: 82Ci (3.04TBq)/mmol.
- b. **Storage:** ^3H -R 1881 will be stored at $-20 \pm 5^\circ\text{C}$. Other substances will be stored according to conditions specified by the supplier.
- c. **Disposition:** All quantities of the test and reference substances which are dispensed will be documented.

9. Test System:

- a. Identification: The test system is rat prostate cytosol. Each tube within the assay will be uniquely labeled as defined in the assay. Cytosol will be stored at $-80 \pm 10^{\circ}\text{C}$.
- b. Justification for selection of the test system: Rat prostate cytosol is used because of the extensive data that exist for comparison and the inability to identify appropriate recombinant system(s) without false negative and positive acting chemicals in the *in vitro* binding assay.
- c. Source: The rat prostate cytosol will be prepared by Battelle – Richland per Battelle SOPs. The ventral prostate tissues are collected from 140 Sprague-Dawley male rats (60 to 90 days of age) castrated 24 hours prior to being humanely killed. Weighed and trimmed prostate tissues are placed in ice-cold buffer prepared with tris, ethylenediaminetetraacetic acid and glycerol (TEDG) with phenylmethylsulfonyl fluoride (PMSF) at a ratio of 0.1 g of tissue per 1.0 ml TEDG buffer with PMSF. Homogenize the tissue using an appropriate homogenizer. Cytosol pooled and stored at $-80 \pm 10^{\circ}\text{C}$.

10. Experimental Design:

- a. Assay to be Performed: Competitive binding of dexamethasone to the androgen receptor using rat prostate cytosol, compared to R 1881 will be performed (Appendix 1). The radio tracer for the assay will be Radiolabeled R 1881 Tracer. Prior to conducting the competitive binding assay, a saturation assay will be performed to demonstrate that the assay is properly standardized (Appendix 1). Each assay (competitive and saturation binding assay) will be run in triplicate (one each day on three separate days by the same technician).
- b. Frequency of Tests: Three tubes will be run per concentration and each assay will be run three times for the saturation and competitive binding assays. The assays are described in detail in Appendix 1.
- c. Route of administration and Reason for its choice: The cytosol is added directly to the test and reference substances in assay tubes in the appropriate sequence with the other reagents in the assay. The direct application and sequence is required for this assay type.
- d. Analysis of Data: Nonlinear curve fitting of unlabeled R 1881 (nM) (X axis) and total radiolabeled binding (DPM) (Y axis) to obtain K_d and $B_{\max}$ and then IC_{50} , Relative Binding Activity ratio (RBA) for each test and reference substance using GraphPad program.

11. **Quality Assurance:** This study will be audited by the Quality Assurance Unit to assure adherence to Good Laboratory Practice Regulations, adherence to the study protocol and compliance with Battelle Standard Operating Procedures. The Quality Assurance Unit will conduct a review of the raw data for accuracy and traceability and will audit the final report.
12. **Reports:** A Report will be prepared at the completion of the study. The report will include, but not be limited to, the following:
 - a. Design of the study and the results obtained.
 - b. Name and address of the facility performing the study.
 - c. Copy of the approved protocol, including all changes and revisions.
 - d. Date of the completed report.
 - e. Instances of ambiguity or unclear direction.
 - f. Prism or other data files.
 - g. Description of all circumstances that may have affected the quality or integrity of data.
 - h. Name, chemical structure, Chemical Abstract Service Registry Number (if known), physical nature and purity (if known) of the test and reference substances.
 - i. Justification for choice of solvent/vehicle if other than water or ethanol, and information to demonstrate that the solvent/vehicle, if other than an established solvent does not bind to or otherwise affect the Androgen Receptor (AR).
 - j. Type and source of AR, its isolation from tissues, protein concentration of AR preparation and method of storage.
 - k. Test conditions.
 - l. Results including extent of precipitation of test and reference substance, K_d and IC_{50} values with confidence limits for R 1881 and test substance, and RBA values for the test substance.
13. **Alteration of Design:** Alterations of the protocol may be made as the study progresses. Changes will be documented as required by Battelle SOPs.
14. **Data Notebooks:** All original data will be maintained in data notebooks. These will include, but not necessarily be limited to the following:
 - a. The original signed protocol and all amendments.
 - b. Test system records.
 - c. Test and reference substances receipt and use records.
 - d. Test and reference substances preparation data.
 - e. Sample preparation data.
 - f. Scintillation counting data.
 - g. Calculations to determine final reported values.
15. **Records to be Maintained:** The protocol, any amendments, the final report and all raw data collected as a result of this study will be archived by Battelle-Richland. The associated facility records will also be archived as required by Battelle-Richland SOPs.

16. **Personnel:** *Curricula vitae* for all personnel involved in the execution of the study are on file at Battelle, Pacific Northwest Division.
17. **Compliance Statement:** This study will be conducted in compliance with the U.S. EPA Good Laboratory Practice Regulations as set forth in Part 160 Title 40 of the Code of Federal Regulations.

Appendix 1

Assay Protocol for the *In Vitro* Androgen Receptor (AR) Saturation and Competitive Binding Assay Using Rat Ventral Prostate Cytosol (RVPC)

OP No. NHEERL-H/RTD/EB/VW/2002-03-000

1.0 Purpose and Applicability

Determine ability of compound to compete with [³H] ligand for binding in rat ventral prostate tissue homogenate.

2.0 Safety and Operating Precautions

All procedures with radioisotopes should follow the regulations and procedures as described in the Hazardous Agent Protocol and in the Radiation Safety Manual and Protocols for U.S. EPA.

3.0 Animal Use

Follow U.S. EPA approved animal use protocols

4.0 Equipment and Materials**4.1 Equipment**

Corning Stir/hot Plates
Pipettes
Balance
Sample rotor
Polytron PT 35/10 Tissue Homogenizer
Vacuum Concentrator
Refrigerated General Laboratory Centrifuge
pH Meter with Tris Compatible Electrode
Scintillation Counter
Refrigerators and freezers (-20° and -80°)

4.2 Chemicals

Tris HCL & Tris Base
Phenylmethylsulfonyl Fluoride (PMSF)
Glycerol 99%+
Sodium Molybdate
Ethylenediaminetetraacetic acid (EDTA); Disodium salt
Dithiothreitol (DTT)
Hydroxylapatite (HAP; BIO-RAD)
Scintillation Cocktail (Optifluor)
Ethyl Alcohol, anhydrous

[³H]-R1881 (NEN; Purity >97%)
Radioinert R1881 (NEN)
Triamcinolone Acetonide

- 4.3 Supplies
20 ml Polypropylene Scintillation Vials
12 x 75 mm Borosilicate Glass Test Tubes
1000 ml graduated cylinders
100 ml Erlenmeyer or plastic containers
pipette tips

5.0 Stock Preparations

5.1. Preparation of Stock Solutions for making TEDG Buffer

5.1.1. *EDTA Stock Solution*: Add 7.444g disodium EDTA to 100 ml ddH₂O = 200mM. Store at 4+ 2°C. Use 750 ul/100ml TEDG buffer = 1.5 mM.

5.1.2. *PMSF Stock Solution*: Add 1.742 g PMSF to 100 ml ethanol = 100 mM. Store at 4+ 2°C. Use 1.00 ml/100ml TEDG buffer = 1.0 mM.

5.1.3. *Sodium Molybdate Stock*: Add 2.419 g sodium molybdate to 8.0 ml ddH₂O in a 10 ml volumetric flask; bring the total volume to 10 mls = 1.0 M. Store at 4°C. Use 100ul/100ml TEDG buffer = 1.0 mM.

5.1.4. *1 M Tris Buffer*: Add 147.24 g Tris-HCL + 8.0 g Tris base to 800mls ddH₂O in a volumetric flask; bring the final volume to 1.0 liter. Refrigerate to 4°C and pH the cooled solution to 7.4. Store at 4+ 2°C. Use 1.0 ml/100 ml TEDG buffer = 10mM. (50 mM Tris = 50 ml 1 M Tris/1 L ddH₂O)

5.1.5. *Triamcinolone Acetonide (TRIAM) Stock*: Add 0.0653grams to 250 ml ethanol = 0.6 mM. Store at 4+ 2°C. Use 100ul/1.0ml TEDG buffer = 60 uM.

5.1.6. Add 15.4 mg DTT directly to 100 ml TEDG buffer the morning of the receptor isolation = 1.0 mM.

5.2. Preparation of Low-Salt TEDG Buffer (pH 7.4)

To make 100 ml of low-salt TEDG buffer add the following together in this order:

87.15 ml ddH₂O
1.0 ml 1M TRIS
10.0 ml glycerol
100 ul 1 M sodium molybdate
750 ul 200mM EDTA
1.0 ml 100mM PMSF
15.4 mg DTT (add immediately before use)

Check pH of the final solution to make sure it is 7.4 at $4 \pm 2^\circ \text{C}$.

5.3 Preparation of 50 mM TRIS Buffer

Add 50.0 ml of 1.0 M TRIS to 950 ml ddH₂O. Store at $4 \pm 2^\circ \text{C}$. Check pH of the final solution to make sure it is 7.4 at $4 \pm 2^\circ \text{C}$.

5.4 Preparation of 60% Hydroxylapatite (HAP) Slurry

5.4.1. Shake BIO-RAD HT-GEL until all the HAP is in suspension (i.e., looks like milk). The evening before the receptor extraction, pour 100 ml (or an appropriate volume) into a 100 ml graduated cylinder, parafilm seal the top and place in the refrigerator for at least 2h.

5.4.2. Pour off the phosphate buffer supernatant, and bring the volume to 100 ml with 50 mM TRIS. Suspend the HAP by parafilm sealing the top of the graduated cylinder and inverting the cylinder several times. Decant supernatant and repeat wash step times 2 with fresh 50 mM TRIS buffer.

5.4.3. Place in the refrigerator overnight.

5.4.4. Decant supernatant. Add enough 50 mM TRIS to make the final solution a 60% slurry (i.e., if the volume of the settled HAP is 60 ml bring the final volume of the slurry to 100 mls with 50 mM TRIS).

5.4.5. Store at $4 \pm 2^\circ \text{C}$ until ready for use in the extraction.

5.5 Preparation of [³H]-R1881 Stock Solutions

Dilute the original 1.0 mCi/ml stock of [³H]-R1881 to 0.1 μM (i.e., $1 \times 10^{-7} \text{ M}$). This is most easily accomplished by pipetting 1 μl of the stock solution for every specific activity unit (Ci/mmol) and diluting this to 10.0 mls with ethanol. Thus, if the specific activity of the stock vial is 86 Ci/mmol, then pipette 86.0 μl into an amber colored vial (i.e., R1881 is photosensitive) and add 10.0 ml ethanol to the vial; this solution is $1 \times 10^{-7} \text{ M}$.

Note: [³H]-R1881 stock solution and dilutions should be stored at $-20 \pm 4^\circ \text{C}$. Store stock solution in original protective vial and store dilutions in amber glass vials. This product is light-sensitive; care should be taken to minimize exposure to light.

5.6 Calculation Check and Dilutions

$$\begin{aligned} 86 \mu\text{l} \times 1.0 \text{ mCi}/1000 \mu\text{l} &= 86 \times 10^{-3} \text{ mCi R1881} = 86 \times 10^{-6} \text{ Ci R1881} \\ 86 \times 10^{-6} \text{ Ci} \div 86.0 \text{ Ci/mmol} &= 1 \times 10^{-6} \text{ mmol R1881} = 1 \times 10^{-9} \text{ moles R1881} \\ 1 \times 10^{-9} \text{ moles R1881} \div 0.010 \text{ liters} &= 1 \times 10^{-7} \text{ moles/liter} = 0.1 \mu\text{M} \end{aligned}$$

To prepare the 1×10^{-8} M stock simply make a 10-fold dilution of the 1×10^{-7} M stock (i.e., pipette 1.0 ml of the 1×10^{-7} M stock into a clean amber colored vial and add 9 ml ethanol = 0.01 uM).

To prepare the 1×10^{-9} M stock simply make a 10-fold dilution of the 1×10^{-8} M stock (i.e., pipette 1.0 ml of the 1×10^{-8} M stock into a clean amber colored vial and add 9 ml ethanol = 0.001 uM).

5.7 Preparation of 100X Radioinert R1881 Solutions

The R1881 comes as a 5.00 mg quantity. Dilute the original stock to 5.0 ml with ethanol = 3.52 mM. Take 56.82 μ l and dilute to 20 ml in an amber vial with ethanol = 1×10^{-5} M R1881. This is the 10 μ M radioinert R1881 stock.

To make the 1.0 μ M radioinert R1881 stock, pipette 2 ml of the 10 μ M stock into an amber vial and dilute to 20 ml with ethanol = 1×10^{-6} M = 1.0 μ M radioinert R1881 stock. To make the 0.10 μ M radioinert R1881 stock, pipette 2 ml of the 1 μ M stock into an amber vial and dilute to 20 ml with ethanol = 1×10^{-7} M = 0.10 μ M radioinert R1881 stock.

5.8 Compound Stock Preparations

5.8.1. Make stocks 30X above desired final concentration (this accounts for the use of 10 μ l stock in 300 μ l cytosol). Initial Stock of each test chemical solution will be diluted in 100% ethanol at a concentration of 3.0×10^2 M (i.e., 30 mM).

EXAMPLE:

4 (t) octyl phenol FW 206.33

1M = 206.33 g/L

1mM = 0.20633 mg/ml $\times 30$ (30 mM desired final stock conc.) = 6.1899 mg/ml

2 ml Stock = 6.1899 mg $\times 2$ = 12.37mg/2ml

5.8.2. Prepare serial dilutions of R1881 for standard curve in ethanol (100%) to yield the Initial Concentrations as indicated in Table 1.

Table 1: Standard Curve		
<i>Standards</i>	<i>Initial R1881 Concentration (Molar)</i>	<i>*Final R1881 Concentration (Molar) in AR assay tube</i>
Negative Control	0	
0	0 (EtOH)	0
NSB	1×10^{-5}	1×10^{-6}
S1	3×10^{-6}	1×10^{-7}
S2	3×10^{-7}	1×10^{-8}
S3	3×10^{-8}	1×10^{-9}
S4	3×10^{-9}	1×10^{-10}
S5	3×10^{-10}	1×10^{-11}
* Final concentration = 10 ul of each standard is added to the assay tube, except for the NSB which is 30 ul.		

5.8.3. Prepare serial dilutions of the test chemicals as indicated in Table 2.

Table 2: Test Chemical Concentrations (this subject to adjustment)		
<i>Serial Dilutions of the Test Chemical</i>	<i>Initial Concentration (Molar)</i>	<i>*Final Concentration (Molar) in AR assay tube</i>
Concentration 1	3×10^{-3}	1×10^{-4}
Concentration 2	3×10^{-4}	1×10^{-5}
Concentration 3	3×10^{-5}	1×10^{-6}
Concentration 4	3×10^{-6}	1×10^{-7}
Concentration 5	3×10^{-7}	1×10^{-8}
Concentration 6	3×10^{-8}	1×10^{-9}
Tube 7	0 (vehicle only)	0
* Final concentration = 10 ul of each Initial Concentration of test chemical is added to the assay tube along with 300 ul of ventral prostate cytosol.		

6.0 Tissue Homogenate Collection

6.1. Castrate 90 day old rats (60-90 day old acceptable; 90 day old preferred) as per laboratory animal protocols.

6.2. 24 hours after castration, make low salt TEDG buffer and place in an ice-water bucket.

6.3. Kill rat and excise ventral prostate. Tissue should be trimmed of fat, weighed and the weights recorded.

6.4. Add low-salt TEDG buffer at 10ml/g tissue.

6.5. Mince tissues with Metzenbaum scissors until all pieces are small 1-2 mm cubes. Then homogenize the tissues using an ice bath with a Polytron homogenizer using three to five 5-sec bursts of the Polytron. [Note: place probe of the Polytron in TEDG buffer in an ice-water bath to cool it down prior to its use for homogenization. Re-cool probe as needed.]

6.6. Transfer homogenates to pre-cooled centrifuge tubes, balance, and centrifuge at 30,000x g for 30 minutes (i.e., 15, 262 rpm using JA-17/JA-21 Beckman rotors).

6.7. The supernatant contains the low-salt cytosolic receptor. Pool the supernatant from all rats. Aliquot as needed for proposed studies and store $-80 \pm 10^\circ\text{C}$ until needed for assay. Discard after 6 months.

6.8. Determine the protein content for each batch of cytosol according to the method by Bradford (1976) using the commercially available BioRad Protein Assay Kit (BioRad Chemical Division, Richmond, CA). Protein concentrations usually range from 5.5 - 8 mg/ml in undiluted cytosol.

7.0. Assay procedure for chemicals: Day 1

7.1. Set up tubes: 12x75 mm glass tubes

7.1.1. Label sufficient glass tubes as needed for the assay.

7.1.2. Add 30 μL of 0.01 μM [^3H] R1881 ($1 \times 10^{-8}\text{M}$) and 50 μL triamcinolone acetone (60 μM stock) to ALL tubes.

7.1.3. For 3 tubes (NSB) at beginning of assay and at end of assay, also add 100x inert R1881 (30 μL of 1.0 μM , ie $1 \times 10^{-6}\text{M}$). These tubes are for determining nonspecific binding.

7.1.4. Place tubes in speed-vac and dry the tubes according to instructions. Remove when dry.

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)													
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (μL)	Tracer (Hot R1881) Volume (μL)	Competitor Volume (μL)	triamcinolone Volume (μL)	Competitor Final Concentration (M)	Aliquot (μL)	HAP (500 μL)
1	1	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
2	2	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
3	3	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
4	1	Inert R1881	NSB		E-1-S0	$1.00\text{E-}05$	300	30	30	50	$1.0\text{E-}06$	100	500
5	2	Inert R1881	NSB		E-1-S0	$1.00\text{E-}05$	300	30	30	50	$1.0\text{E-}06$	100	500
6	3	Inert R1881	NSB		E-1-S0	$1.00\text{E-}05$	300	30	30	50	$1.0\text{E-}06$	100	500
7	1	Inert R1881	S	1	E-1-S1	$3.00\text{E-}06$	300	30	10	50	$1.0\text{E-}07$	100	500
8	2	Inert R1881	S	1	E-1-S1	$3.00\text{E-}06$	300	30	10	50	$1.0\text{E-}07$	100	500
9	3	Inert R1881	S	1	E-1-S1	$3.00\text{E-}06$	300	30	10	50	$1.0\text{E-}07$	100	500
10	1	Inert R1881	S	2	E-1-S2	$3.00\text{E-}07$	300	30	10	50	$1.0\text{E-}08$	100	500
11	2	Inert R1881	S	2	E-1-S2	$3.00\text{E-}07$	300	30	10	50	$1.0\text{E-}08$	100	500
12	3	Inert R1881	S	2	E-1-S2	$3.00\text{E-}07$	300	30	10	50	$1.0\text{E-}08$	100	500

13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	1.0E-09	100	500
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	1.0E-09	100	500
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	1.0E-09	100	500
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	1.0E-10	100	500
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	1.0E-10	100	500
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	1.0E-10	100	500
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	1.0E-11	100	500
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	1.0E-11	100	500
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	1.0E-11	100	500
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	1.E-03	100	500
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	1.E-03	100	500
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	1.E-03	100	500
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	1.E-04	100	500
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	1.E-04	100	500
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	1.E-04	100	500
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	1.E-05	100	500
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	1.E-05	100	500
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	1.E-05	100	500
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	1.E-06	100	500
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	1.E-06	100	500
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	1.E-06	100	500
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	1.E-07	100	500
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	1.0E-07	100	500
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	1.0E-07	100	500
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	1.0E-08	100	500
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	1.0E-08	100	500
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	1.0E-08	100	500
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	1.0E-09	100	500
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	1.0E-09	100	500
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	1.0E-09	100	500
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	1.0E-10	100	500
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	1.0E-10	100	500
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	1.0E-10	100	500
46	1	unknown 1	C	1	E-1-C11	3.00E-02	300	30	10	50	1.0E-03	100	500
47	2	unknown 1	C	1	E-1-C11	3.00E-02	300	30	10	50	1.0E-03	100	500
48	3	unknown 1	C	1	E-1-C11	3.00E-02	300	30	10	50	1.0E-03	100	500
49	1	unknown 1	C	2	E-1-C12	3.00E-03	300	30	10	50	1.0E-04	100	500
50	2	unknown 1	C	2	E-1-C12	3.00E-03	300	30	10	50	1.0E-04	100	500
51	3	unknown 1	C	2	E-1-C12	3.00E-03	300	30	10	50	1.0E-04	100	500
52	1	unknown 1	C	3	E-1-C13	3.00E-04	300	30	10	50	1.0E-05	100	500
53	2	unknown 1	C	3	E-1-C13	3.00E-04	300	30	10	50	1.0E-05	100	500
54	3	unknown 1	C	3	E-1-C13	3.00E-04	300	30	10	50	1.0E-05	100	500
55	1	unknown 1	C	4	E-1-C14	3.00E-05	300	30	10	50	1.0E-06	100	500

56	2	unknown 1	C	4	E-1-C14	3.00E-05	300	30	10	50	1.0E-06	100	500
57	3	unknown 1	C	4	E-1-C14	3.00E-05	300	30	10	50	1.0E-06	100	500
58	1	unknown 1	C	5	E-1-C15	3.00E-06	300	30	10	50	1.0E-07	100	500
59	2	unknown 1	C	5	E-1-C15	3.00E-06	300	30	10	50	1.0E-07	100	500
60	3	unknown 1	C	5	E-1-C15	3.00E-06	300	30	10	50	1.0E-07	100	500
61	1	unknown 1	C	6	E-1-C16	3.00E-07	300	30	10	50	1.0E-08	100	500
62	2	unknown 1	C	6	E-1-C16	3.00E-07	300	30	10	50	1.0E-08	100	500
63	3	unknown 1	C	6	E-1-C16	3.00E-07	300	30	10	50	1.0E-08	100	500
64	1	unknown 1	C	7	E-1-C17	3.00E-08	300	30	10	50	1.0E-09	100	500
65	2	unknown 1	C	7	E-1-C17	3.00E-08	300	30	10	50	1.0E-09	100	500
66	3	unknown 1	C	7	E-1-C17	3.00E-08	300	30	10	50	1.0E-09	100	500
67	1	unknown 1	C	8	E-1-C18	3.00E-09	300	30	10	50	1.0E-10	100	500
68	2	unknown 1	C	8	E-1-C18	3.00E-09	300	30	10	50	1.0E-10	100	500
69	3	unknown 1	C	8	E-1-C18	3.00E-09	300	30	10	50	1.0E-10	100	500
70	1	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
71	2	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
72	3	ethanol	EtOH	0	—	—	300	30	10	50	—	100	500
73	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	1.0E-06	100	500
74	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	1.0E-06	100	500
75	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	1.0E-06	100	500
76	1	none	Hot		—	—	—	30	—	—	—	—	—
77	2	none	Hot		—	—	—	30	—	—	—	—	—
78	3	none	Hot		—	—	—	30	—	—	—	—	—
79	1	none	Hot		—	—	—	30	—	—	—	—	—
80	2	none	Hot		—	—	—	30	—	—	—	—	—
81	3	none	Hot		—	—	—	30	—	—	—	—	—

7.2. Add 10ul of compound stocks (see 5.8 for concentrations 1-7 in triplicate)

7.3. Remove aliquot of prostate cytosol and thaw on ice. Cytosol should be diluted with ice-cold low-salt TEDG buffer to give a protein concentration of ~1 mg per 300 ul assay tube. The amount of cytosol protein is subject to adjustment based on activity identified in saturation binding assays.

7.4. Add 300 ul of diluted cytosol to every tube ON ICE. Gently vortex and place tubes in refrigerator overnight in rotor (18-20hr).

Note: Make sure that all components are concentrated at the bottom of tube. If any of the liquid remains on the side of the tube, centrifuge assay tubes for 1 minute at 600 x g (4°C) to concentrate fluid at bottom of tube.

7.5. Before leaving for the day, prepare the washes of the HAP slurry as described in section 5.4 above.

7.6. Label the HAP tubes and the scintillation vials to be used the following day - see underlines below.

8.0 Assay procedure: Day 2

8.1. The following morning, wash the HAP as described in section 5.4 above, dilute with 50 mM TRIS to yield a 60% slurry, and transfer contents to a plastic or glass container. Place a stir bar in the container and place in a beaker containing ice-water; stir the HAP slurry by placing the beaker on a magnetic stir plate.

8.2. While the HAP slurry is constantly being stirred, pipette 500 μ l of the HAP slurry into clean pre-labelled 12 x 75 mm glass test tubes. Place these tubes in a rack in an ice-water bath prior to pipetting the HAP slurry and keep them in the ice-water bath for the remainder of the assay.

8.3. One HAP tube should be prepared for each incubation tube.

8.4. Take the incubation tubes from the refrigerator and place them in an ice-water bath with the HAP tubes. Pipette 100 μ l from each of the incubation tubes into the appropriate pre-labelled tubes containing HAP. Repeat for all tubes. Quickly take each rack from the ice-water bath and vortex each rack of tubes using the whole-rack vortex unit. Place racks back into the ice-water bath and vortex as above every 5 minutes for 20 minutes.

8.5. Centrifuge the HAP tubes for 10-11 minutes at $4 \pm 2^{\circ}\text{C}$ and 600 x g (1780 rpm in a Beckman GLC refrigerated centrifuge). Place the tubes back into the rack and into the ice-water bath.

8.6. While the tubes remain in the ice-water bath, aspirate or decant the supernatant from each tube. If aspirating, use a 9 inch pipette connected to an aspiration apparatus as per the radiation safety protocol.

8.7. Add 2 ml of 50 mM TRIS to each tube, vortex and centrifuge at 600 x g as above. Place the tubes into decanting racks in an ice-water bath and decant the supernatant TRIS wash into the radiation safety container. Gently tap the tube openings on a clean adsorbent diaper, place the rack back in the ice-water bath and add 2 mls of 50 mM TRIS.

8.8. Repeat the TRIS washing procedure 3 or 4 times (to be determined empirically) keeping the tubes on ice at all times.

8.9. Following the last wash and decanting, add 2 mls of ethanol to each tube, vortex 3 times at 5 minute intervals and centrifuge the tubes at 600 x g for 10 minutes. Decant the supernatants into pre-labelled 20 ml scintillation vials containing 14 ml of Optifluor scintillation cocktail. Count samples using the single label DPM program with quench correction.

9.0. Saturation Radioligand Binding Assay

Prior to routinely conducting the AR competitive binding assays, the methods should be standardized within each laboratory. A series of saturation radioligand binding assays should be conducted to demonstrate AR specificity and saturation. Nonlinear regression analysis of these data and subsequent Scatchard plots will document AR binding affinity (K_d) and maximum specific binding number (B_{max}). Scatchard assay is to be conducted as follows:

Day 1 9.1. Set up tubes: 12x75 glass tubes and label for 8 concentrations in triplicate each with and without 100X inert (48 tubes total 1 through 48 below).

9.2. Add [^3H] R1881 from the appropriate stock solutions to tubes as listed below:

9.3. Place 50 μ l of 60 uM stock triamcinolone acetonide to ALL tubes.

9.4 An aliquot of each concentration of [^3H]R1881 should also be counted on scintillation counter to determine total counts added (tube # 49-72 below).

Saturation Assay Tube Layout

<i>Position</i>	<i>Replicate</i>	<i>Tube Type Code</i>	<i>Hot Initial Concentration (nM)</i>	<i>Hot R1881 Volume (uL)</i>	<i>Hot Final Concentration (nM)</i>	<i>Cold Initial Concentration (uM)</i>	<i>Cold Volume (uL)</i>	<i>Cold Final Concentration (nM)</i>	<i>Triamcelenone Acetate (uL)</i>	<i>Cytosol (ul)</i>
1	1	H	10.0	7.5	0.25	—	—	—	50	300
2	2	H	10.0	7.5	0.25	—	—	—	50	300
3	3	H	10.0	7.5	0.25	—	—	—	50	300
4	1	H	10.0	15	0.50	—	—	—	50	300
5	2	H	10.0	15	0.50	—	—	—	50	300
6	3	H	10.0	15	0.50	—	—	—	50	300
7	1	H	10.0	21	0.70	—	—	—	50	300
8	2	H	10.0	21	0.70	—	—	—	50	300
9	3	H	10.0	21	0.70	—	—	—	50	300
10	1	H	10.0	30	1.00	—	—	—	50	300
11	2	H	10.0	30	1.00	—	—	—	50	300
12	3	H	10.0	30	1.00	—	—	—	50	300
13	1	H	10.0	45	1.50	—	—	—	50	300
14	2	H	10.0	45	1.50	—	—	—	50	300
15	3	H	10.0	45	1.50	—	—	—	50	300
16	1	H	100.0	7.5	2.50	—	—	—	50	300
17	2	H	100.0	7.5	2.50	—	—	—	50	300
18	3	H	100.0	7.5	2.50	—	—	—	50	300
19	1	H	100.0	15	5.00	—	—	—	50	300
20	2	H	100.0	15	5.00	—	—	—	50	300
21	3	H	100.0	15	5.00	—	—	—	50	300
22	1	H	100.0	30	10.00	—	—	—	50	300
23	2	H	100.0	30	10.00	—	—	—	50	300
24	3	H	100.0	30	10.00	—	—	—	50	300
25	1	HC	10.0	7.5	0.25	1.00	7.5	25	50	300
26	2	HC	10.0	7.5	0.25	1.00	7.5	25	50	300
27	3	HC	10.0	7.5	0.25	1.00	7.5	25	50	300
28	1	HC	10.0	15	0.5	1.00	15	50	50	300
29	2	HC	10.0	15	0.5	1.00	15	50	50	300
30	3	HC	10.0	15	0.5	1.00	15	50	50	300
31	1	HC	10.0	21	0.7	1.00	21	70	50	300
32	2	HC	10.0	21	0.7	1.00	21	70	50	300
33	3	HC	10.0	21	0.7	1.00	21	70	50	300
34	1	HC	10.0	30	1	1.00	30	100	50	300
35	2	HC	10.0	30	1	1.00	30	100	50	300
36	3	HC	10.0	30	1	1.00	30	100	50	300

37	1	HC	10.0	45	1.5	1.00	45	150	50	300
38	2	HC	10.0	45	1.5	1.00	45	150	50	300
39	3	HC	10.0	45	1.5	1.00	45	150	50	300
40	1	HC	100.0	7.5	2.5	10.00	7.5	250	50	300
41	2	HC	100.0	7.5	2.5	10.00	7.5	250	50	300
42	3	HC	100.0	7.5	2.5	10.00	7.5	250	50	300
43	1	HC	100.0	15	5	10.00	15	500	50	300
44	2	HC	100.0	15	5	10.00	15	500	50	300
45	3	HC	100.0	15	5	10.00	15	500	50	300
46	1	HC	100.0	30	10	10.00	30	1000	50	300
47	2	HC	100.0	30	10	10.00	30	1000	50	300
48	3	HC	100.0	30	10	10.00	30	1000	50	300
49	1	Hot	10.0	7.5	0.03	—	—	—	—	—
50	2	Hot	10.0	7.5	0.03	—	—	—	—	—
51	3	Hot	10.0	7.5	0.03	—	—	—	—	—
52	1	Hot	10.0	15	0.06	—	—	—	—	—
53	2	Hot	10.0	15	0.06	—	—	—	—	—
54	3	Hot	10.0	15	0.06	—	—	—	—	—
55	1	Hot	10.0	21	0.08	—	—	—	—	—
56	2	Hot	10.0	21	0.08	—	—	—	—	—
57	3	Hot	10.0	21	0.08	—	—	—	—	—
58	1	Hot	10.0	30	0.10	—	—	—	—	—
59	2	Hot	10.0	30	0.10	—	—	—	—	—
60	3	Hot	10.0	30	0.10	—	—	—	—	—
61	1	Hot	10.0	45	0.30	—	—	—	—	—
62	2	Hot	10.0	45	0.30	—	—	—	—	—
63	3	Hot	10.0	45	0.30	—	—	—	—	—
64	1	Hot	100.0	7.5	0.60	—	—	—	—	—
65	2	Hot	100.0	7.5	0.60	—	—	—	—	—
66	3	Hot	100.0	7.5	0.60	—	—	—	—	—
67	1	Hot	100.0	15	1.00	—	—	—	—	—
68	2	Hot	100.0	15	1.00	—	—	—	—	—
69	3	Hot	100.0	15	1.00	—	—	—	—	—
70	1	Hot	100.0	30	3.00	—	—	—	—	—
71	2	Hot	100.0	30	3.00	—	—	—	—	—
72	3	Hot	100.0	30	3.00	—	—	—	—	—

9.5. Place tubes in speed-vac (Tubes 1-48) and dry the tubes according to instructions. Remove when dry and place on ice.

9.6. Cytosol should be diluted with the low salt TEDG buffer to a protein concentration of ~ 0.6 mg per 300 ul assay (The 0.6 mg is for initial assessment, it may be necessary to adjust depending upon the linearity of the Scatchard plot). Add 300 ul of diluted prostate cytosol to all tubes (1-48). Keep tubes and cytosol on ice at all times during this procedure. Gently vortex and place tubes in refrigerator overnight in rotor (18-20hr).

9.7 Before leaving for the day, conduct washes of the HAP slurry as described in section 5.4 above. If desired, label the HAP tubes and the scintillation vials to be used the following day.

Day 2

9.8. Continue as with Day 2 protocol for competitive binding assay above in section 8.0.

10.0 Data Processing

10.1 Free Concentration of [³H]-R1881

Multiply the DPM in the total counts tubes by 1.8047×10^{-5} . This value will yield the free concentration (i.e., nM) of [³H]-R1881 initially present in each incubation tube.

Calculation Check -

$$\begin{array}{rcll} \text{X DPM} & = & 4.5045 \times 10^{-13} \text{ Ci} = 5.4141 \times 10^{-15} \text{ mmole} = 5.4141 \times 10^{-18} \text{ moles} \\ 2.22 \times 10^{12} \text{ dpm/Ci} & * & 83.2 \text{ Ci/mmol} & 1000 \text{ mmole/mole} & 0.0003 \text{ liters} \end{array}$$

$$= 1.8047 \times 10^{-14} \text{ moles/liter} = \text{X} (1.8047 \times 10^{-5}) \text{ nM} \\ 1 \times 10^{-9} \text{ moles/nmole}$$

*Note this value will be the Specific activity of the radioligand ([³H]R1881) used in the assay.

10.2 Calculation of Total, Nonspecific and Specific [³H]-R1881 Binding

10.2.1. Total binding is calculated by multiplying the DPM from the tubes that contained only radiolabelled R1881 x (1.6242×10^{-2}) . This value will be total binding in fmoles.

10.2.2. Nonspecific binding is calculated by multiplying the DPM from the tubes containing radiolabelled R1881 + 100-fold molar excess of radioinert R1881 x (1.6242×10^{-2}) . This value will be nonspecific binding in fmoles.

10.2.3. Specific binding is calculated by subtracting nonspecific binding from total binding i.e., fmoles total binding - fmoles nonspecific binding = specific binding in fmoles.

10.3 Graphical Presentation of the Data

10.3.1. Standard Curve and Test Chemical Competitive Binding Curves: Data for the standard curve and each test chemical will be plotted as the percent ³H_R1881 bound versus the molar concentration. Estimates of the IC₅₀s will be determined using appropriate non linear curve fitting software such as GraphPad Prism (GraphPad

Software, Inc., San Diego, CA). A Scatchard Analysis may also be performed for the standard curve using R1881 to demonstrate that the assay meets acceptable QA standards.

10.3.2. Relative Binding Affinity: The RBA for each competitor should be calculated by dividing the IC_{50} for R1881 by the IC_{50} of the competitor and expressing as a percent (e.g., RBA for R1881 = 100 %).

10.3.3. Maximal binding capacity (B_{max}) and association/dissociation constants (K_a / K_d) can be estimated using a number of commercially available iterative nonlinear regression analysis programs. One of the better programs was developed by Munson and Rodbard and is called LIGAND.

10.4 References

- 1) Nonneman, D.J., Ganjam, V.K., Welshons, W.V., and Vom Saal, F.S. (1992) *Biol. Reprod.* **47**, 723-729
- 2) Segel, I.H. (1975) *Enzyme Kinetics: Behavior and Analysis of Rapid Equilibrium and Steady-State Enzyme Systems*. 1st Ed, John Wiley and Sons, Inc., New York, NY
- 3) Munson, P.J., and Rodbard, D. (1980) *Anal. Biochem.* **107**, 220-239.
- 4) Tekpetey, F.R., and Amann, R.P. (1988) *Biol. Reprod.* **38**, 1051-1060.
- 5) Wilson, V.S., Lambright, C.S., Ostby, J. and Gray, Jr., L.E.. *In vitro* and *in vivo* effects of 17-beta trenbolone: A feedlot effluent contaminant. (2002). *Toxicol. Sci.* **70**(2):202-211..
- 6) Bradford, M. (1976). *Anal. Biochem.* **72**, 248-254.

PROTOCOL AMENDMENT
 STUDY NUMBER: SR-04-WA-4-11-07
 AMENDMENT NUMBER: A-1
 DATE: September 30, 2005
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ENDOCRINE DISRUPTOR SCREENING PROGRAM AMENDMENT REPORT

STUDY NUMBER: SR-04-WA-4-11-07		DATE: September 30, 2005	
AMENDMENT NUMBER: 1		WAL/STUDY DIRECTOR: ML Blanton /JE Morris	
NOTEBOOK NUMBER: N/A			
TITLE OF STUDY: Validation of an Androgen Receptor Binding Assay-Task 7			
QAPP/PROTOCOL ID: Work Assignment 4-11			
AMENDMENT RELATING TO:			
☐	QAPP	☐	QMP
☐	SOP	☐	Method
		☒	Protocol

ORIGINAL DOCUMENT SPECIFICATIONS:

Entries that are earmarked for change in this amendment are presented as bold.

1. Protocol section 8. Test, marker and reference substances a.1 Test Substance:

Dexamethasone (CAS # 50-02-2) will be prepared by and supplied by the Chemical Repository, Battelle, Sequim, Washington. Dexamethasone is also, identified as weak positive. There are 30 additional test substances identified by the following bar codes (code numbers): **CR43240, CR43241, CR43242, CR42343, CR43244, CR43245, CR43246, CR43247, CR43248, CR43249, CR43250, CR42351, CR42352, CR42353, CR423254, CR423255, CR42356, CR42357, CR42358, CR42359, CR42360, CR42361, CR42362, CR43263, CR43264, CR42365, CR42366, CR42367, CR42368 and CR42369.**

2. Protocol section 4. Objective and section 8. Test, marker and reference substances a.1. Test Substance:

Three unknown chemicals, CR42356, CR42364, and CR42366, are deleted from the test list for a total of 27 test substances.

3. The study number was incorrectly entered on the study protocol for WA 4-11 Task 7 as **SR-04-WA 4-11-01** and in appendix I was listed as **SR-02-WA-4-11-04**.
4. Protocol section 6. Proposed Study Dates: b. Completion of In Vitro Studies: **September 9, 2005.**

AMENDMENT:

1. Dexamethasone (CAS # 50-02-2) will be prepared by and supplied by the Chemical Repository, Battelle, Sequim, Washington. Dexamethasone is also, identified as weak positive. **There are** 30 additional test substances identified by the following bar codes (code numbers): **CR42340, CR42341, CR42342, CR42343, CR42344, CR42345, CR42346, CR42347,**

PROTOCOL AMENDMENT
STUDY NUMBER: SR-04-WA-4-11-07
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CR42348, CR42349, CR42350, CR42351, CR42352, CR42353, CR42354, CR42355, CR42356, CR42357, CR42358, CR42359, CR42360, CR42361, CR42362, CR42363, CR42364, CR42365, CR42366, CR42367, CR42368 and CR42369.

2. Dexamethasone (CAS # 50-02-2) will be prepared by and supplied by the Chemical Repository, Battelle, Sequim, Washington. Dexamethasone is also, identified as weak positive. There are 30 additional test substances identified by the following bar codes (code numbers): CR42340, CR42341, CR42342, CR42343, CR42344, CR42345, CR42346, CR42347, CR42348, CR42349, CR42350, CR42351, CR42352, CR42353, CR42354, CR42355, CR42357, CR42358, CR42359, CR42360, CR42361, CR42362, CR42363, CR42365, CR42367, CR42368 and CR42369.
3. Study number should be **SR-04-WA-4-11-07**.
4. Proposed completion date will be **October 21, 2005**.

REASON FOR CHANGE:

1. Wrong bar codes were entered for identified chemicals in bold as noted in item 1 of amendment.
2. The bar codes for 3 unknown chemicals have been removed from the study because of solubility issues and at the request of EPA.
3. Incorrect Battelle study number was entered on the protocol for Task 7 for WA 4-11.
4. Additional study assignments forced delays in completing task.

Approval:

Work Assignment Leader

Michael L. Burton

Date 10-31-05

Study Director

James E. Morris

Date 10-3-05

EDSP QA Representative

Mary E. Lutz

Date 10/7/05

EDSP Program Management

Doris P. Rombus

Date 9/30/05

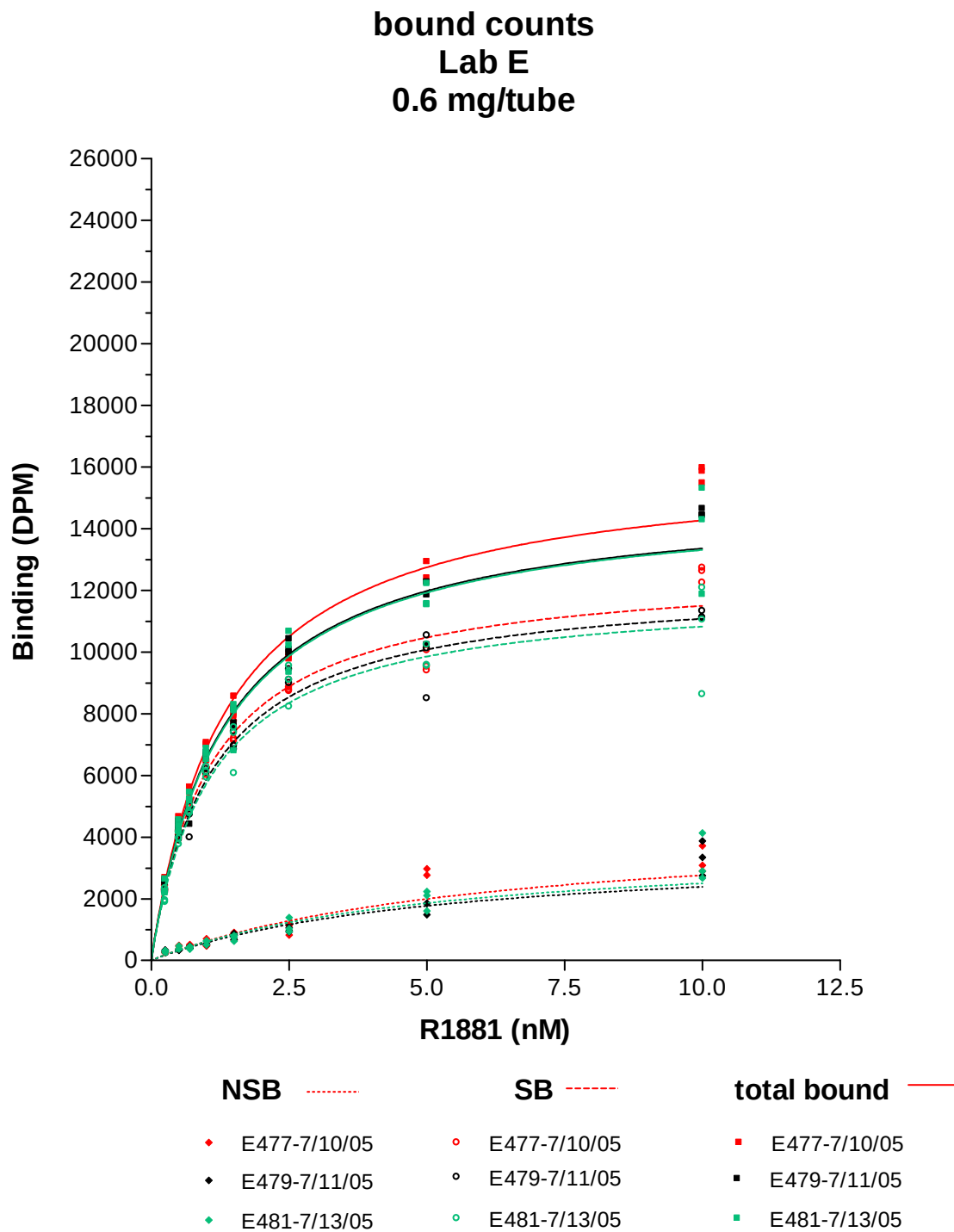
EDSP Battelle QAM

Cheri L. Pollock

Date 9-30-05

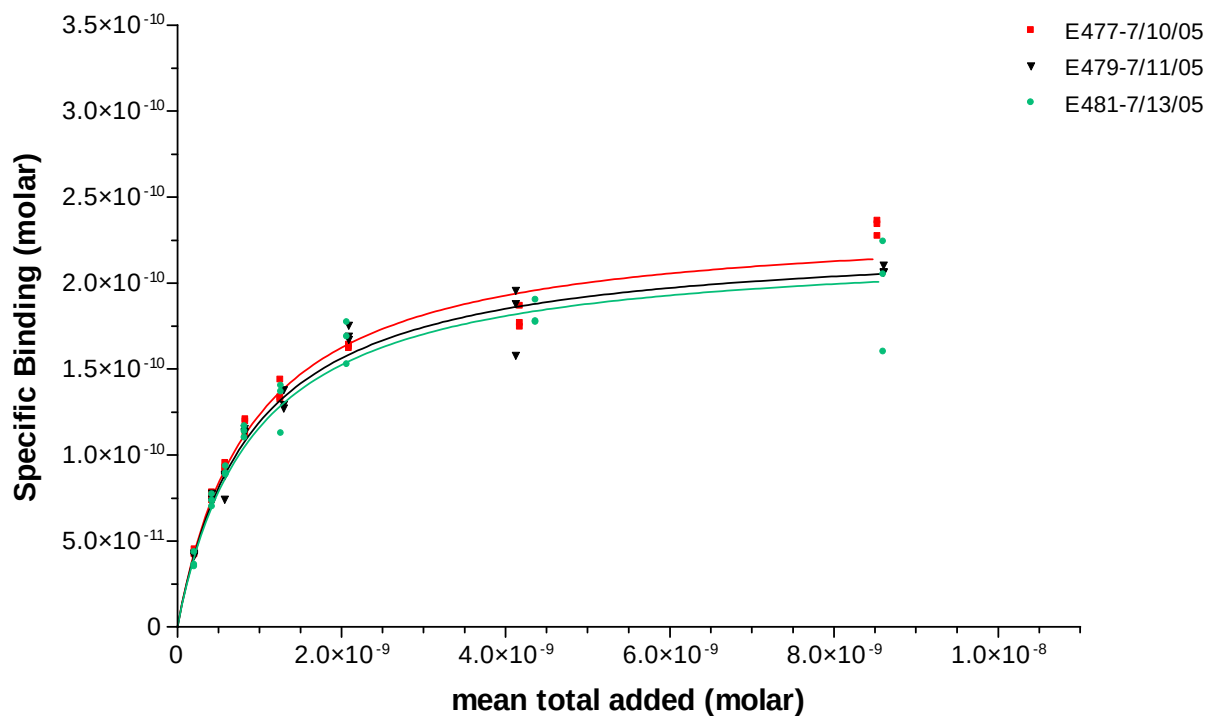
cc: Send final approved copies to:
MSL QA Representative
EDSP Battelle QAM

Appendix 2: Prism Files for Saturation Binding Experiments



Lab E

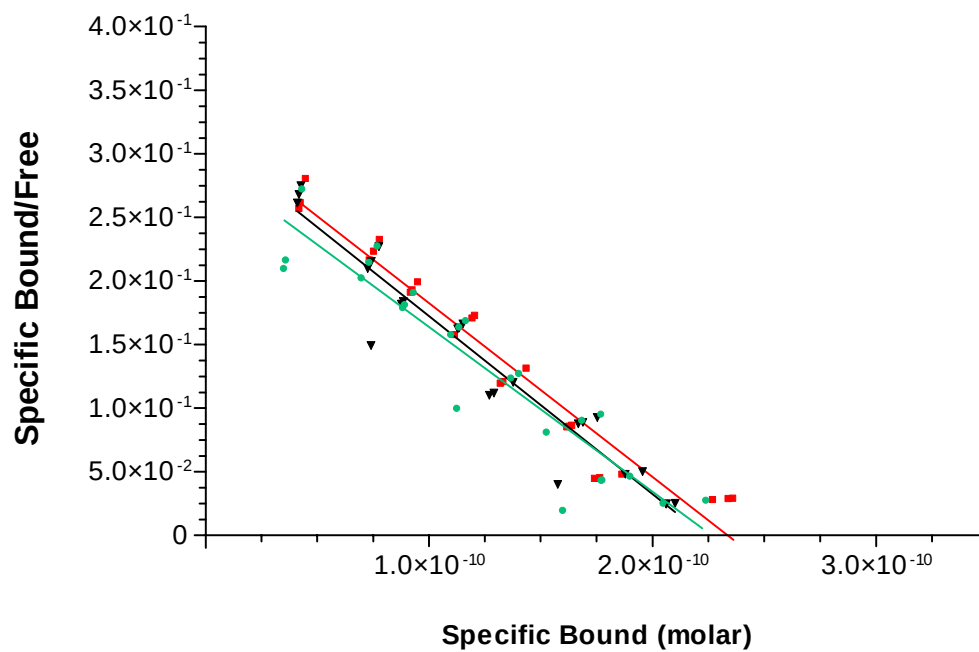
0.6 mg/tube



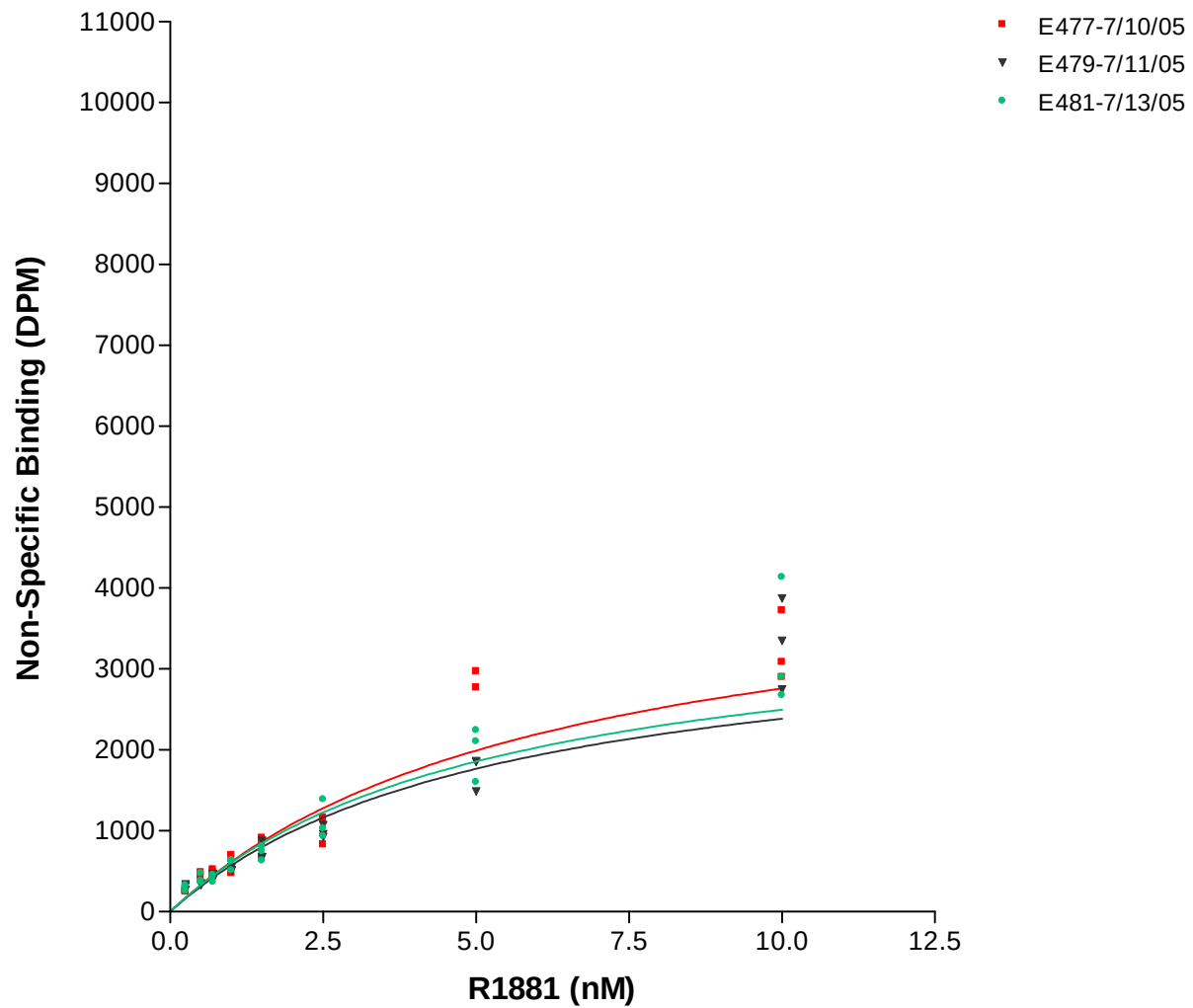
Specific bound	E477-7/10/05	E479-7/11/05	E481-7/13/05
BMAX	2.370e-010	2.268e-010	2.222e-010
KD	9.194e-010	9.039e-010	9.156e-010
Std. Error			
BMAX	5.754e-012	7.052e-012	9.612e-012
KD	4.358e-011	5.508e-011	7.680e-011
95% Confidence Intervals			
BMAX	2.251e-010 to 2.490e-010	2.122e-010 to 2.414e-010	2.023e-010 to 2.422e-010
KD	8.290e-010 to 1.010e-009	7.897e-010 to 1.018e-009	7.563e-010 to 1.075e-009
Goodness of Fit			
Degrees of Freedom	22	22	22
R ² (unweighted)	0.9735	0.9742	0.9417
Weighted Sum of Squares (1/Y ²)	0.06464	0.1082	0.2198
Absolute Sum of Squares	2.078e-021	1.823e-021	3.947e-021
Sy.x	9.718e-012	9.102e-012	1.339e-011
Data			
Number of X values	24	24	24
Number of Y replicates	1	1	1
Total number of values	24	24	24
Number of missing values	0	0	0

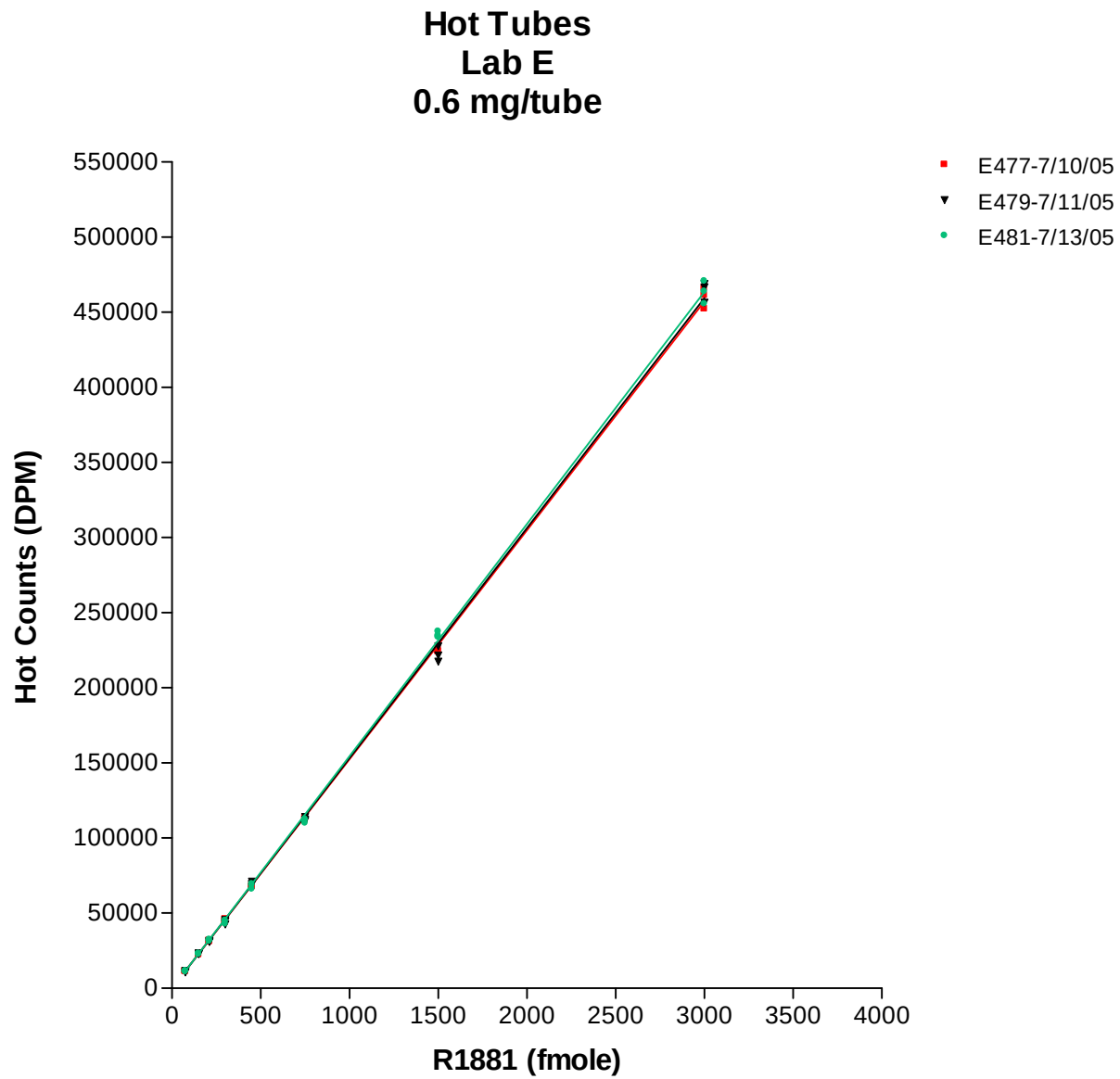
Scatchard Display
Lab E
0.6 mg/tube

- E477-7/10/05
- ▼ E479-7/11/05
- E481-7/13/05



NSB Tubes
Lab E
0.6 mg/tube





Appendix 3: Excel Files for Saturation Binding Experiments:

Laboratory E

AR Saturation Assay (cold R1881 dilutions supplied by Battelle)

72 assay tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in columns O and DK

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Provide a reason in column R

The value in column Q will automatically change to FALSE

For your convenience, data reduction is performed in columns

U through BZ, and the values needed for analysis are presented
in columns CF through CN

Cells in column S are presented with a grey background

if the total binding exceeds 10% of the hot added at that concentration,
the cytosol concentration is probably too high for good competitive assays

Laboratory Code: E

Run identification: 477

Assay start date: 7/10/2005

Tracer lot number: 3559-507

Specific activity on day of assay: 80.96 Ci/mole

Cytosol lot or vial number: 051905

protein (cytosol) per tube: 600 ug

protein (cytosol) per tube: 0.6 mg

KD 9.19E-01 nM

Bmax 11.85 fmole/100 ug

total volume in tubes 300 uL

volume of ethanol counted: 2 mL

multiply DPM in sample by : 3

Receptor Notes

diluted to 2 mg/ml for use (0.6 mg/300 ul)

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Saturation Assay Tube Layout																			
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetenone Acetate (uL)	Cytosol (ul)	Significant portion of label on Vial	dpm as counted	corrected DPM for 2mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	Ten Percent Rule	Saturation X values	Bound y values	NSB y values
1	1	H	10.0	7.5	0.25	—	—	—	50	300	—	851.52	2554.56	TRUE		22.5%	0.25	2554.6	255.1
2	2	H	10.0	7.5	0.25	—	—	—	50	300	—	894.52	2683.56	TRUE		23.6%	0.25	2683.6	255.1
3	3	H	10.0	7.5	0.25	—	—	—	50	300	—	840.57	2521.71	TRUE		22.2%	0.25	2521.7	255.1
4	1	H	10.0	15	0.50	—	—	—	50	300	—	1505.40	4516.2	TRUE		19.8%	0.5	4516.2	444.4
5	2	H	10.0	15	0.50	—	—	—	50	300	—	1551.10	4653.3	TRUE		20.4%	0.5	4653.3	444.4
6	3	H	10.0	15	0.50	—	—	—	50	300	—	1471.10	4413.3	TRUE		19.4%	0.5	4413.3	444.4
7	1	H	10.0	21	0.70	—	—	—	50	300	—	1812.30	5436.9	TRUE		17.3%	0.7	5436.9	482.7
8	2	H	10.0	21	0.70	—	—	—	50	300	—	1872.40	5617.2	TRUE		17.9%	0.7	5617.2	482.7
9	3	H	10.0	21	0.70	—	—	—	50	300	—	1825.50	5476.5	TRUE		17.4%	0.7	5476.5	482.7
10	1	H	10.0	30	1.00	—	—	—	50	300	—	2351.90	7055.7	TRUE		15.7%	1	7055.7	551.9
11	2	H	10.0	30	1.00	—	—	—	50	300	—	2189.80	6569.4	TRUE		14.7%	1	6569.4	551.9
12	3	H	10.0	30	1.00	—	—	—	50	300	—	2332.20	6996.6	TRUE		15.6%	1	6996.6	551.9
13	1	H	10.0	45	1.50	—	—	—	50	300	—	2646.30	7938.9	TRUE		11.7%	1.5	7938.9	812.5
14	2	H	10.0	45	1.50	—	—	—	50	300	—	2855.10	8565.3	TRUE		12.6%	1.5	8565.3	812.5
15	3	H	10.0	45	1.50	—	—	—	50	300	—	2668.00	8004	TRUE		11.8%	1.5	8004.0	812.5
16	1	H	100.0	7.5	2.50	—	—	—	50	300	—	3275.40	9826.2	TRUE		8.7%	2.5	9826.2	1042.8
17	2	H	100.0	7.5	2.50	—	—	—	50	300	—	3297.80	9893.4	TRUE		8.8%	2.5	9893.4	1042.8
18	3	H	100.0	7.5	2.50	—	—	—	50	300	—	3257.70	9773.1	TRUE		8.7%	2.5	9773.1	1042.8
19	1	H	100.0	15	5.00	—	—	—	50	300	—	4309.70	12929.1	TRUE		5.7%	5	12929.1	2870.2
20	2	H	100.0	15	5.00	—	—	—	50	300	—	4132.30	12396.9	TRUE		5.5%	5	12396.9	2870.2
21	3	H	100.0	15	5.00	—	—	—	50	300	—	4090.50	12271.5	TRUE		5.5%	5	12271.5	2870.2
22	1	H	100.0	30	10.00	—	—	—	50	300	—	5286.20	15858.6	TRUE		3.4%	10	15858.6	3234.8
23	2	H	100.0	30	10.00	—	—	—	50	300	—	5323.70	15971.1	TRUE		3.5%	10	15971.1	3234.8
24	3	H	100.0	30	10.00	—	—	—	50	300	—	5161.00	15483	TRUE		3.4%	10	15483.0	3234.8

Saturation Assay Tube Layout												dpm as counted	corrected DPM for 2mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	Ten Percent Rule	Saturation X values	Bound y values	NSB y values
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetonone Acetate (uL)	Cytosol (uL)	Significant portion of label on Vial								
25	1	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	81.83	245.49	TRUE					
26	2	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	82.78	248.34	TRUE					
27	3	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	90.50	271.5	TRUE					
28	1	HC	10.0	15	0.5	1.00	15	50	50	300	C7	153.02	459.06	TRUE					
29	2	HC	10.0	15	0.5	1.00	15	50	50	300	C7	161.77	485.31	TRUE					
30	3	HC	10.0	15	0.5	1.00	15	50	50	300	C7	129.65	388.95	TRUE					
31	1	HC	10.0	21	0.7	1.00	21	70	50	300	C6	173.58	520.74	TRUE					
32	2	HC	10.0	21	0.7	1.00	21	70	50	300	C6	145.57	436.71	TRUE					
33	3	HC	10.0	21	0.7	1.00	21	70	50	300	C6	163.59	490.77	TRUE					
34	1	HC	10.0	30	1	1.00	30	100	50	300	C5	157.77	473.31	TRUE					
35	2	HC	10.0	30	1	1.00	30	100	50	300	C5	233.46	700.38	TRUE					
36	3	HC	10.0	30	1	1.00	30	100	50	300	C5	160.67	482.01	TRUE					
37	1	HC	10.0	45	1.5	1.00	45	150	50	300	C4	220.16	660.48	TRUE					
38	2	HC	10.0	45	1.5	1.00	45	150	50	300	C4	288.58	865.74	TRUE					
39	3	HC	10.0	45	1.5	1.00	45	150	50	300	C4	303.72	911.16	TRUE					
40	1	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	387.68	1163.04	TRUE					
41	2	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	275.68	827.04	TRUE					
42	3	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	379.43	1138.29	TRUE					
43	1	HC	100.0	15	5	10.00	15	500	50	300	C2	511.17	1533.51	FALSE	spill				
44	2	HC	100.0	15	5	10.00	15	500	50	300	C2	990.14	2970.42	TRUE					
45	3	HC	100.0	15	5	10.00	15	500	50	300	C2	923.31	2769.93	TRUE					
46	1	HC	100.0	30	10	10.00	30	1000	50	300	C1	965.92	2897.76	TRUE					
47	2	HC	100.0	30	10	10.00	30	1000	50	300	C1	1240.30	3720.9	TRUE					
48	3	HC	100.0	30	10	10.00	30	1000	50	300	C1	1028.58	3085.74	TRUE					
49	1	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11380.7	11380.7	TRUE					
50	2	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11321.1	11321.1	TRUE					
51	3	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11385.1	11385.1	TRUE					
52	1	Hot	10.0	15	0.5	—	—	—	—	—	—	23012.0	23012	TRUE					
53	2	Hot	10.0	15	0.5	—	—	—	—	—	—	22959.0	22959	TRUE					
54	3	Hot	10.0	15	0.5	—	—	—	—	—	—	22401.0	22401	TRUE					
55	1	Hot	10.0	21	0.7	—	—	—	—	—	—	31011.0	31011	TRUE					
56	2	Hot	10.0	21	0.7	—	—	—	—	—	—	31801.0	31801	TRUE					
57	3	Hot	10.0	21	0.7	—	—	—	—	—	—	31527.0	31527	TRUE					
58	1	Hot	10.0	30	1	—	—	—	—	—	—	44722.0	44722	TRUE					
59	2	Hot	10.0	30	1	—	—	—	—	—	—	43823.0	43823	TRUE					
60	3	Hot	10.0	30	1	—	—	—	—	—	—	45910.0	45910	TRUE					
61	1	Hot	10.0	45	1.5	—	—	—	—	—	—	67656.0	67656	TRUE					
62	2	Hot	10.0	45	1.5	—	—	—	—	—	—	68111.0	68111	TRUE					
63	3	Hot	10.0	45	1.5	—	—	—	—	—	—	67622.0	67622	TRUE					
64	1	Hot	100.0	7.5	2.5	—	—	—	—	—	—	112317	112317	TRUE					
65	2	Hot	100.0	7.5	2.5	—	—	—	—	—	—	113821	113821	TRUE					
66	3	Hot	100.0	7.5	2.5	—	—	—	—	—	—	112310	112310	TRUE					
67	1	Hot	100.0	15	5	—	—	—	—	—	—	226752	226752	TRUE					
68	2	Hot	100.0	15	5	—	—	—	—	—	—	224386	224386	TRUE					
69	3	Hot	100.0	15	5	—	—	—	—	—	—	224037	224037	TRUE					
70	1	Hot	100.0	30	10	—	—	—	—	—	—	461331	461331	TRUE					
71	2	Hot	100.0	30	10	—	—	—	—	—	—	466101	466101	TRUE					
72	3	Hot	100.0	30	10	—	—	—	—	—	—	452231	452231	TRUE					

Total Binding -- Positions 1-24 radiolabeled R1881 plus cytosol (Panel A)												
Run	Position	Tube Identification			Assay tube contents							
		Rep	Tube Type Code	Conc. Code	Hot Conc. Initial	Hot R1881 Volume	Cold R1881 Conc. Initial	Cold R1881 volume	Triamcetenone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)
477	1	1	H	c1	10.0	7.5	—	—	—	300	0.25	—
477	2	2	H	c1	10.0	7.5	—	—	—	300	0.25	—
477	3	3	H	c1	10.0	7.5	—	—	—	300	0.25	—
477	4	1	H	c2	10.0	15	—	—	—	300	0.50	—
477	5	2	H	c2	10.0	15	—	—	—	300	0.50	—
477	6	3	H	c2	10.0	15	—	—	—	300	0.50	—
477	7	1	H	c3	10.0	21	—	—	—	300	0.70	—
477	8	2	H	c3	10.0	21	—	—	—	300	0.70	—
477	9	3	H	c3	10.0	21	—	—	—	300	0.70	—
477	10	1	H	c4	10.0	30	—	—	—	300	1.00	—
477	11	2	H	c4	10.0	30	—	—	—	300	1.00	—
477	12	3	H	c4	10.0	30	—	—	—	300	1.00	—
477	13	1	H	c5	10.0	45	—	—	—	300	1.50	—
477	14	2	H	c5	10.0	45	—	—	—	300	1.50	—
477	15	3	H	c5	10.0	45	—	—	—	300	1.50	—
477	16	1	H	c6	100.0	7.5	—	—	—	300	2.50	—
477	17	2	H	c6	100.0	7.5	—	—	—	300	2.50	—
477	18	3	H	c6	100.0	7.5	—	—	—	300	2.50	—
477	19	1	H	c7	100.0	15	—	—	—	300	5.00	—
477	20	2	H	c7	100.0	15	—	—	—	300	5.00	—
477	21	3	H	c7	100.0	15	—	—	—	300	5.00	—
477	22	1	H	c8	100.0	30	—	—	—	300	10.00	—
477	23	2	H	c8	100.0	30	—	—	—	300	10.00	—
477	24	3	H	c8	100.0	30	—	—	—	300	10.00	—
												Total Volume
												(ul)

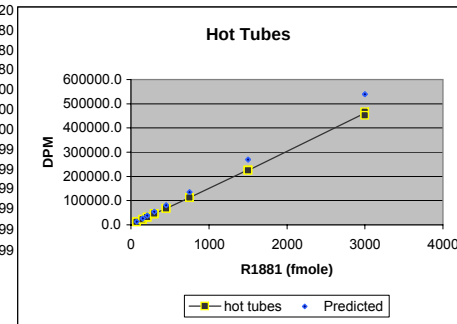
Run	Position								Number of molecules					Ratio
		Total Counts	Non Specific Binding (Mean of reps in pos. 25-48)	Specific Binding (Total - Non Specific)	Ratio of NSB/ total binding	Ratio Total binding/ Hot	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Total Binding molecules	Non Specific Binding molecules	Specific Binding molecules	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Specific Bound / Free
		(dpm)	(dpm)	(dpm)			(dpm)	(dpm)	(fmole)	(fmole)	(fmole)	(fmole)	(fmole)	
477	1	2554.6	255.1	2299.5	10.0%	22.5%	11362.3	8807.7	17	2	15	75	58	0.26
477	2	2683.6	255.1	2428.5	9.5%	23.6%	11362.3	8678.7	18	2	16	75	57	0.28
477	3	2521.7	255.1	2266.6	10.1%	22.2%	11362.3	8840.6	17	2	15	75	58	0.26
477	4	4516.2	444.4	4071.8	9.8%	19.8%	22790.7	18274.5	30	3	27	149	120	0.22
477	5	4653.3	444.4	4208.9	9.6%	20.4%	22790.7	18137.4	31	3	28	149	119	0.23
477	6	4413.3	444.4	3968.9	10.1%	19.4%	22790.7	18377.4	29	3	26	149	121	0.22
477	7	5436.9	482.7	4954.2	8.9%	17.3%	31446.3	26009.4	36	3	32	206	171	0.19
477	8	5617.2	482.7	5134.5	8.6%	17.9%	31446.3	25829.1	37	3	34	206	169	0.20
477	9	5476.5	482.7	4993.8	8.8%	17.4%	31446.3	25969.8	36	3	33	206	170	0.19
477	10	7055.7	551.9	6503.8	7.8%	15.7%	44818.3	37762.6	46	4	43	294	248	0.17
477	11	6569.4	551.9	6017.5	8.4%	14.7%	44818.3	38248.9	43	4	39	294	251	0.16
477	12	6996.6	551.9	6444.7	7.9%	15.6%	44818.3	37821.7	46	4	42	294	248	0.17
477	13	7938.9	812.5	7126.4	10.2%	11.7%	67796.3	59857.4	52	5	47	445	393	0.12
477	14	8565.3	812.5	7752.8	9.5%	12.6%	67796.3	59231.0	56	5	51	445	388	0.13
477	15	8004.0	812.5	7191.5	10.2%	11.8%	67796.3	59792.3	52	5	47	445	392	0.12
477	16	9826.2	1042.8	8783.4	10.6%	8.7%	112816.0	102989.8	64	7	58	740	675	0.09
477	17	9893.4	1042.8	8850.6	10.5%	8.8%	112816.0	102922.6	65	7	58	740	675	0.09
477	18	9773.1	1042.8	8730.3	10.7%	8.7%	112816.0	103042.9	64	7	57	740	676	0.08
477	19	12929.1	2870.2	10058.9	22.2%	5.7%	225058.3	212129.2	85	19	66	1476	1391	0.05
477	20	12396.9	2870.2	9526.7	23.2%	5.5%	225058.3	212661.4	81	19	62	1476	1395	0.04
477	21	12271.5	2870.2	9401.3	23.4%	5.5%	225058.3	212786.8	80	19	62	1476	1396	0.04
477	22	15858.6	3234.8	12623.8	20.4%	3.4%	459887.7	444029.1	104	21	83	3016	2912	0.03
477	23	15971.1	3234.8	12736.3	20.3%	3.5%	459887.7	443916.6	105	21	84	3016	2911	0.03
477	24	15483.0	3234.8	12248.2	20.9%	3.4%	459887.7	444404.7	102	21	80	3016	2915	0.03

Run	Position	Non Specific Binding -- Positions 25-48 radiolabeled R1881 plus 100 X inert R1881 plus cytosol												
		Tube Identification			Assay tube contents							Scintillation Results		
		Rep	Tube Type Code	Conc. Code	Hot Conc. R1881 Initial	Hot	Cold R1881 Conc. Initial	Cold	Triamcetonone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final	Counts per Scintillation Vial (Total Binding)	Non Specific Binding (Mean of reps in pos. 25-48)
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)	(dpm)	(dpm)
477	25	1	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	245.5	255.1
477	26	2	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	248.3	255.1
477	27	3	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	271.5	255.1
477	28	1	HC	c2	10.0	15	1.00	15	50	300	0.5	50	459.1	444.4
477	29	2	HC	c2	10.0	15	1.00	15	50	300	0.5	50	485.3	444.4
477	30	3	HC	c2	10.0	15	1.00	15	50	300	0.5	50	389.0	444.4
477	31	1	HC	c3	10.0	21	1.00	21	50	300	0.7	70	520.7	482.7
477	32	2	HC	c3	10.0	21	1.00	21	50	300	0.7	70	436.7	482.7
477	33	3	HC	c3	10.0	21	1.00	21	50	300	0.7	70	490.8	482.7
477	34	1	HC	c4	10.0	30	1.00	30	50	300	1	100	473.3	551.9
477	35	2	HC	c4	10.0	30	1.00	30	50	300	1	100	700.4	551.9
477	36	3	HC	c4	10.0	30	1.00	30	50	300	1	100	482.0	551.9
477	37	1	HC	c5	10.0	45	1.00	45	50	300	1.5	150	660.5	812.5
477	38	2	HC	c5	10.0	45	1.00	45	50	300	1.5	150	865.7	812.5
477	39	3	HC	c5	10.0	45	1.00	45	50	300	1.5	150	911.2	812.5
477	40	1	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	1163.0	1042.8
477	41	2	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	827.0	1042.8
477	42	3	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	1138.3	1042.8
477	43	1	HC	c7	100.0	15	10.00	15	50	300	5	500		2870.2
477	44	2	HC	c7	100.0	15	10.00	15	50	300	5	500	2970.4	2870.2
477	45	3	HC	c7	100.0	15	10.00	15	50	300	5	500	2769.9	2870.2
477	46	1	HC	c8	100.0	30	10.00	30	50	300	10	1000	2897.8	3234.8
477	47	2	HC	c8	100.0	30	10.00	30	50	300	10	1000	3720.9	3234.8
477	48	3	HC	c8	100.0	30	10.00	30	50	300	10	1000	3085.7	3234.8

Run	Position	Free -- Positions 49-72, radiolabeled R1881 without cytosol								
		Rep	Tube Type Code	Conc. Code	Hot R1881 Conc. Initial	Hot R1881 Volume	Molecules of R1881	Counts per Scintillation Vial	Experimental number of molecules	Total Added (Mean of reps in pos. 49-72)
					(nM)	(ul)	(fmole)	(dpm)	(fmole)	(dpm)
477	49	1	Hot	c1	10	7.5	75	11380.7	75	11362.3
477	50	2	Hot	c1	10	7.5	75	11321.1	74	11362.3
477	51	3	Hot	c1	10	7.5	75	11385.1	75	11362.3
477	52	1	Hot	c2	10	15	150	23012.0	151	22790.7
477	53	2	Hot	c2	10	15	150	22959.0	151	22790.7
477	54	3	Hot	c2	10	15	150	22401.0	147	22790.7
477	55	1	Hot	c3	10	21	210	31011.0	203	31446.3
477	56	2	Hot	c3	10	21	210	31801.0	209	31446.3
477	57	3	Hot	c3	10	21	210	31527.0	207	31446.3
477	58	1	Hot	c4	10	30	300	44722.0	293	44818.3
477	59	2	Hot	c4	10	30	300	43823.0	287	44818.3
477	60	3	Hot	c4	10	30	300	45910.0	301	44818.3
477	61	1	Hot	c5	10	45	450	67656.0	444	67796.3
477	62	2	Hot	c5	10	45	450	68111.0	447	67796.3
477	63	3	Hot	c5	10	45	450	67622.0	444	67796.3
477	64	1	Hot	c6	100	7.5	750	112317.0	737	112816.0
477	65	2	Hot	c6	100	7.5	750	113821.0	747	112816.0
477	66	3	Hot	c6	100	7.5	750	112310.0	737	112816.0
477	67	1	Hot	c7	100	15	1500	226752.0	1487	225058.3
477	68	2	Hot	c7	100	15	1500	224386.0	1472	225058.3
477	69	3	Hot	c7	100	15	1500	224037.0	1469	225058.3
477	70	1	Hot	c8	100	30	3000	461331.0	3026	459887.7
477	71	2	Hot	c8	100	30	3000	466101.0	3057	459887.7
477	72	3	Hot	c8	100	30	3000	452231.0	2966	459887.7

predicted dpm

Computation Check	
7/10/05	specific activity date
80.96	Ci/mMole 3H R1881
2.22E+12	DPM/Ci (definition)
1.7973E+14	DPM/mMole
1.7973E+11	DPM/nMole
179.7	DPM/fmole
0.005564	fMole/DPM



Linear regression results (LINEST function)	
(Regression line forced through 0,0)	
Slope	152.4724108 dpm/fmole
1/slope	0.006558564 fmole/dpm
x	y
origin	0
end point	3057.0 466101
SLOPE function, used if missing HOT tubes	
Slope	153.1 dpm/fmole
1/slope	0.006533 fmole/dpm
x	y
origin	0
end point	3045.1 466101

Prism input for bound/free		Prism input for specific bound	
specific bound/molar	bound/free	average total added molar	specific bound/molar
4.26457E-11	0.26107	2.10726E-10	4.26457E-11
4.50381E-11	0.27982	2.10726E-10	4.50381E-11
4.20364E-11	0.25639	2.10726E-10	4.20364E-11
7.5515E-11	0.22281	4.22676E-10	7.5515E-11
7.80576E-11	0.23205	4.22676E-10	7.80576E-11
7.36066E-11	0.21596	4.22676E-10	7.36066E-11
9.188E-11	0.19048	5.83205E-10	9.188E-11
9.52238E-11	0.19879	5.83205E-10	9.52238E-11
9.26144E-11	0.19229	5.83205E-10	9.26144E-11
1.2062E-10	0.17223	8.31202E-10	1.2062E-10
1.11601E-10	0.15732	8.31202E-10	1.11601E-10
1.19524E-10	0.17040	8.31202E-10	1.19524E-10
1.32167E-10	0.11906	1.25735E-09	1.32167E-10
1.43784E-10	0.13089	1.25735E-09	1.43784E-10
1.33375E-10	0.12028	1.25735E-09	1.33375E-10
1.62897E-10	0.08528	2.09229E-09	1.62897E-10
1.64144E-10	0.08599	2.09229E-09	1.64144E-10
1.61913E-10	0.08473	2.09229E-09	1.61913E-10
1.86553E-10	0.04742	4.17394E-09	1.86553E-10
1.76683E-10	0.04480	4.17394E-09	1.76683E-10
1.74357E-10	0.04418	4.17394E-09	1.74357E-10
2.34121E-10	0.02843	8.52909E-09	2.34121E-10
2.36208E-10	0.02869	8.52909E-09	2.36208E-10
2.27155E-10	0.02756	8.52909E-09	2.27155E-10

Bmax molar	2.37E-10	KD molar	9.19E-10
mole to molar conversion value	0.0003	molar to nM conversion	1.00E+09
DPM/mole = (DPM/mmol)*1000	1.80E+17	kd nM =	9.19E-01
Bmax molar to Bmax moles	7.1112E-14		
= DPM/((DPM/mmol)*1000)	7.1112E-14		
=Bmax DPM	12781.17279		
assay date	7/10/2005		
Bmax(dpm)	12781.17279		
DPM/Ci (definition)	2.22E+12		
Ci/mmol	80.96		
DPM/mmol	1.80E+14		
DPM/pmol	1.80E+05		
1/(DPM/mmol)	5.56E-15		
1/(DPM/pmol)	5.56E-06		
SA(dpm/pmol)	1.80E+05		
protein/tube (ug)	600		
protein./tube(mg)	0.6		
bmax pmole	0.071112		
bmax pmole/mg	0.11852		
Bmax fmole/mg	118.52		
Bmax (fmole/100 ug)	11.852		
Bmax(fmole/100 ug)/Bmax molar	5.00E+10		

Laboratory E

AR Saturation Assay (cold R1881 dilutions supplied by Battelle)

72 assay tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in columns O and DK

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Provide a reason in column R

The value in column Q will automatically change to FALSE

For your convenience, data reduction is performed in columns

U through BZ, and the values needed for analysis are presented
in columns CF through CN

Cells in column S are presented with a grey background

if the total binding exceeds 10% of the hot added at that concentration,
the cytosol concentration is probably too high for good competitive assays

Laboratory Code: E

Run identification: 479

Assay start date: 7/11/2005

Tracer lot number: 3559-507

Specific activity on day of assay: 80.95 Ci/mole

Cytosol lot or vial number: 051905

protein (cytosol) per tube: 600 ug

protein (cytosol) per tube: 0.6 mg

KD 9.04E-01 nM

Bmax 11.34 fmole/100 ug

total volume in tubes 300 uL

volume of ethanol counted: 2 mL

multiply DPM in sample by : 3

Receptor Notes

diluted to 2 mg/ml for use (0.6 mg/300 ul)

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Saturation Assay Tube Layout																				
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetenone Acetate (uL)	Cytosol (ul)	Significant portion of label on Vial	dpm as counted								corrected DPM for 2mL
1	1	H	10.0	7.5	0.25	—	—	—	50	300	—	869.35	2608.05	TRUE			23.7%	0.25	2608.1	306.8
2	2	H	10.0	7.5	0.25	—	—	—	50	300	—	854.35	2563.05	TRUE			23.3%	0.25	2563.1	306.8
3	3	H	10.0	7.5	0.25	—	—	—	50	300	—	839.25	2517.75	TRUE			22.9%	0.25	2517.8	306.8
4	1	H	10.0	15	0.50	—	—	—	50	300	—	1416.70	4250.1	TRUE			18.6%	0.5	4250.1	337.9
5	2	H	10.0	15	0.50	—	—	—	50	300	—	1504.30	4512.9	TRUE			19.7%	0.5	4512.9	337.9
6	3	H	10.0	15	0.50	—	—	—	50	300	—	1445.40	4336.2	TRUE			18.9%	0.5	4336.2	337.9
7	1	H	10.0	21	0.70	—	—	—	50	300	—	1472.10	4416.3	TRUE			14.2%	0.7	4416.3	427.0
8	2	H	10.0	21	0.70	—	—	—	50	300	—	1716.60	5149.8	TRUE			16.5%	0.7	5149.8	427.0
9	3	H	10.0	21	0.70	—	—	—	50	300	—	1731.60	5194.8	TRUE			16.7%	0.7	5194.8	427.0
10	1	H	10.0	30	1.00	—	—	—	50	300	—	2243.10	6729.3	TRUE			15.3%	1	6729.3	522.5
11	2	H	10.0	30	1.00	—	—	—	50	300	—	2211.50	6634.5	TRUE			15.0%	1	6634.5	522.5
12	3	H	10.0	30	1.00	—	—	—	50	300	—	2200.70	6602.1	TRUE			15.0%	1	6602.1	522.5
13	1	H	10.0	45	1.50	—	—	—	50	300	—	2528.90	7586.7	TRUE			10.9%	1.5	7586.7	741.2
14	2	H	10.0	45	1.50	—	—	—	50	300	—	2565.60	7696.8	TRUE			11.0%	1.5	7696.8	741.2
15	3	H	10.0	45	1.50	—	—	—	50	300	—	2719.50	8158.5	TRUE			11.7%	1.5	8158.5	741.2
16	1	H	100.0	7.5	2.50	—	—	—	50	300	—	3325.10	9975.3	TRUE			8.9%	2.5	9975.3	983.2
17	2	H	100.0	7.5	2.50	—	—	—	50	300	—	3475.20	10425.6	TRUE			9.3%	2.5	10425.6	983.2
18	3	H	100.0	7.5	2.50	—	—	—	50	300	—	3360.80	10082.4	TRUE			9.0%	2.5	10082.4	983.2
19	1	H	100.0	15	5.00	—	—	—	50	300	—	3409.20	10227.6	TRUE			4.6%	5	10227.6	1730.5
20	2	H	100.0	15	5.00	—	—	—	50	300	—	3949.70	11849.1	TRUE			5.3%	5	11849.1	1730.5
21	3	H	100.0	15	5.00	—	—	—	50	300	—	4089.00	12267	TRUE			5.5%	5	12267.0	1730.5
22	1	H	100.0	30	10.00	—	—	—	50	300	—	4812.40	14437.2	TRUE			3.1%	10	14437.2	3322.4
23	2	H	100.0	30	10.00	—	—	—	50	300	—	4883.40	14650.2	TRUE			3.2%	10	14650.2	3322.4
24	3	H	100.0	30	10.00	—	—	—	50	300	—	4808.60	14425.8	TRUE			3.1%	10	14425.8	3322.4

Saturation Assay Tube Layout												dpm as counted	corrected DPM for 2mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	Ten Percent Rule	Saturation X values	Bound y values	NSB y values
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetenone Acetate (uL)	Cytosol (ul)	Significant portion of label on Vial								
25	1	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	104.60	313.8	TRUE					
26	2	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	112.05	336.15	TRUE					
27	3	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	90.13	270.39	TRUE					
28	1	HC	10.0	15	0.5	1.00	15	50	50	300	C7	112.41	337.23	TRUE					
29	2	HC	10.0	15	0.5	1.00	15	50	50	300	C7	109.13	327.39	TRUE					
30	3	HC	10.0	15	0.5	1.00	15	50	50	300	C7	116.36	349.08	TRUE					
31	1	HC	10.0	21	0.7	1.00	21	70	50	300	C6	140.92	422.76	TRUE					
32	2	HC	10.0	21	0.7	1.00	21	70	50	300	C6	154.61	463.83	TRUE					
33	3	HC	10.0	21	0.7	1.00	21	70	50	300	C6	131.49	394.47	TRUE					
34	1	HC	10.0	30	1	1.00	30	100	50	300	C5	171.04	513.12	TRUE					
35	2	HC	10.0	30	1	1.00	30	100	50	300	C5	182.67	548.01	TRUE					
36	3	HC	10.0	30	1	1.00	30	100	50	300	C5	168.80	506.4	TRUE					
37	1	HC	10.0	45	1.5	1.00	45	150	50	300	C4	224.84	674.52	TRUE					
38	2	HC	10.0	45	1.5	1.00	45	150	50	300	C4	224.23	672.69	TRUE					
39	3	HC	10.0	45	1.5	1.00	45	150	50	300	C4	292.09	876.27	TRUE					
40	1	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	355.69	1067.07	TRUE					
41	2	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	307.34	922.02	TRUE					
42	3	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	320.14	960.42	TRUE					
43	1	HC	100.0	15	5	10.00	15	500	50	300	C2	619.69	1859.07	TRUE					
44	2	HC	100.0	15	5	10.00	15	500	50	300	C2	495.15	1485.45	TRUE					
45	3	HC	100.0	15	5	10.00	15	500	50	300	C2	615.70	1847.1	TRUE					
46	1	HC	100.0	30	10	10.00	30	1000	50	300	C1	1290.50	3871.5	TRUE					
47	2	HC	100.0	30	10	10.00	30	1000	50	300	C1	1116.00	3348	TRUE					
48	3	HC	100.0	30	10	10.00	30	1000	50	300	C1	915.87	2747.61	TRUE					
49	1	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11492.2	11492.2	TRUE					
50	2	Hot	10.0	7.5	0.25	—	—	—	—	—	—	10478.2	10478.2	TRUE					
51	3	Hot	10.0	7.5	0.25	—	—	—	—	—	—	10974.0	10974	TRUE					
52	1	Hot	10.0	15	0.5	—	—	—	—	—	—	23303.0	23303	TRUE					
53	2	Hot	10.0	15	0.5	—	—	—	—	—	—	22698.0	22698	TRUE					
54	3	Hot	10.0	15	0.5	—	—	—	—	—	—	22712.0	22712	TRUE					
55	1	Hot	10.0	21	0.7	—	—	—	—	—	—	30789.0	30789	TRUE					
56	2	Hot	10.0	21	0.7	—	—	—	—	—	—	31196.0	31196	TRUE					
57	3	Hot	10.0	21	0.7	—	—	—	—	—	—	31430.0	31430	TRUE					
58	1	Hot	10.0	30	1	—	—	—	—	—	—	45413.0	45413	TRUE					
59	2	Hot	10.0	30	1	—	—	—	—	—	—	44380.0	44380	TRUE					
60	3	Hot	10.0	30	1	—	—	—	—	—	—	42457.0	42457	TRUE					
61	1	Hot	10.0	45	1.5	—	—	—	—	—	—	70912.0	70912	TRUE					
62	2	Hot	10.0	45	1.5	—	—	—	—	—	—	69410.0	69410	TRUE					
63	3	Hot	10.0	45	1.5	—	—	—	—	—	—	69246.0	69246	TRUE					
64	1	Hot	100.0	7.5	2.5	—	—	—	—	—	—	111379	111379	TRUE					
65	2	Hot	100.0	7.5	2.5	—	—	—	—	—	—	112051	112051	TRUE					
66	3	Hot	100.0	7.5	2.5	—	—	—	—	—	—	114006	114006	TRUE					
67	1	Hot	100.0	15	5	—	—	—	—	—	—	221591	221591	TRUE					
68	2	Hot	100.0	15	5	—	—	—	—	—	—	227633	227633	TRUE					
69	3	Hot	100.0	15	5	—	—	—	—	—	—	217422	217422	TRUE					
70	1	Hot	100.0	30	10	—	—	—	—	—	—	456488	456488	TRUE					
71	2	Hot	100.0	30	10	—	—	—	—	—	—	468707	468707	TRUE					
72	3	Hot	100.0	30	10	—	—	—	—	—	—	466608	466608	TRUE					

Total Binding -- Positions 1-24 radiolabeled R1881 plus cytosol (Panel A)												
Run	Position	Tube Identification			Assay tube contents							
		Rep	Tube Type Code	Conc. Code	Hot Conc. Initial	Hot R1881 Volume	Cold R1881 Conc. Initial	Cold R1881 volume	Triamcetenone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)
479	1	1	H	c1	10.0	7.5	—	—	—	300	0.25	—
479	2	2	H	c1	10.0	7.5	—	—	—	300	0.25	—
479	3	3	H	c1	10.0	7.5	—	—	—	300	0.25	—
479	4	1	H	c2	10.0	15	—	—	—	300	0.50	—
479	5	2	H	c2	10.0	15	—	—	—	300	0.50	—
479	6	3	H	c2	10.0	15	—	—	—	300	0.50	—
479	7	1	H	c3	10.0	21	—	—	—	300	0.70	—
479	8	2	H	c3	10.0	21	—	—	—	300	0.70	—
479	9	3	H	c3	10.0	21	—	—	—	300	0.70	—
479	10	1	H	c4	10.0	30	—	—	—	300	1.00	—
479	11	2	H	c4	10.0	30	—	—	—	300	1.00	—
479	12	3	H	c4	10.0	30	—	—	—	300	1.00	—
479	13	1	H	c5	10.0	45	—	—	—	300	1.50	—
479	14	2	H	c5	10.0	45	—	—	—	300	1.50	—
479	15	3	H	c5	10.0	45	—	—	—	300	1.50	—
479	16	1	H	c6	100.0	7.5	—	—	—	300	2.50	—
479	17	2	H	c6	100.0	7.5	—	—	—	300	2.50	—
479	18	3	H	c6	100.0	7.5	—	—	—	300	2.50	—
479	19	1	H	c7	100.0	15	—	—	—	300	5.00	—
479	20	2	H	c7	100.0	15	—	—	—	300	5.00	—
479	21	3	H	c7	100.0	15	—	—	—	300	5.00	—
479	22	1	H	c8	100.0	30	—	—	—	300	10.00	—
479	23	2	H	c8	100.0	30	—	—	—	300	10.00	—
479	24	3	H	c8	100.0	30	—	—	—	300	10.00	—
												Total Volume
												(ul)

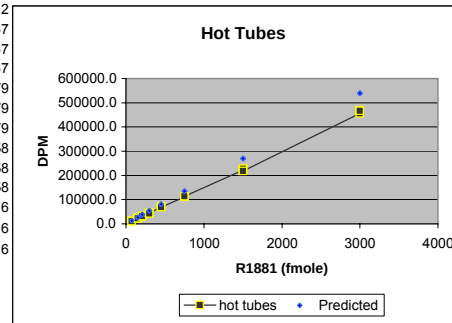
Run	Position							Number of molecules						Ratio
		Total Counts	Non Specific Binding (Mean of reps in pos. 25-48)	Specific Binding (Total - Non Specific)	Ratio of NSB/ total binding	Ratio Total binding/ Hot	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Total Binding molecules	Non Specific Binding molecules	Specific Binding molecules	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Specific Bound / Free
		(dpm)	(dpm)	(dpm)			(dpm)	(dpm)	(fmole)	(fmole)	(fmole)	(fmole)	(fmole)	
479	1	2608.1	306.8	2301.3	11.8%	23.7%	10981.5	8373.4	17	2	15	72	55	0.27
479	2	2563.1	306.8	2256.3	12.0%	23.3%	10981.5	8418.4	17	2	15	72	55	0.27
479	3	2517.8	306.8	2211.0	12.2%	22.9%	10981.5	8463.7	16	2	14	72	55	0.26
479	4	4250.1	337.9	3912.2	8.0%	18.6%	22904.3	18654.2	28	2	26	150	122	0.21
479	5	4512.9	337.9	4175.0	7.5%	19.7%	22904.3	18391.4	29	2	27	150	120	0.23
479	6	4336.2	337.9	3998.3	7.8%	18.9%	22904.3	18568.1	28	2	26	150	121	0.22
479	7	4416.3	427.0	3989.3	9.7%	14.2%	31138.3	26722.0	29	3	26	203	174	0.15
479	8	5149.8	427.0	4722.8	8.3%	16.5%	31138.3	25988.5	34	3	31	203	170	0.18
479	9	5194.8	427.0	4767.8	8.2%	16.7%	31138.3	25943.5	34	3	31	203	169	0.18
479	10	6729.3	522.5	6206.8	7.8%	15.3%	44083.3	37354.0	44	3	41	288	244	0.17
479	11	6634.5	522.5	6112.0	7.9%	15.0%	44083.3	37448.8	43	3	40	288	245	0.16
479	12	6602.1	522.5	6079.6	7.9%	15.0%	44083.3	37481.2	43	3	40	288	245	0.16
479	13	7586.7	741.2	6845.5	9.8%	10.9%	69856.0	62269.3	50	5	45	456	407	0.11
479	14	7696.8	741.2	6955.6	9.6%	11.0%	69856.0	62159.2	50	5	45	456	406	0.11
479	15	8158.5	741.2	7417.3	9.1%	11.7%	69856.0	61697.5	53	5	48	456	403	0.12
479	16	9975.3	983.2	8992.1	9.9%	8.9%	112478.7	102503.4	65	6	59	734	669	0.09
479	17	10425.6	983.2	9442.4	9.4%	9.3%	112478.7	102053.1	68	6	62	734	666	0.09
479	18	10082.4	983.2	9099.2	9.8%	9.0%	112478.7	102396.3	66	6	59	734	669	0.09
479	19	10227.6	1730.5	8497.1	16.9%	4.6%	222215.3	211987.7	67	11	55	1451	1384	0.04
479	20	11849.1	1730.5	10118.6	14.6%	5.3%	222215.3	210366.2	77	11	66	1451	1374	0.05
479	21	12267.0	1730.5	10536.5	14.1%	5.5%	222215.3	209948.3	80	11	69	1451	1371	0.05
479	22	14437.2	3322.4	11114.8	23.0%	3.1%	463934.3	449497.1	94	22	73	3029	2935	0.02
479	23	14650.2	3322.4	11327.8	22.7%	3.2%	463934.3	449284.1	96	22	74	3029	2934	0.03
479	24	14425.8	3322.4	11103.4	23.0%	3.1%	463934.3	449508.5	94	22	73	3029	2935	0.02

Run	Position	Non Specific Binding -- Positions 25-48 radiolabeled R1881 plus 100 X inert R1881 plus cytosol												
		Tube Identification			Assay tube contents							Scintillation Results		
		Rep	Tube Type Code	Conc. Code	Hot Conc. R1881 Initial	Hot	Cold R1881 Conc. Initial	Cold	Triamcetonone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final	Counts per Scintillation Vial (Total Binding)	Non Specific Binding (Mean of reps in pos. 25-48)
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)	(dpm)	(dpm)
479	25	1	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	313.8	306.8
479	26	2	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	336.2	306.8
479	27	3	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	270.4	306.8
479	28	1	HC	c2	10.0	15	1.00	15	50	300	0.5	50	337.2	337.9
479	29	2	HC	c2	10.0	15	1.00	15	50	300	0.5	50	327.4	337.9
479	30	3	HC	c2	10.0	15	1.00	15	50	300	0.5	50	349.1	337.9
479	31	1	HC	c3	10.0	21	1.00	21	50	300	0.7	70	422.8	427.0
479	32	2	HC	c3	10.0	21	1.00	21	50	300	0.7	70	463.8	427.0
479	33	3	HC	c3	10.0	21	1.00	21	50	300	0.7	70	394.5	427.0
479	34	1	HC	c4	10.0	30	1.00	30	50	300	1	100	513.1	522.5
479	35	2	HC	c4	10.0	30	1.00	30	50	300	1	100	548.0	522.5
479	36	3	HC	c4	10.0	30	1.00	30	50	300	1	100	506.4	522.5
479	37	1	HC	c5	10.0	45	1.00	45	50	300	1.5	150	674.5	741.2
479	38	2	HC	c5	10.0	45	1.00	45	50	300	1.5	150	672.7	741.2
479	39	3	HC	c5	10.0	45	1.00	45	50	300	1.5	150	876.3	741.2
479	40	1	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	1067.1	983.2
479	41	2	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	922.0	983.2
479	42	3	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	960.4	983.2
479	43	1	HC	c7	100.0	15	10.00	15	50	300	5	500	1859.1	1730.5
479	44	2	HC	c7	100.0	15	10.00	15	50	300	5	500	1485.5	1730.5
479	45	3	HC	c7	100.0	15	10.00	15	50	300	5	500	1847.1	1730.5
479	46	1	HC	c8	100.0	30	10.00	30	50	300	10	1000	3871.5	3322.4
479	47	2	HC	c8	100.0	30	10.00	30	50	300	10	1000	3348.0	3322.4
479	48	3	HC	c8	100.0	30	10.00	30	50	300	10	1000	2747.6	3322.4

Run	Position	Free -- Positions 49-72, radiolabeled R1881 without cytosol								
		Rep	Tube Type Code	Conc. Code	Hot R1881 Conc. Initial	Hot R1881 Volume	Molecules of R1881	Counts per Scintillation Vial	Experimental number of molecules	Total Added (Mean of reps in pos. 49-72)
					(nM)	(ul)	(fmole)	(dpm)	(fmole)	(dpm)
479	49	1	Hot	c1	10	7.5	75	11492.2	75	10981.5
479	50	2	Hot	c1	10	7.5	75	10478.2	68	10981.5
479	51	3	Hot	c1	10	7.5	75	10974.0	72	10981.5
479	52	1	Hot	c2	10	15	150	23303.0	152	22904.3
479	53	2	Hot	c2	10	15	150	22698.0	148	22904.3
479	54	3	Hot	c2	10	15	150	22712.0	148	22904.3
479	55	1	Hot	c3	10	21	210	30789.0	201	31138.3
479	56	2	Hot	c3	10	21	210	31196.0	204	31138.3
479	57	3	Hot	c3	10	21	210	31430.0	205	31138.3
479	58	1	Hot	c4	10	30	300	45413.0	297	44083.3
479	59	2	Hot	c4	10	30	300	44380.0	290	44083.3
479	60	3	Hot	c4	10	30	300	42457.0	277	44083.3
479	61	1	Hot	c5	10	45	450	70912.0	463	69856.0
479	62	2	Hot	c5	10	45	450	69410.0	453	69856.0
479	63	3	Hot	c5	10	45	450	69246.0	452	69856.0
479	64	1	Hot	c6	100	7.5	750	111379.0	727	112478.7
479	65	2	Hot	c6	100	7.5	750	112051.0	732	112478.7
479	66	3	Hot	c6	100	7.5	750	114006.0	744	112478.7
479	67	1	Hot	c7	100	15	1500	221591.0	1447	222215.3
479	68	2	Hot	c7	100	15	1500	227633.0	1486	222215.3
479	69	3	Hot	c7	100	15	1500	217422.0	1420	222215.3
479	70	1	Hot	c8	100	30	3000	456488.0	2981	463934.3
479	71	2	Hot	c8	100	30	3000	468707.0	3060	463934.3
479	72	3	Hot	c8	100	30	3000	466608.0	3047	463934.3

predicted dpm

Computation Check	
7/11/05	specific activity date
80.95	Ci/mMole 3H R1881
2.22E+12	DPM/Ci (definition)
1.7971E+14	DPM/mMole
1.7971E+11	DPM/nMole
179.7	DPM/fmole
0.005565	fmole/DPM



Linear regression results (LINEST function)	
(Regression line forced through 0,0)	
Slope	153.1501233 dpm/fmole
1/slope	0.006529541 fmole/dpm
x	y
origin	0
end point	3060.4 468707
SLOPE function, used if missing HOT tubes	
Slope	154.1 dpm/fmole
1/slope	0.006491 fmole/dpm
x	y
origin	0
end point	3042.3 468707

Prism input for bound/free		Prism input for specific bound	
specific bound/molar	bound/free	average total added molar	specific bound/molar
4.2686E-11	0.27483	2.03694E-10	4.2686E-11
4.18513E-11	0.26802	2.03694E-10	4.18513E-11
4.1011E-11	0.26123	2.03694E-10	4.1011E-11
7.25669E-11	0.20972	4.2485E-10	7.25669E-11
7.74416E-11	0.22701	4.2485E-10	7.74416E-11
7.4164E-11	0.21533	4.2485E-10	7.4164E-11
7.39967E-11	0.14929	5.77581E-10	7.39967E-11
8.76023E-11	0.18173	5.77581E-10	8.76023E-11
8.8437E-11	0.18378	5.77581E-10	8.8437E-11
1.15129E-10	0.16616	8.17696E-10	1.15129E-10
1.13371E-10	0.16321	8.17696E-10	1.13371E-10
1.1277E-10	0.16220	8.17696E-10	1.1277E-10
1.26977E-10	0.10993	1.29575E-09	1.26977E-10
1.29019E-10	0.11190	1.29575E-09	1.29019E-10
1.37583E-10	0.12022	1.29575E-09	1.37583E-10
1.66794E-10	0.08773	2.08635E-09	1.66794E-10
1.75146E-10	0.09252	2.08635E-09	1.75146E-10
1.68781E-10	0.08886	2.08635E-09	1.68781E-10
1.57611E-10	0.04008	4.12185E-09	1.57611E-10
1.87688E-10	0.04810	4.12185E-09	1.87688E-10
1.9544E-10	0.05019	4.12185E-09	1.9544E-10
2.06168E-10	0.02473	8.60546E-09	2.06168E-10
2.10119E-10	0.02521	8.60546E-09	2.10119E-10
2.05956E-10	0.02470	8.60546E-09	2.05956E-10

Bmax molar	2.27E-10	KD molar	9.04E-10
mole to molar conversion value	0.0003	molar to nM conversion	1.00E+09
DPM/mole = (DPM/mmol)*1000	1.80E+17	kd nM =	9.04E-01
Bmax molar to Bmax moles	6.804E-14		
= DPM/((DPM/mmol)*1000)	6.804E-14		
=Bmax DPM	12227.15402		
assay date	7/11/2005		
Bmax(dpm)	12227.15402		
DPM/Ci (definition)	2.22E+12		
Ci/mmol	80.95		
DPM/mmol	1.80E+14		
DPM/pmol	1.80E+05		
1/(DPM/mmol)	5.56E-15		
1/(DPM/pmol)	5.56E-06		
SA(dpm/pmol)	1.80E+05		
protein./tube (ug)	600		
protein./tube(mg)	0.6		
bmax pmole	0.068040		
bmax pmole/mg	0.1134		
Bmax fmole/mg	113.4		
Bmax (fmole/100 ug)	11.34		
Bmax(fmole/100 ug)/Bmax molar	5.00E+10		

Laboratory E

AR Saturation Assay (cold R1881 dilutions supplied by Battelle)

72 assay tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in columns O and DK

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Provide a reason in column R

The value in column Q will automatically change to FALSE

For your convenience, data reduction is performed in columns

U through BZ, and the values needed for analysis are presented
in columns CF through CN

Cells in column S are presented with a grey background

if the total binding exceeds 10% of the hot added at that concentration,
the cytosol concentration is probably too high for good competitive assays

Laboratory Code:

E

Run identification:

481

Assay start date:

7/13/2005

Tracer lot number:

3559-507

Specific activity on day of assay:

80.92

Ci/mmmole

Cytosol lot or vial number:

051905

protein (cytosol) per tube:

600

ug

protein (cytosol) per tube:

0.6

mg

KD

9.16E-01

nM

Bmax

11.11

fmole/100 ug

total volume in tubes

300

uL

volume of ethanol counted:

2

mL

multiply DPM in sample by :

3

Receptor Notes

diluted to 2 mg/ml for use (0.6 mg/300 ul)

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Saturation Assay Tube Layout																			
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetenone Acetate (uL)	Cytosol (ul)	Significant portion of label on Vial	dpm as counted	corrected DPM for 2mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	Ten Percent Rule	Saturation X values	Bound y values	NSB y values
1	1	H	10.0	7.5	0.25	—	—	—	50	300	—	730.51	2191.53	TRUE		19.5%	0.25	2191.5	296.4
2	2	H	10.0	7.5	0.25	—	—	—	50	300	—	747.45	2242.35	TRUE		19.9%	0.25	2242.4	296.4
3	3	H	10.0	7.5	0.25	—	—	—	50	300	—	878.85	2636.55	TRUE		23.4%	0.25	2636.6	296.4
4	1	H	10.0	15	0.50	—	—	—	50	300	—	1392.20	4176.6	TRUE		18.3%	0.5	4176.6	408.0
5	2	H	10.0	15	0.50	—	—	—	50	300	—	1455.50	4366.5	TRUE		19.1%	0.5	4366.5	408.0
6	3	H	10.0	15	0.50	—	—	—	50	300	—	1519.50	4558.5	TRUE		19.9%	0.5	4558.5	408.0
7	1	H	10.0	21	0.70	—	—	—	50	300	—	1728.20	5184.6	TRUE		16.3%	0.7	5184.6	418.8
8	2	H	10.0	21	0.70	—	—	—	50	300	—	1744.20	5232.6	TRUE		16.4%	0.7	5232.6	418.8
9	3	H	10.0	21	0.70	—	—	—	50	300	—	1816.20	5448.6	TRUE		17.1%	0.7	5448.6	418.8
10	1	H	10.0	30	1.00	—	—	—	50	300	—	2291.20	6873.6	TRUE		15.5%	1	6873.6	590.6
11	2	H	10.0	30	1.00	—	—	—	50	300	—	2173.50	6520.5	TRUE		14.7%	1	6520.5	590.6
12	3	H	10.0	30	1.00	—	—	—	50	300	—	2237.80	6713.4	TRUE		15.2%	1	6713.4	590.6
13	1	H	10.0	45	1.50	—	—	—	50	300	—	2266.50	6799.5	TRUE		10.0%	1.5	6799.5	726.6
14	2	H	10.0	45	1.50	—	—	—	50	300	—	2700.60	8101.8	TRUE		11.9%	1.5	8101.8	726.6
15	3	H	10.0	45	1.50	—	—	—	50	300	—	2762.80	8288.4	TRUE		12.2%	1.5	8288.4	726.6
16	1	H	100.0	7.5	2.50	—	—	—	50	300	—	3115.70	9347.1	TRUE		8.4%	2.5	9347.1	1117.1
17	2	H	100.0	7.5	2.50	—	—	—	50	300	—	3555.50	10666.5	TRUE		9.6%	2.5	10666.5	1117.1
18	3	H	100.0	7.5	2.50	—	—	—	50	300	—	3403.20	10209.6	TRUE		9.2%	2.5	10209.6	1117.1
19	1	H	100.0	15	5.00	—	—	—	50	300	—	3853.00	11559	TRUE		4.9%	5	11559.0	1982.8
20	2	H	100.0	15	5.00	—	—	—	50	300	—	3845.40	11536.2	TRUE		4.9%	5	11536.2	1982.8
21	3	H	100.0	15	5.00	—	—	—	50	300	—	4075.20	12225.6	TRUE		5.2%	5	12225.6	1982.8
22	1	H	100.0	30	10.00	—	—	—	50	300	—	5105.60	15316.8	TRUE		3.3%	10	15316.8	3237.3
23	2	H	100.0	30	10.00	—	—	—	50	300	—	3955.10	11865.3	TRUE		2.6%	10	11865.3	3237.3
24	3	H	100.0	30	10.00	—	—	—	50	300	—	4761.80	14285.4	TRUE		3.1%	10	14285.4	3237.3

Saturation Assay Tube Layout																			
Position	Replicate	Tube Type Code	Hot Initial Concentration (nM)	Hot R1881 Volume (uL)	Hot Final Concentration (nM)	Cold Initial Concentration (uM)	Cold R1881 Volume (uL)	Cold Final Concentration (nM)	Triamcetenone Acetate (uL)	Cytosol (ul)	Significant portion of label on Vial	dpm as counted	corrected DPM for 2mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	Ten Percent Rule	Saturation X values	Bound y values	NSB y values
25	1	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	108.37	325.11	TRUE					
26	2	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	84.59	253.77	TRUE					
27	3	HC	10.0	7.5	0.25	1.00	7.5	25	50	300	C8	103.46	310.38	TRUE					
28	1	HC	10.0	15	0.5	1.00	15	50	50	300	C7	157.82	473.46	TRUE					
29	2	HC	10.0	15	0.5	1.00	15	50	50	300	C7	124.82	374.46	TRUE					
30	3	HC	10.0	15	0.5	1.00	15	50	50	300	C7	125.38	376.14	TRUE					
31	1	HC	10.0	21	0.7	1.00	21	70	50	300	C6	123.29	369.87	TRUE					
32	2	HC	10.0	21	0.7	1.00	21	70	50	300	C6	151.81	455.43	TRUE					
33	3	HC	10.0	21	0.7	1.00	21	70	50	300	C6	143.71	431.13	TRUE					
34	1	HC	10.0	30	1	1.00	30	100	50	300	C5	207.97	623.91	TRUE					
35	2	HC	10.0	30	1	1.00	30	100	50	300	C5	212.25	636.75	TRUE					
36	3	HC	10.0	30	1	1.00	30	100	50	300	C5	170.37	511.11	TRUE					
37	1	HC	10.0	45	1.5	1.00	45	150	50	300	C4	210.01	630.03	TRUE					
38	2	HC	10.0	45	1.5	1.00	45	150	50	300	C4	248.20	744.6	TRUE					
39	3	HC	10.0	45	1.5	1.00	45	150	50	300	C4	268.36	805.08	TRUE					
40	1	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	463.12	1389.36	TRUE					
41	2	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	311.35	934.05	TRUE					
42	3	HC	100.0	7.5	2.5	10.00	7.5	250	50	300	C3	342.66	1027.98	TRUE					
43	1	HC	100.0	15	5	10.00	15	500	50	300	C2	701.26	2103.78	TRUE					
44	2	HC	100.0	15	5	10.00	15	500	50	300	C2	534.00	1602	TRUE					
45	3	HC	100.0	15	5	10.00	15	500	50	300	C2	747.49	2242.47	TRUE					
46	1	HC	100.0	30	10	10.00	30	1000	50	300	C1	966.63	2899.89	TRUE					
47	2	HC	100.0	30	10	10.00	30	1000	50	300	C1	1378.60	4135.8	TRUE					
48	3	HC	100.0	30	10	10.00	30	1000	50	300	C1	892.02	2676.06	TRUE					
49	1	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11449.5	11449.5	TRUE					
50	2	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11204.8	11204.8	TRUE					
51	3	Hot	10.0	7.5	0.25	—	—	—	—	—	—	11100.3	11100.3	TRUE					
52	1	Hot	10.0	15	0.5	—	—	—	—	—	—	23154.0	23154	TRUE					
53	2	Hot	10.0	15	0.5	—	—	—	—	—	—	22697.0	22697	TRUE					
54	3	Hot	10.0	15	0.5	—	—	—	—	—	—	22707.0	22707	TRUE					
55	1	Hot	10.0	21	0.7	—	—	—	—	—	—	31416.0	31416	TRUE					
56	2	Hot	10.0	21	0.7	—	—	—	—	—	—	31867.0	31867	TRUE					
57	3	Hot	10.0	21	0.7	—	—	—	—	—	—	32339.0	32339	TRUE					
58	1	Hot	10.0	30	1	—	—	—	—	—	—	42879.0	42879	TRUE					
59	2	Hot	10.0	30	1	—	—	—	—	—	—	45013.0	45013	TRUE					
60	3	Hot	10.0	30	1	—	—	—	—	—	—	44787.0	44787	TRUE					
61	1	Hot	10.0	45	1.5	—	—	—	—	—	—	69306.0	69306	TRUE					
62	2	Hot	10.0	45	1.5	—	—	—	—	—	—	68642.0	68642	TRUE					
63	3	Hot	10.0	45	1.5	—	—	—	—	—	—	66107.0	66107	TRUE					
64	1	Hot	100.0	7.5	2.5	—	—	—	—	—	—	111878	111878	TRUE					
65	2	Hot	100.0	7.5	2.5	—	—	—	—	—	—	112465	112465	TRUE					
66	3	Hot	100.0	7.5	2.5	—	—	—	—	—	—	110005	110005	TRUE					
67	1	Hot	100.0	15	5	—	—	—	—	—	—	237414	237414	TRUE					
68	2	Hot	100.0	15	5	—	—	—	—	—	—	233806	233806	TRUE					
69	3	Hot	100.0	15	5	—	—	—	—	—	—	234692	234692	TRUE					
70	1	Hot	100.0	30	10	—	—	—	—	—	—	455700	455700	TRUE					
71	2	Hot	100.0	30	10	—	—	—	—	—	—	470855	470855	TRUE					
72	3	Hot	100.0	30	10	—	—	—	—	—	—	463848	463848	TRUE					

Total Binding -- Positions 1-24 radiolabeled R1881 plus cytosol (Panel A)												
Run	Position	Tube Identification			Assay tube contents							
		Rep	Tube Type Code	Conc. Code	Hot Conc. Initial	Hot R1881 Volume	Cold R1881 Conc. Initial	Cold R1881 volume	Triamcetenone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)
481	1	1	H	c1	10.0	7.5	—	—	—	300	0.25	—
481	2	2	H	c1	10.0	7.5	—	—	—	300	0.25	—
481	3	3	H	c1	10.0	7.5	—	—	—	300	0.25	—
481	4	1	H	c2	10.0	15	—	—	—	300	0.50	—
481	5	2	H	c2	10.0	15	—	—	—	300	0.50	—
481	6	3	H	c2	10.0	15	—	—	—	300	0.50	—
481	7	1	H	c3	10.0	21	—	—	—	300	0.70	—
481	8	2	H	c3	10.0	21	—	—	—	300	0.70	—
481	9	3	H	c3	10.0	21	—	—	—	300	0.70	—
481	10	1	H	c4	10.0	30	—	—	—	300	1.00	—
481	11	2	H	c4	10.0	30	—	—	—	300	1.00	—
481	12	3	H	c4	10.0	30	—	—	—	300	1.00	—
481	13	1	H	c5	10.0	45	—	—	—	300	1.50	—
481	14	2	H	c5	10.0	45	—	—	—	300	1.50	—
481	15	3	H	c5	10.0	45	—	—	—	300	1.50	—
481	16	1	H	c6	100.0	7.5	—	—	—	300	2.50	—
481	17	2	H	c6	100.0	7.5	—	—	—	300	2.50	—
481	18	3	H	c6	100.0	7.5	—	—	—	300	2.50	—
481	19	1	H	c7	100.0	15	—	—	—	300	5.00	—
481	20	2	H	c7	100.0	15	—	—	—	300	5.00	—
481	21	3	H	c7	100.0	15	—	—	—	300	5.00	—
481	22	1	H	c8	100.0	30	—	—	—	300	10.00	—
481	23	2	H	c8	100.0	30	—	—	—	300	10.00	—
481	24	3	H	c8	100.0	30	—	—	—	300	10.00	—
												Total Volume
												(ul)

Run	Position								Number of molecules						Ratio
		Total Counts	Non Specific Binding (Mean of reps in pos. 25-48)	Specific Binding (Total - Non Specific)	Ratio of NSB/ total binding	Ratio Total binding/ Hot	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Total Binding molecules	Non Specific Binding molecules	Specific Binding molecules	Total Added (Mean of reps in pos. 49-72)	Free (total added - bound)	Specific Bound / Free	
		(dpm)	(dpm)	(dpm)			(dpm)	(dpm)	(fmole)	(fmole)	(fmole)	(fmole)	(fmole)		
481	1	2191.5	296.4	1895.1	13.5%	19.5%	11251.5	9060.0	14	2	12	73	59	0.21	
481	2	2242.4	296.4	1945.9	13.2%	19.9%	11251.5	9009.2	15	2	13	73	58	0.22	
481	3	2636.6	296.4	2340.1	11.2%	23.4%	11251.5	8615.0	17	2	15	73	56	0.27	
481	4	4176.6	408.0	3768.6	9.8%	18.3%	22852.7	18676.1	27	3	24	148	121	0.20	
481	5	4366.5	408.0	3958.5	9.3%	19.1%	22852.7	18486.2	28	3	26	148	120	0.21	
481	6	4558.5	408.0	4150.5	9.0%	19.9%	22852.7	18294.2	29	3	27	148	118	0.23	
481	7	5184.6	418.8	4765.8	8.1%	16.3%	31874.0	26689.4	34	3	31	206	173	0.18	
481	8	5232.6	418.8	4813.8	8.0%	16.4%	31874.0	26641.4	34	3	31	206	172	0.18	
481	9	5448.6	418.8	5029.8	7.7%	17.1%	31874.0	26425.4	35	3	33	206	171	0.19	
481	10	6873.6	590.6	6283.0	8.6%	15.5%	44226.3	37352.7	44	4	41	286	242	0.17	
481	11	6520.5	590.6	5929.9	9.1%	14.7%	44226.3	37705.8	42	4	38	286	244	0.16	
481	12	6713.4	590.6	6122.8	8.8%	15.2%	44226.3	37512.9	43	4	40	286	243	0.16	
481	13	6799.5	726.6	6072.9	10.7%	10.0%	68018.3	61218.8	44	5	39	440	396	0.10	
481	14	8101.8	726.6	7375.2	9.0%	11.9%	68018.3	59916.5	52	5	48	440	388	0.12	
481	15	8288.4	726.6	7561.8	8.8%	12.2%	68018.3	59729.9	54	5	49	440	387	0.13	
481	16	9347.1	1117.1	8230.0	12.0%	8.4%	111449.3	102102.2	60	7	53	721	661	0.08	
481	17	10666.5	1117.1	9549.4	10.5%	9.6%	111449.3	100782.8	69	7	62	721	652	0.09	
481	18	10209.6	1117.1	9092.5	10.9%	9.2%	111449.3	101239.7	66	7	59	721	655	0.09	
481	19	11559.0	1982.8	9576.3	17.2%	4.9%	235304.0	223745.0	75	13	62	1523	1448	0.04	
481	20	11536.2	1982.8	9553.5	17.2%	4.9%	235304.0	223767.8	75	13	62	1523	1448	0.04	
481	21	12225.6	1982.8	10242.9	16.2%	5.2%	235304.0	223078.4	79	13	66	1523	1444	0.05	
481	22	15316.8	3237.3	12079.6	21.1%	3.3%	463467.7	448150.9	99	21	78	2999	2900	0.03	
481	23	11865.3	3237.3	8628.1	27.3%	2.6%	463467.7	451602.4	77	21	56	2999	2922	0.02	
481	24	14285.4	3237.3	11048.2	22.7%	3.1%	463467.7	449182.3	92	21	71	2999	2907	0.02	

Run	Position	Non Specific Binding -- Positions 25-48 radiolabeled R1881 plus 100 X inert R1881 plus cytosol												
		Tube Identification			Assay tube contents							Scintillation Results		
		Rep	Tube Type Code	Conc. Code	Hot Conc. R1881 Initial	Hot	Cold R1881 Conc. Initial	Cold	Triamcetenone Acetate	Cytosol	Hot Conc. Final	Cold Conc. Final	Counts per Scintillation Vial (Total Binding)	Non Specific Binding (Mean of reps in pos. 25-48)
					(nM)	(ul)	(mM)	(ul)	(ul)	(ul)	(nM)	(nM)		
481	25	1	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	325.1	296.4
481	26	2	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	253.8	296.4
481	27	3	HC	c1	10.0	7.5	1.00	7.5	50	300	0.25	25	310.4	296.4
481	28	1	HC	c2	10.0	15	1.00	15	50	300	0.5	50	473.5	408.0
481	29	2	HC	c2	10.0	15	1.00	15	50	300	0.5	50	374.5	408.0
481	30	3	HC	c2	10.0	15	1.00	15	50	300	0.5	50	376.1	408.0
481	31	1	HC	c3	10.0	21	1.00	21	50	300	0.7	70	369.9	418.8
481	32	2	HC	c3	10.0	21	1.00	21	50	300	0.7	70	455.4	418.8
481	33	3	HC	c3	10.0	21	1.00	21	50	300	0.7	70	431.1	418.8
481	34	1	HC	c4	10.0	30	1.00	30	50	300	1	100	623.9	590.6
481	35	2	HC	c4	10.0	30	1.00	30	50	300	1	100	636.8	590.6
481	36	3	HC	c4	10.0	30	1.00	30	50	300	1	100	511.1	590.6
481	37	1	HC	c5	10.0	45	1.00	45	50	300	1.5	150	630.0	726.6
481	38	2	HC	c5	10.0	45	1.00	45	50	300	1.5	150	744.6	726.6
481	39	3	HC	c5	10.0	45	1.00	45	50	300	1.5	150	805.1	726.6
481	40	1	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	1389.4	1117.1
481	41	2	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	934.1	1117.1
481	42	3	HC	c6	100.0	7.5	10.00	7.5	50	300	2.5	250	1028.0	1117.1
481	43	1	HC	c7	100.0	15	10.00	15	50	300	5	500	2103.8	1982.8
481	44	2	HC	c7	100.0	15	10.00	15	50	300	5	500	1602.0	1982.8
481	45	3	HC	c7	100.0	15	10.00	15	50	300	5	500	2242.5	1982.8
481	46	1	HC	c8	100.0	30	10.00	30	50	300	10	1000	2899.9	3237.3
481	47	2	HC	c8	100.0	30	10.00	30	50	300	10	1000	4135.8	3237.3
481	48	3	HC	c8	100.0	30	10.00	30	50	300	10	1000	2676.1	3237.3

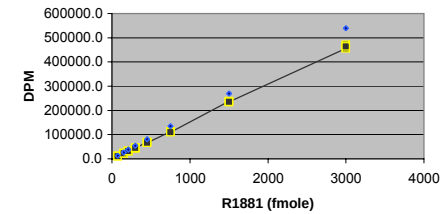
Run	Position	Free -- Positions 49-72, radiolabeled R1881 without cytosol								
		Rep	Tube Type Code	Conc. Code	Hot R1881 Conc. Initial	Hot R1881 Volume	Molecules of R1881	Counts per Scintillation Vial	Experimental number of molecules	Total Added (Mean of reps in pos. 49-72)
					(nM)	(ul)	(fmole)	(dpm)	(fmole)	(dpm)
481	49	1	Hot	c1	10	7.5	75	11449.5	74	11251.5
481	50	2	Hot	c1	10	7.5	75	11204.8	73	11251.5
481	51	3	Hot	c1	10	7.5	75	11100.3	72	11251.5
481	52	1	Hot	c2	10	15	150	23154.0	150	22852.7
481	53	2	Hot	c2	10	15	150	22697.0	147	22852.7
481	54	3	Hot	c2	10	15	150	22707.0	147	22852.7
481	55	1	Hot	c3	10	21	210	31416.0	203	31874.0
481	56	2	Hot	c3	10	21	210	31867.0	206	31874.0
481	57	3	Hot	c3	10	21	210	32339.0	209	31874.0
481	58	1	Hot	c4	10	30	300	42879.0	277	44226.3
481	59	2	Hot	c4	10	30	300	45013.0	291	44226.3
481	60	3	Hot	c4	10	30	300	44787.0	290	44226.3
481	61	1	Hot	c5	10	45	450	69306.0	448	68018.3
481	62	2	Hot	c5	10	45	450	68642.0	444	68018.3
481	63	3	Hot	c5	10	45	450	66107.0	428	68018.3
481	64	1	Hot	c6	100	7.5	750	111878.0	724	111449.3
481	65	2	Hot	c6	100	7.5	750	112465.0	728	111449.3
481	66	3	Hot	c6	100	7.5	750	110005.0	712	111449.3
481	67	1	Hot	c7	100	15	1500	237414.0	1536	235304.0
481	68	2	Hot	c7	100	15	1500	233806.0	1513	235304.0
481	69	3	Hot	c7	100	15	1500	234692.0	1519	235304.0
481	70	1	Hot	c8	100	30	3000	455700.0	2949	463467.7
481	71	2	Hot	c8	100	30	3000	470855.0	3047	463467.7
481	72	3	Hot	c8	100	30	3000	463848.0	3002	463467.7

predicted dpm

Computation Check

7/13/05 specific activity date
 80.92 Ci/mMole 3H R1881
 2.22E+12 DPM/Ci (definition)
 1.7965E+14 DPM/mMole
 1.7965E+11 DPM/nmole
 179.7 DPM/fmole
 0.005566 fmole/DPM

Hot Tubes



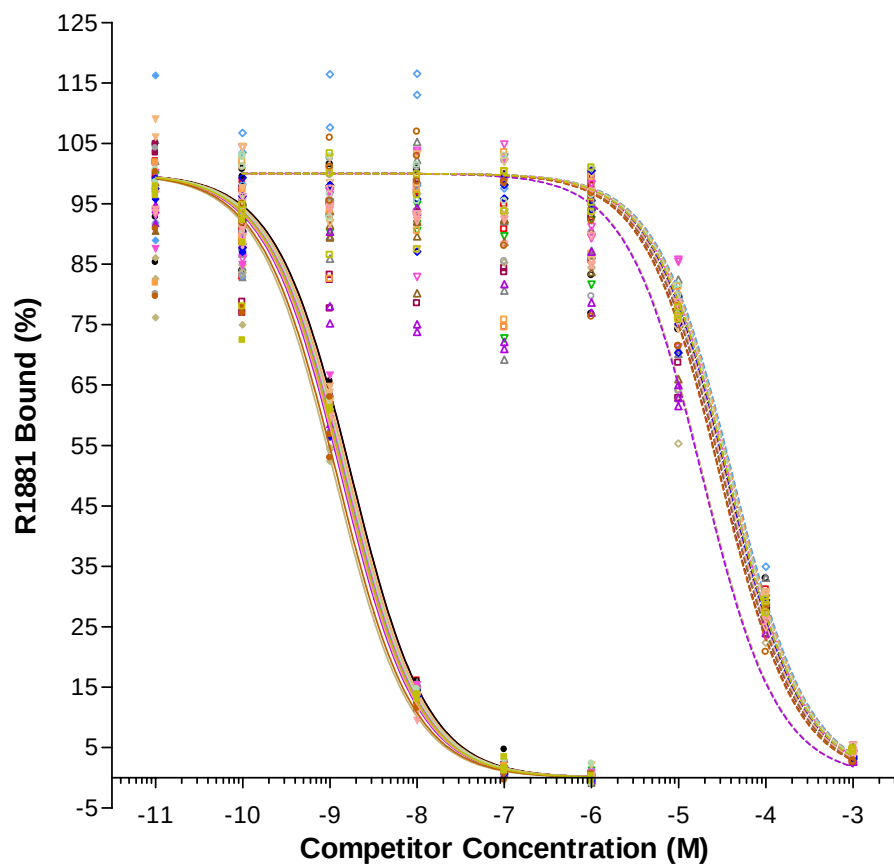
Linear regression results (LINEST function)	
(Regression line forced through 0,0)	
Slope	154.5333567 dpm/fmole
1/slope	0.006471095 fmole/dpm
x	y
origin	0 0
end point	3046.9 470855
SLOPE function, used if missing HOT tubes	
Slope	155.2 dpm/fmole
1/slope	0.006442 fmole/dpm
x	y
origin	0 0
end point	3033.5 470855

Prism input for bound/free		Prism input for specific bound	
specific bound/molar	bound/free	average total added molar	specific bound/molar
3.5163E-11	0.20917	2.08767E-10	3.5163E-11
3.61059E-11	0.21599	2.08767E-10	3.61059E-11
4.34201E-11	0.27163	2.08767E-10	4.34201E-11
6.99244E-11	0.20179	4.24022E-10	6.99244E-11
7.34479E-11	0.21413	4.24022E-10	7.34479E-11
7.70104E-11	0.22687	4.24022E-10	7.70104E-11
8.84272E-11	0.17856	5.91409E-10	8.84272E-11
8.93179E-11	0.18069	5.91409E-10	8.93179E-11
9.33256E-11	0.19034	5.91409E-10	9.33256E-11
1.16579E-10	0.16821	8.20601E-10	1.16579E-10
1.10027E-10	0.15727	8.20601E-10	1.10027E-10
1.13606E-10	0.16322	8.20601E-10	1.13606E-10
1.12681E-10	0.09920	1.26205E-09	1.12681E-10
1.36844E-10	0.12309	1.26205E-09	1.36844E-10
1.40307E-10	0.12660	1.26205E-09	1.40307E-10
1.52704E-10	0.08061	2.0679E-09	1.52704E-10
1.77185E-10	0.09475	2.0679E-09	1.77185E-10
1.68707E-10	0.08981	2.0679E-09	1.68707E-10
1.77683E-10	0.04280	4.36597E-09	1.77683E-10
1.7726E-10	0.04269	4.36597E-09	1.7726E-10
1.90052E-10	0.04592	4.36597E-09	1.90052E-10
2.24131E-10	0.02695	8.59945E-09	2.24131E-10
1.6009E-10	0.01911	8.59945E-09	1.6009E-10
2.04994E-10	0.02460	8.59945E-09	2.04994E-10

Bmax molar	2.22E-10	KD molar	9.16E-10
mole to molar conversion value	0.0003	molar to nM conversion	1.00E+09
DPM/mole = (DPM/mmol)*1000	1.80E+17	kd nM =	9.16E-01
Bmax molar to Bmax moles	6.66E-14		
= DPM/((DPM/mmol)*1000)	6.66E-14		
=Bmax DPM	11975.47965		
assay date	7/13/2005		
Bmax(dpm)	11975.47965		
DPM/Ci (definition)	2.22E+12		
Ci/mmol	80.92		
DPM/mmol	1.80E+14		
DPM/pmol	1.80E+05		
1/(DPM/mmol)	5.57E-15		
1/(DPM/pmol)	5.57E-06		
SA(dpm/pmol)	1.80E+05		
protein./tube (ug)	600		
protein./tube(mg)	0.6		
bmax pmole	0.066660		
bmax pmole/mg	0.1111		
Bmax fmole/mg	111.1		
Bmax (fmole/100 ug)	11.11		
Bmax(fmole/100 ug)/Bmax molar	5.00E+10		

Appendix 4: Prism Files for Competitive Binding Experiments

WA 4-11-7 Competitive

**Standard Curve and 'Weak Positive'
Protein
1.0 mg per tube**

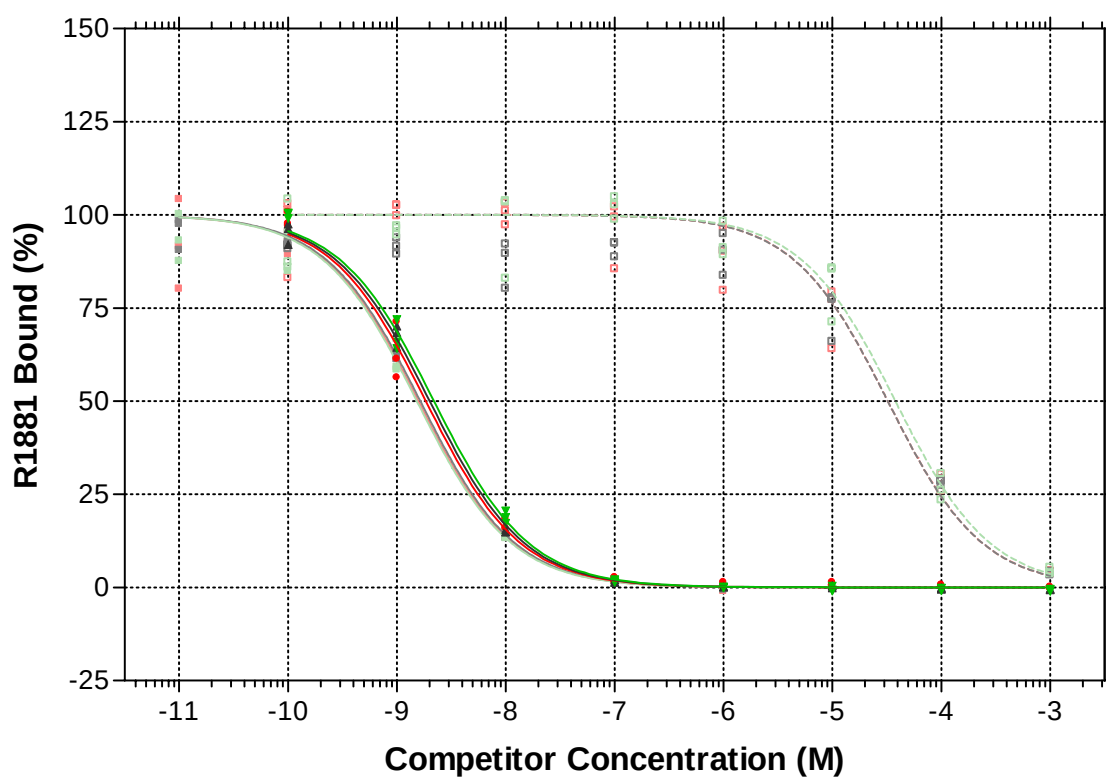
Standard Curve	Weak Positive	Standard Curve	Weak Positive
■ E-489-8/9/05	□ E-489-8/9/05	▼ E-508-9/28/05	▼ E-508-9/28/05
• E-490-8/11/05	◦ E-490-8/11/05	■ E-509-10/03/05	■ E-509-10/03/05
▼ E-491-8/15/05	▼ E-491-8/15/05	▲ E-510-10/04/05	▲ E-510-10/04/05
▲ E-499-9/12/05	▲ E-499-9/12/05	▼ E-511-10/06/05	▼ E-511-10/06/05
◆ E-501-9/13/05	◆ E-501-9/13/05	◆ E-512-10/10/05	◆ E-512-10/10/05
■ E-502-9/14/05	■ E-502-9/14/05	● E-513-10/13/05	● E-513-10/13/05
◆ E-504-9/20/05	◆ E-504-9/20/05	▼ E-514-10/18/05	▼ E-514-10/18/05
● E-506-9/26/05	● E-506-9/26/05	● E-515-10/19/05	● E-515-10/19/05
▲ E-507-9/27/05	▲ E-507-9/27/05	■ E-516-10/27/05	■ E-516-10/27/05

WA 4-11-7 Competitive

Lab E CR42340

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



- E-506-9/26/05
- ▲ E-507-9/27/05
- ▼ E-508-9/28/05

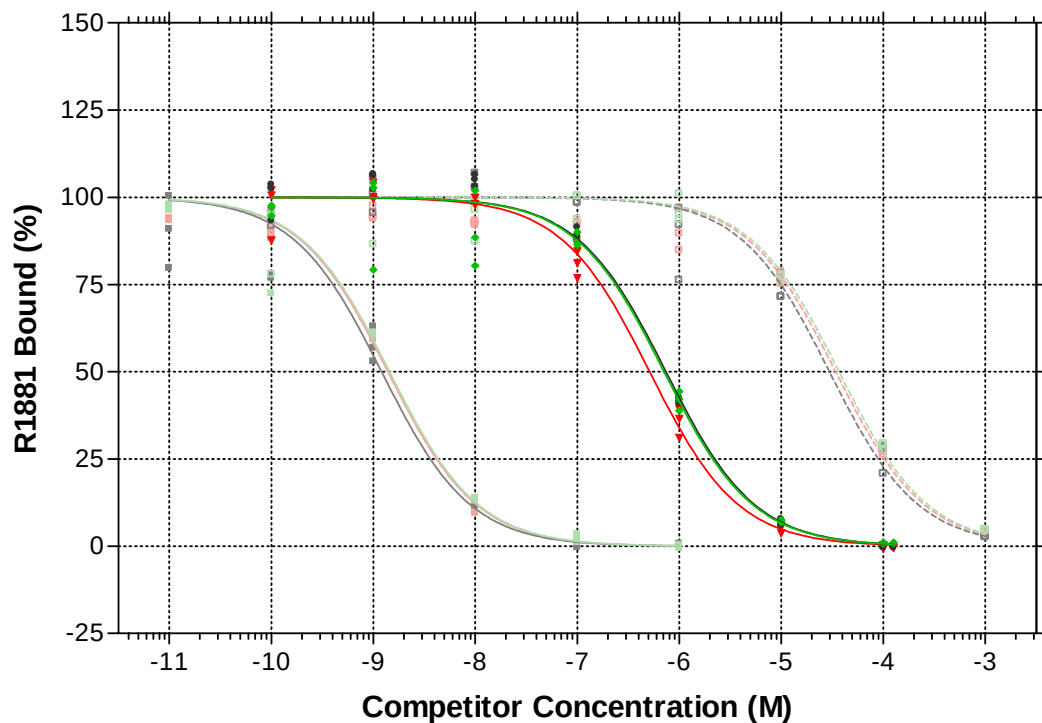
CR42340	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-506-9/26/05	0.000	0.000	100.000	0.000	-8.734	0.027
E-507-9/27/05	0.000	0.000	100.000	0.000	-8.698	0.013
E-508-9/28/05	0.000	0.000	100.000	0.000	-8.659	0.021

WA 4-11-7 Competitive

Lab E CR42341

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



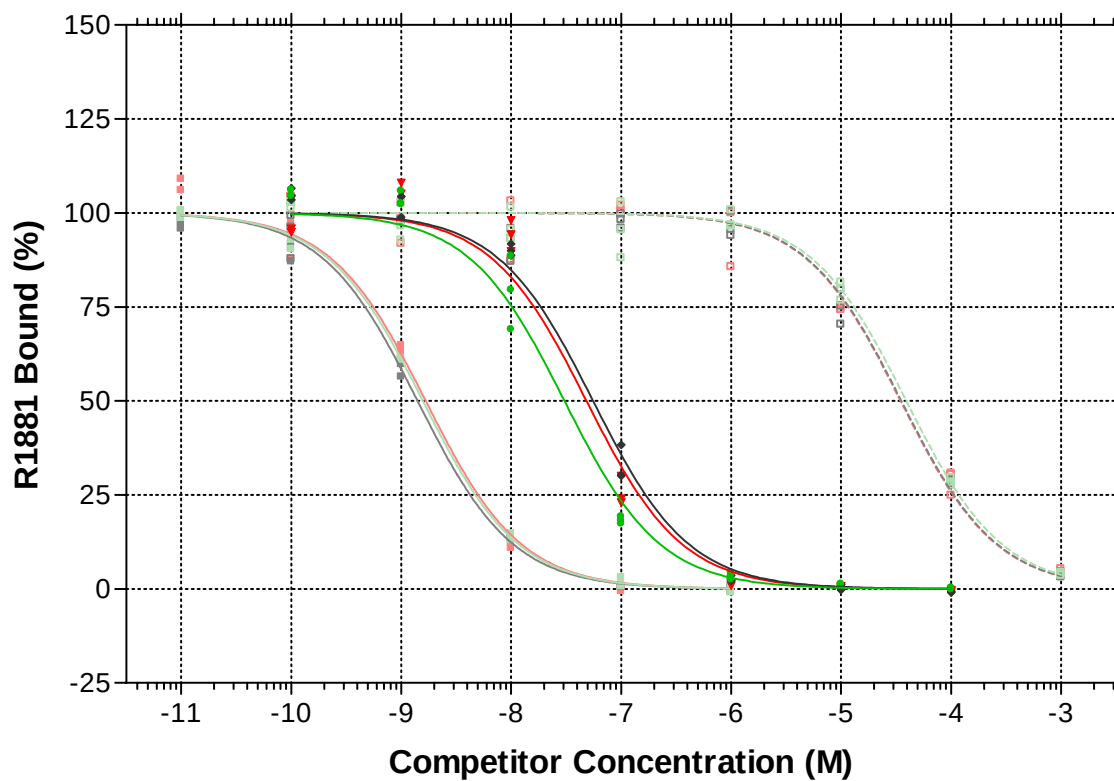
	CR42341	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-514-10/18/05	E-514-10/18/05	0.000	0.000	100.000	0.000	-6.290	0.033
• E-515-10/19/05	E-515-10/19/05	0.000	0.000	100.000	0.000	-6.130	0.033
◆ E-516-10/27/05	E-516-10/27/05	0.000	0.000	100.000	0.000	-6.149	0.059

WA 4-11-7 Competitive

Lab E CR42342

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



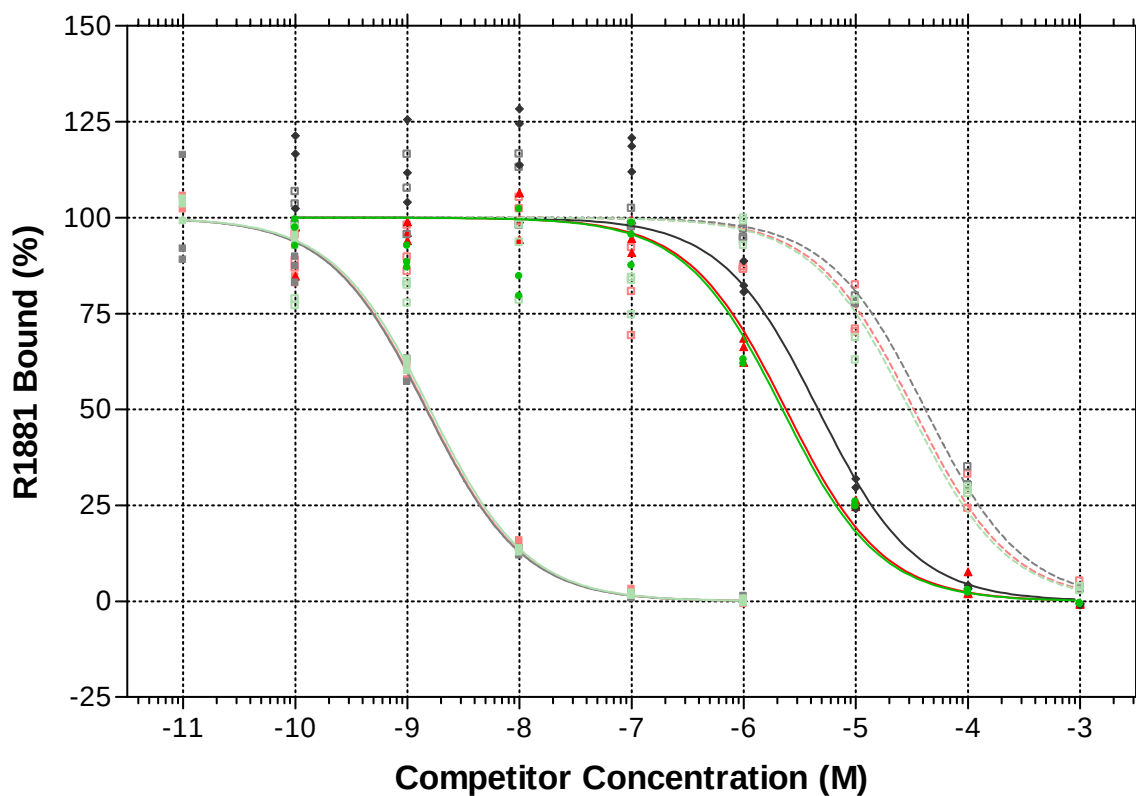
CR42342		BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-511-10/06/05	E-511-10/06/05	0.000	0.000	100.000	0.000	-7.315	0.062
◆ E-512-10/10/05	E-512-10/10/05	0.000	0.000	100.000	0.000	-7.255	0.039
● E-513-10/13/05	E-513-10/13/05	0.000	0.000	100.000	0.000	-7.515	0.050

WA 4-11-7 Competitive

Lab E CR42343

Protein: 1.0 mg per tube

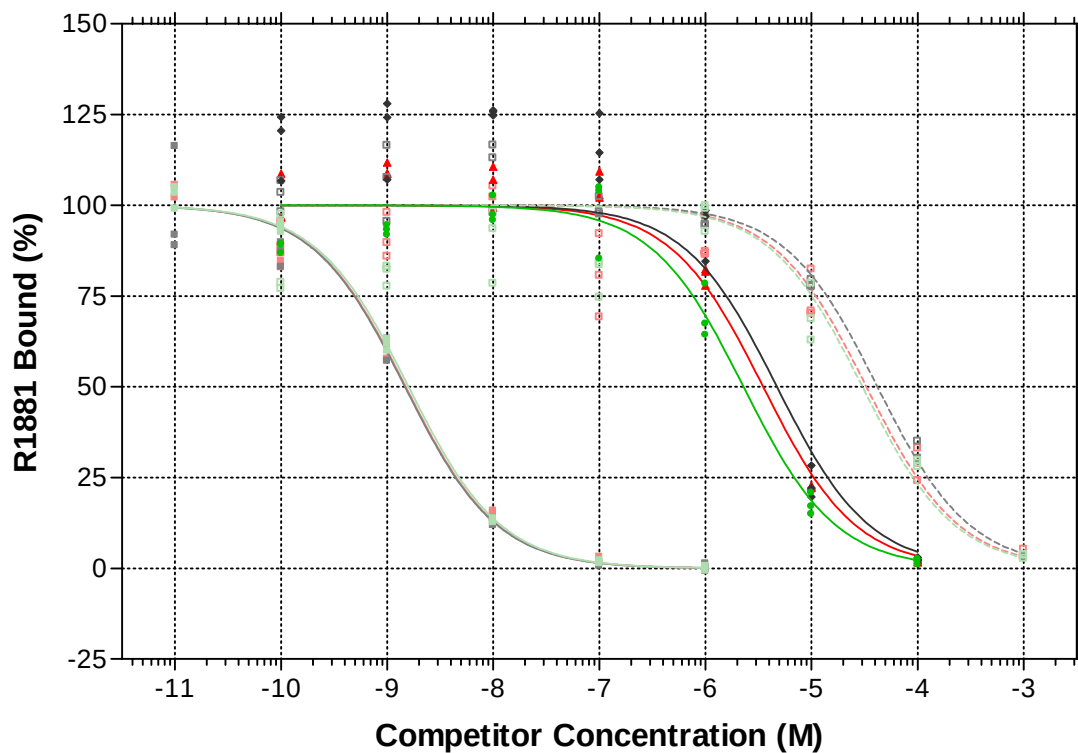
Solid squares = Standard Curve, Open squares = Weak Positive



CR42343		BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▲ E-499-9/12/05	E-499-9/12/05	0.000	0.000	100.000	0.000	-5.623	0.050
◆ E-501-9/13/05	E-501-9/13/05	0.000	0.000	100.000	0.000	-5.335	0.131
● E-502-9/14/05	E-502-9/14/05	0.000	0.000	100.000	0.000	-5.655	0.084

WA 4-11-7 Competitive

Lab E CR42344
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



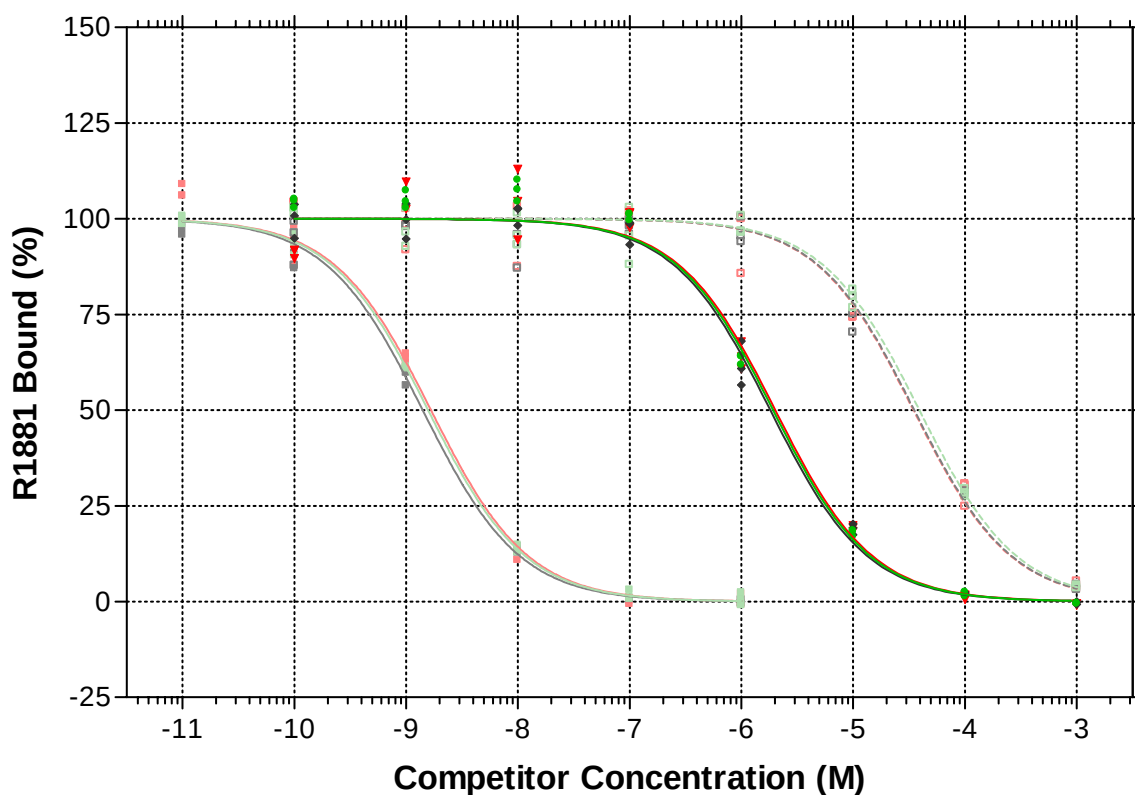
	CR42344	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▲ E-499-9/12/05	E-499-9/12/05	0.000	0.000	100.000	0.000	-5.455	0.062
◆ E-501-9/13/05	E-501-9/13/05	0.000	0.000	100.000	0.000	-5.326	0.168
● E-502-9/14/05	E-502-9/14/05	0.000	0.000	100.000	0.000	-5.640	0.066

WA 4-11-7 Competitive

Lab E CR42345

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



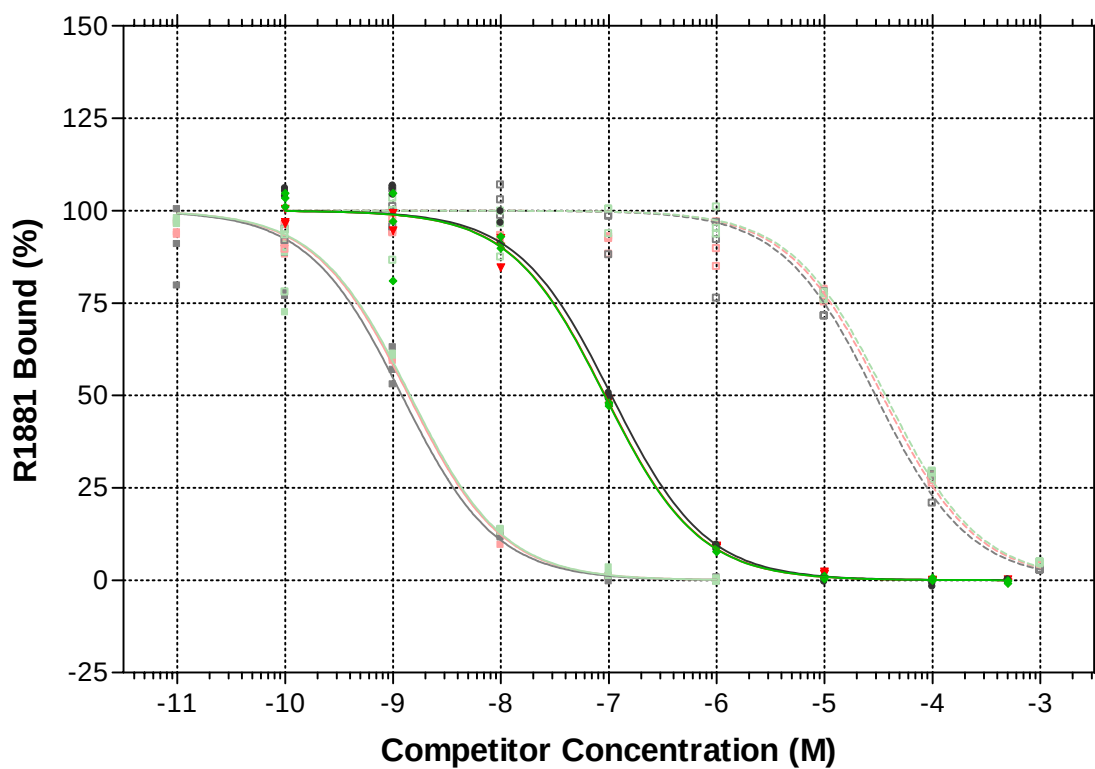
	CR42345	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-511-10/06/05	E-511-10/06/05	0.000	0.000	100.000	0.000	-5.697	0.054
♦ E-512-10/10/05	E-512-10/10/05	0.000	0.000	100.000	0.000	-5.741	0.032
● E-513-10/13/05	E-513-10/13/05	0.000	0.000	100.000	0.000	-5.716	0.043

WA 4-11-7 Competitive

Lab E CR42346

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



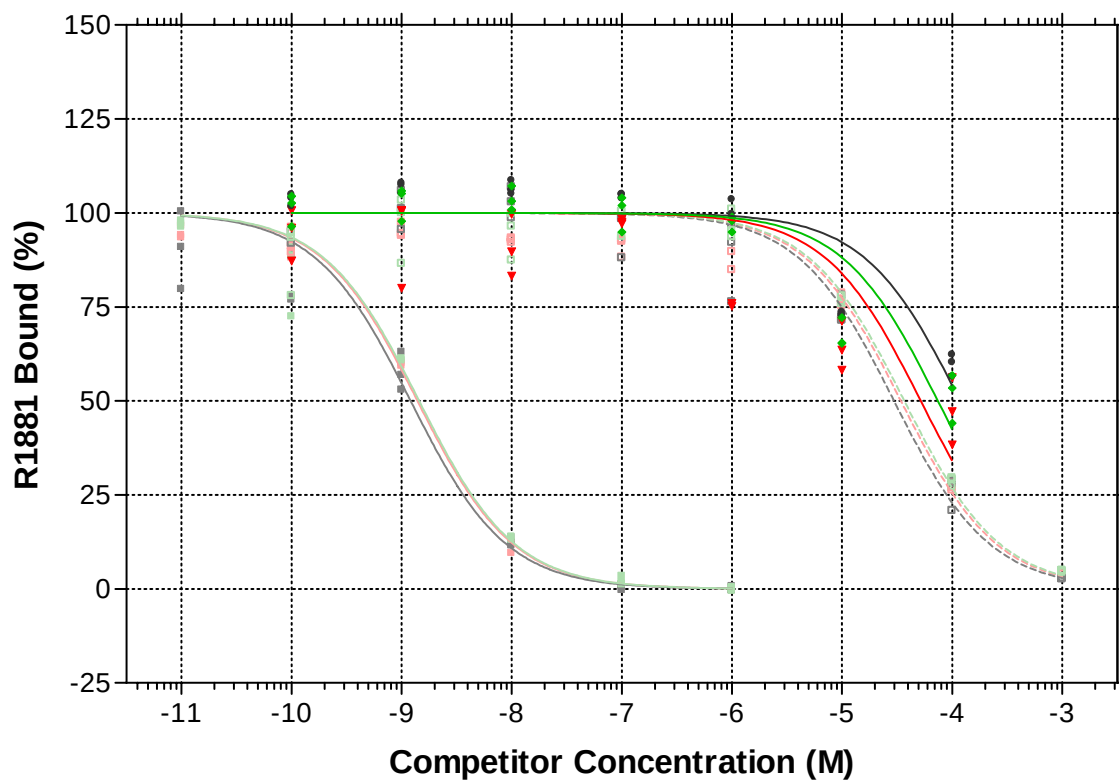
	CR42346	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼	E-514-10/18/05	0.000	0.000	100.000	0.000	-7.035	0.018
•	E-515-10/19/05	0.000	0.000	100.000	0.000	-6.977	0.035
◆	E-516-10/27/05	0.000	0.000	100.000	0.000	-7.039	0.038

WA 4-11-7 Competitive

Lab E CR42347

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



- ▼ E-514-10/18/05
- E-515-10/19/05
- ◆ E-516-10/27/05

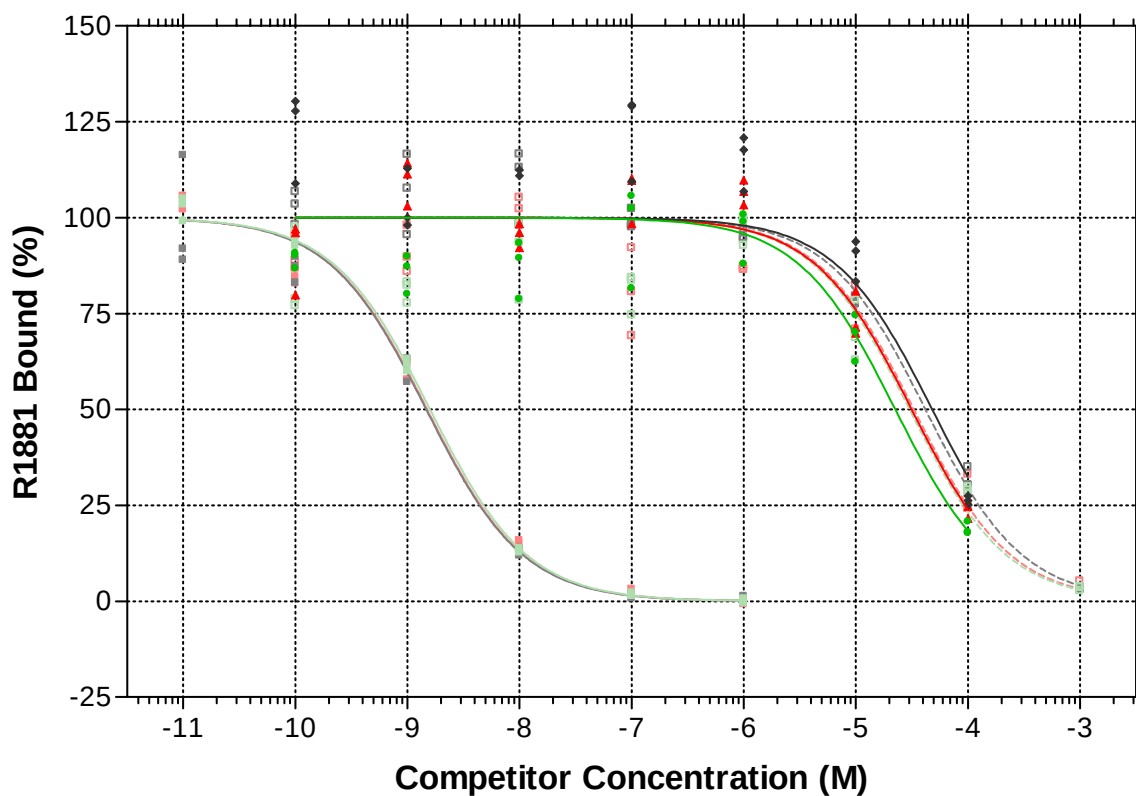
CR42347	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-514-10/18/05	0.000	0.000	100.000	0.000	-4.284	0.137
E-515-10/19/05	0.000	0.000	100.000	0.000	-3.927	0.089
E-516-10/27/05	0.000	0.000	100.000	0.000	-4.129	0.090

WA 4-11-7 Competitive

Lab E CR42348

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive

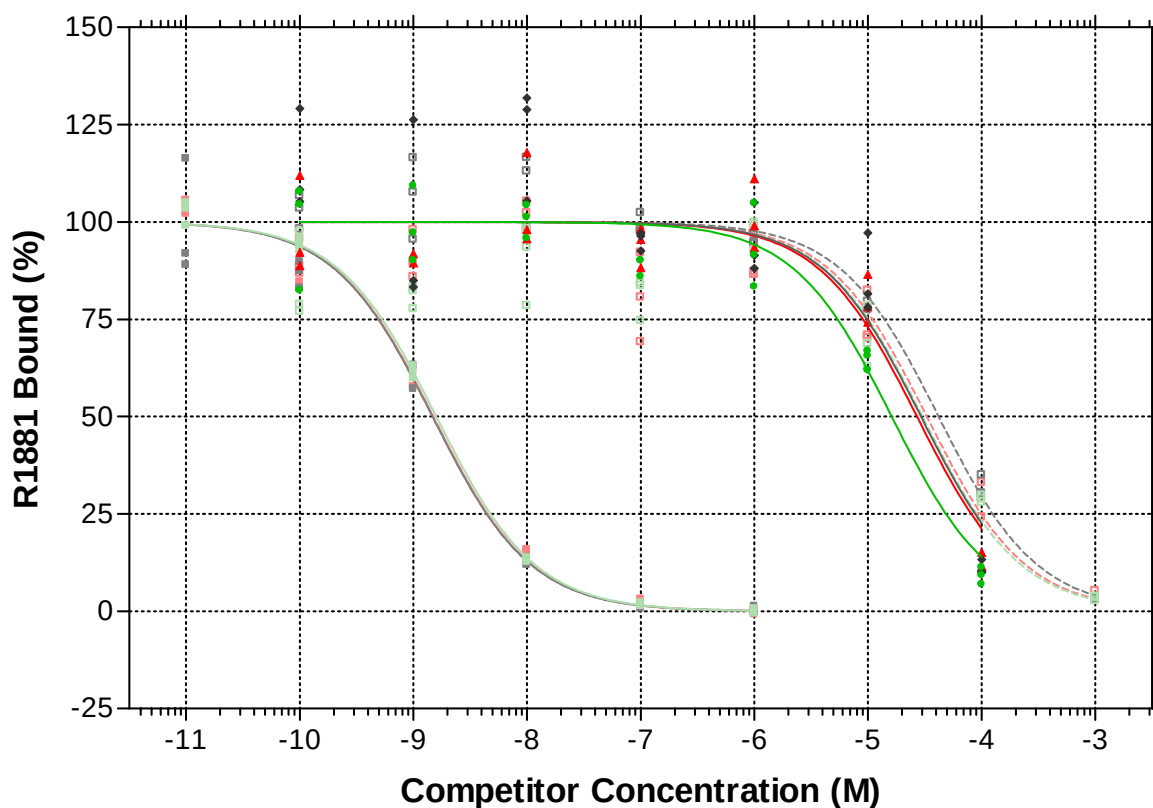


- ▲ E-499-9/12/05
- ◆ E-501-9/13/05
- E-502-9/14/05

CR42348	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-499-9/12/05	0.000	0.000	100.000	0.000	-4.502	0.082
E-501-9/13/05	0.000	0.000	100.000	0.000	-4.318	0.160
E-502-9/14/05	0.000	0.000	100.000	0.000	-4.647	0.099

WA 4-11-7 Competitive

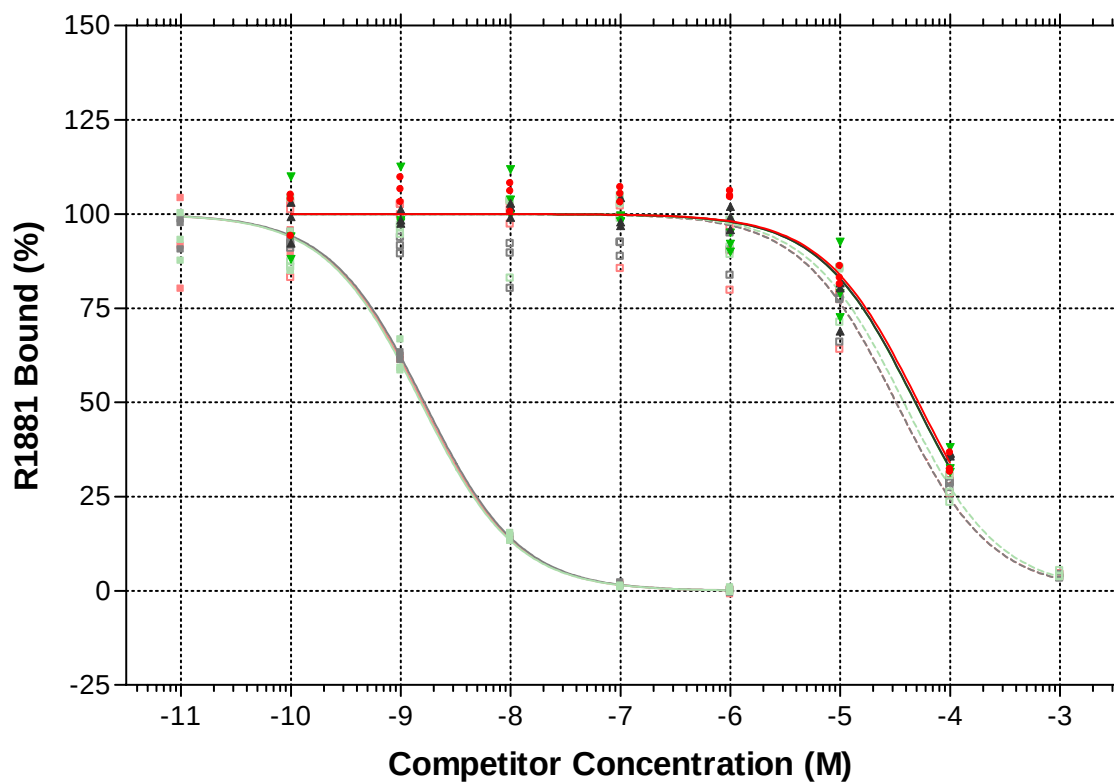
Lab E CR42349
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42349	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▲ E-499-9/12/05	E-499-9/12/05	0.000	0.000	100.000	0.000	-4.568	0.090
◆ E-501-9/13/05	E-501-9/13/05	0.000	0.000	100.000	0.000	-4.533	0.156
● E-502-9/14/05	E-502-9/14/05	0.000	0.000	100.000	0.000	-4.790	0.076

WA 4-11-7 Competitive

Lab E CR42350
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



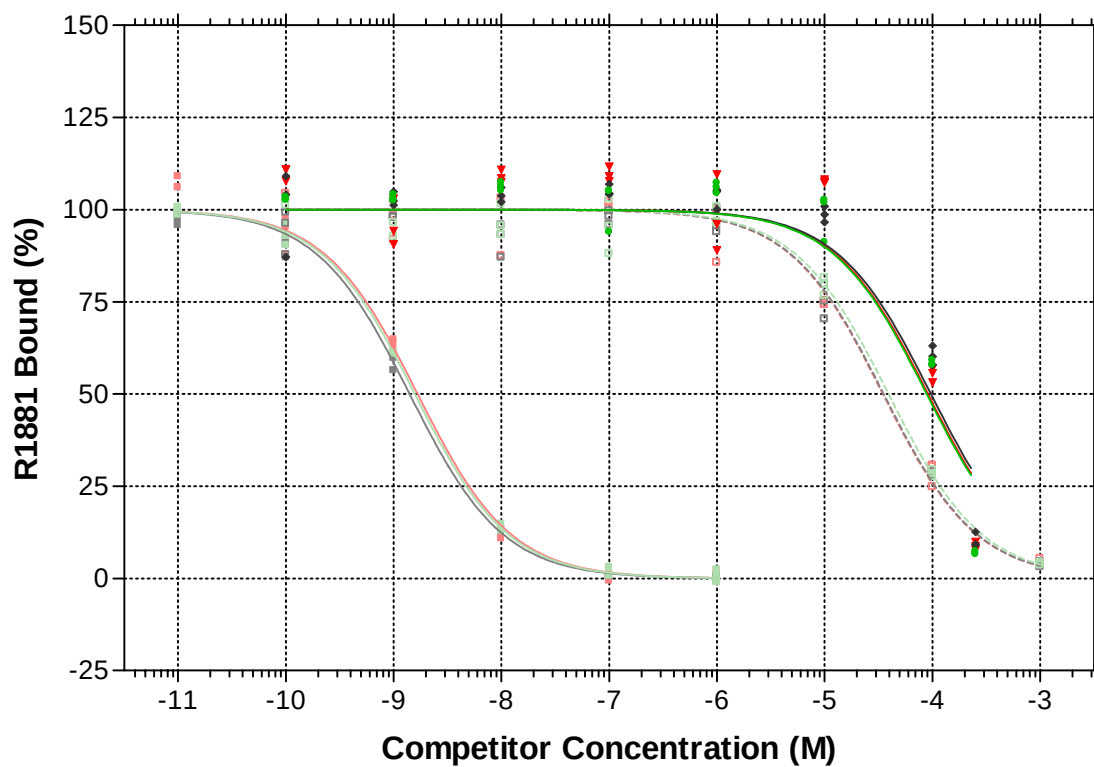
	CR42350	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
• E-506-9/26/05	E-506-9/26/05	0.000	0.000	100.000	0.000	-4.288	0.052
▲ E-507-9/27/05	E-507-9/27/05	0.000	0.000	100.000	0.000	-4.315	0.042
▼ E-508-9/28/05	E-508-9/28/05	0.000	0.000	100.000	0.000	-4.318	0.066

WA 4-11-7 Competitive

Lab E CR42351

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



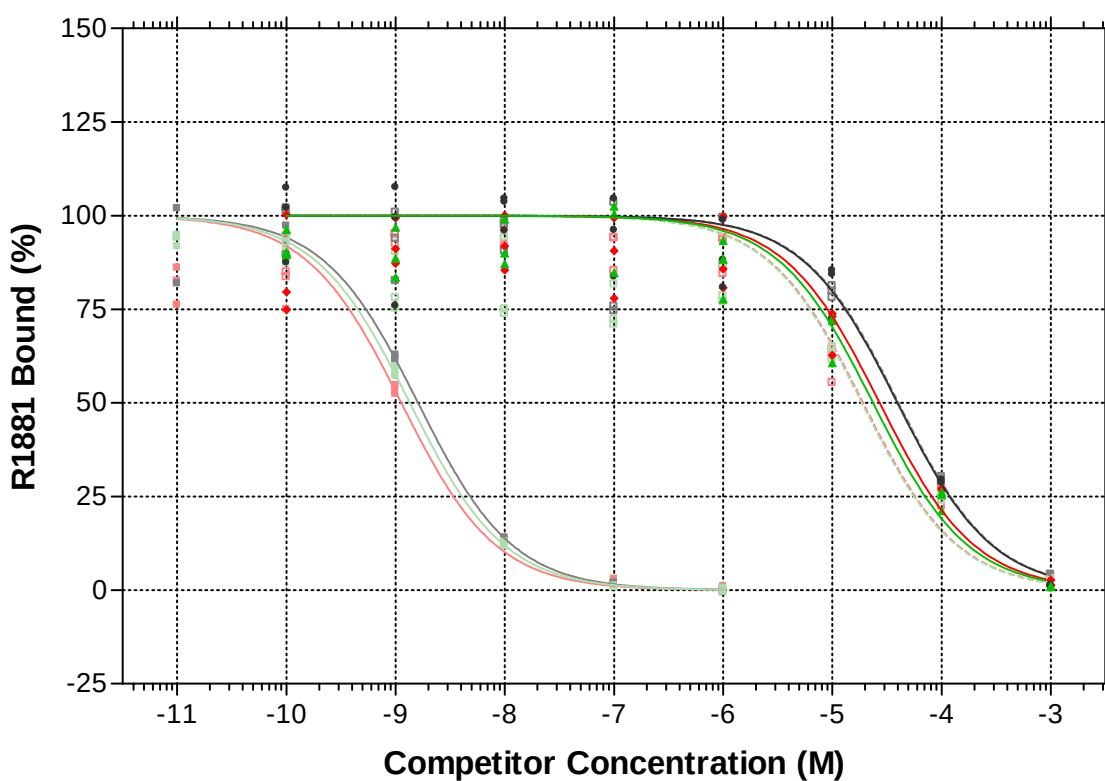
	CR42351	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼	E-511-10/06/05	0.000	0.000	100.000	0.000	-4.042	0.090
◆	E-512-10/10/05	0.000	0.000	100.000	0.000	-4.013	0.071
●	E-513-10/13/05	0.000	0.000	100.000	0.000	-4.053	0.075

WA 4-11-7 Competitive

Lab E CR42352

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



- ♦ E-504-9/20/05
- E-509-10/03/05
- ▲ E-510-10/04/05

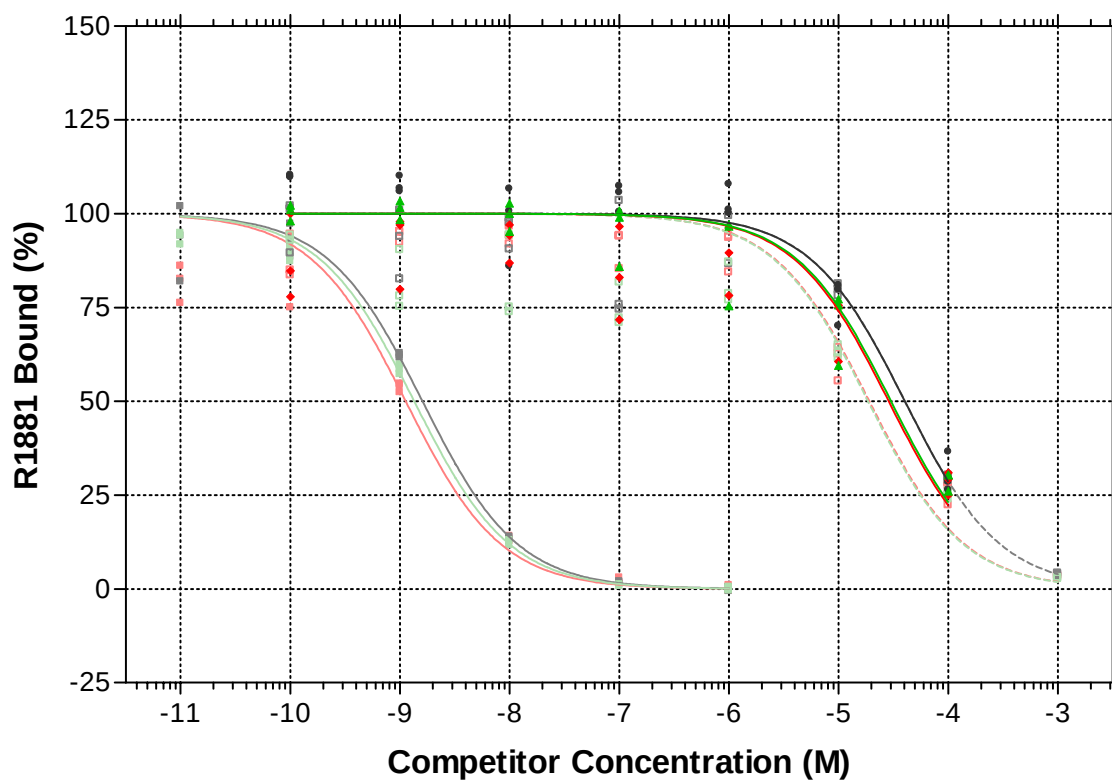
CR42352	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-504-9/20/05	0.000	0.000	100.000	0.000	-4.567	0.104
E-509-10/03/05	0.000	0.000	100.000	0.000	-4.404	0.082
E-510-10/04/05	0.000	0.000	100.000	0.000	-4.627	0.082

WA 4-11-7 Competitive

Lab E CR42353

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive

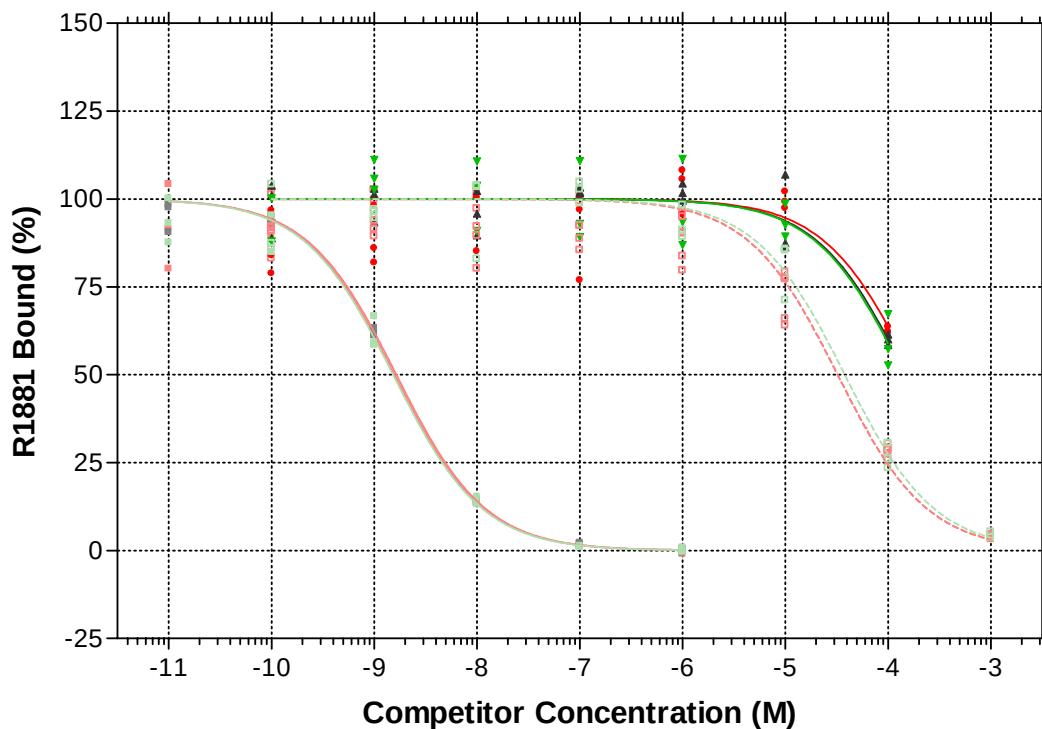


- ♦ E-504-9/20/05
- E-509-10/03/05
- ▲ E-510-10/04/05

CR42353	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-504-9/20/05	0.000	0.000	100.000	0.000	-4.543	0.120
E-509-10/03/05	0.000	0.000	100.000	0.000	-4.395	0.072
E-510-10/04/05	0.000	0.000	100.000	0.000	-4.521	0.070

WA 4-11-7 Competitive

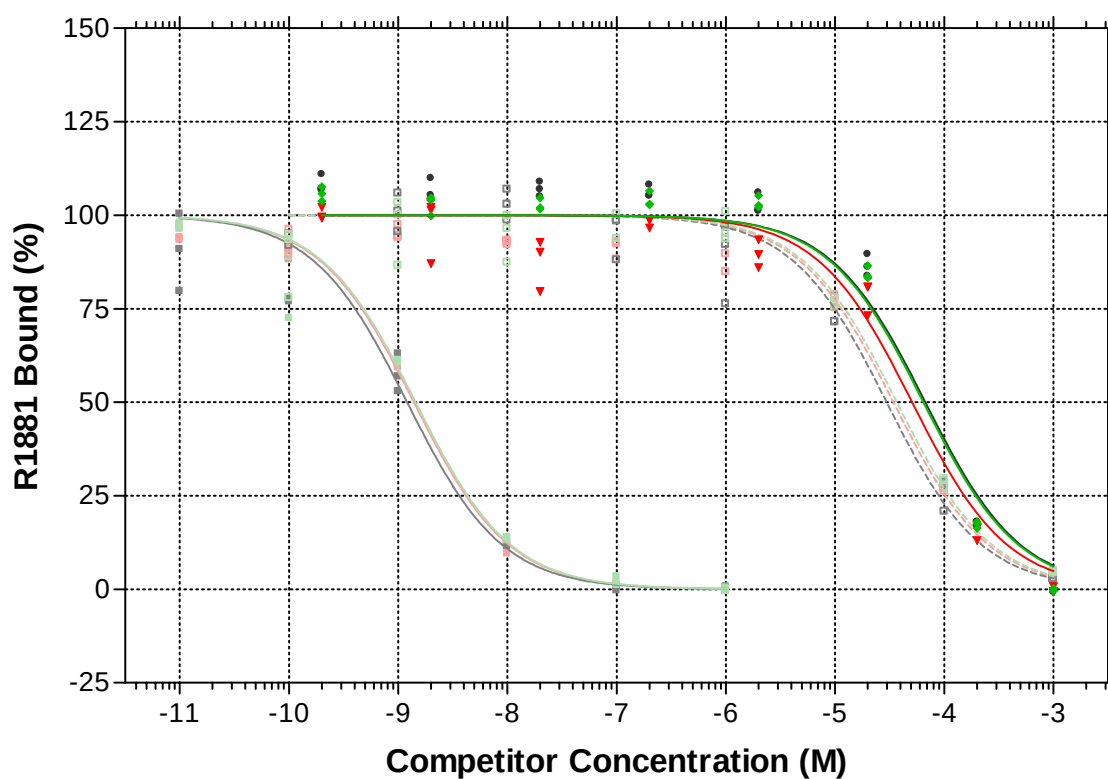
Lab E CR42354
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42354	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
•	E-506-9/26/05	0.000	0.000	100.000	0.000	-3.755	0.112
▲	E-507-9/27/05	0.000	0.000	100.000	0.000	-3.823	0.058
▼	E-508-9/28/05	0.000	0.000	100.000	0.000	-3.842	0.082

WA 4-11-7 Competitive

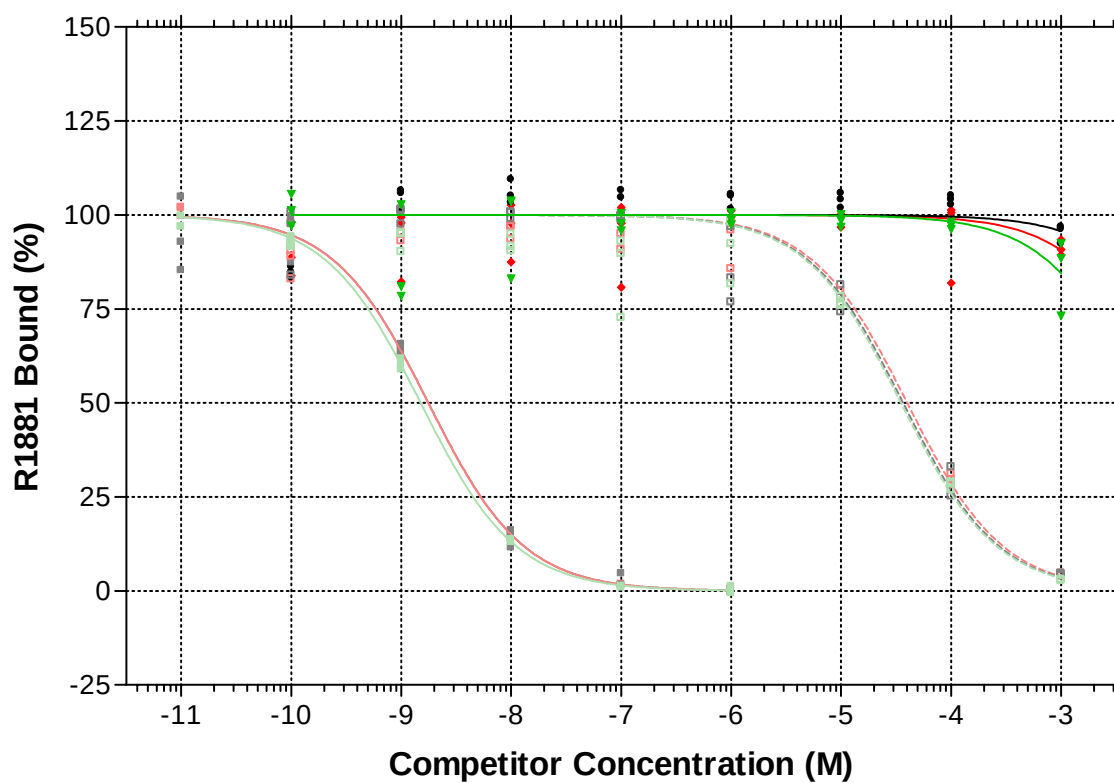
Lab E CR42355
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42355	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-514-10/18/05	E-514-10/18/05	0.000	0.000	100.000	0.000	-4.294	0.069
• E-515-10/19/05	E-515-10/19/05	0.000	0.000	100.000	0.000	-4.172	0.072
◆ E-516-10/27/05	E-516-10/27/05	0.000	0.000	100.000	0.000	-4.191	0.057

WA 4-11-7 Competitive

Lab E CR42357
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



- ♦ E-489-8/9/05
- E-490-8/11/05
- ▼ E-491-8/15/05

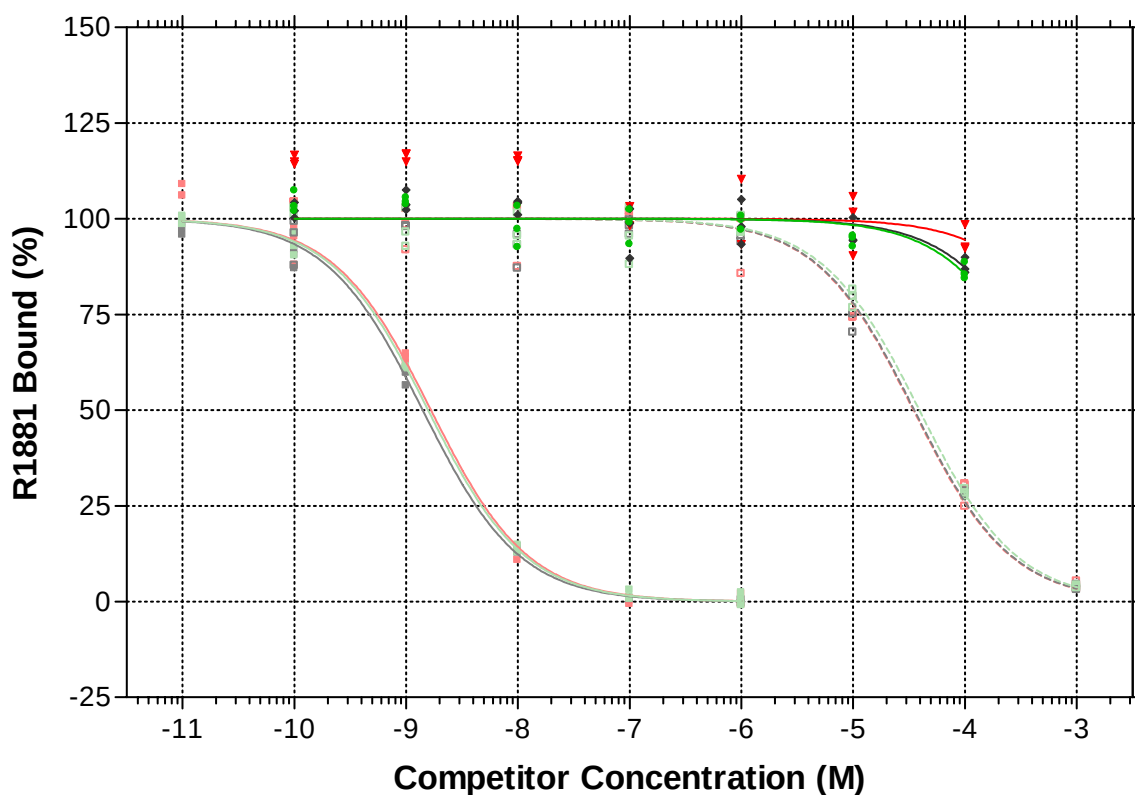
CR42357	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-489-8/9/05	0.000	0.000	100.000	0.000	-2.015	0.243
E-490-8/11/05	0.000	0.000	100.000	0.000	-1.656	0.427
E-491-8/15/05	0.000	0.000	100.000	0.000	-2.264	0.151

WA 4-11-7 Competitive

Lab E CR42358

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



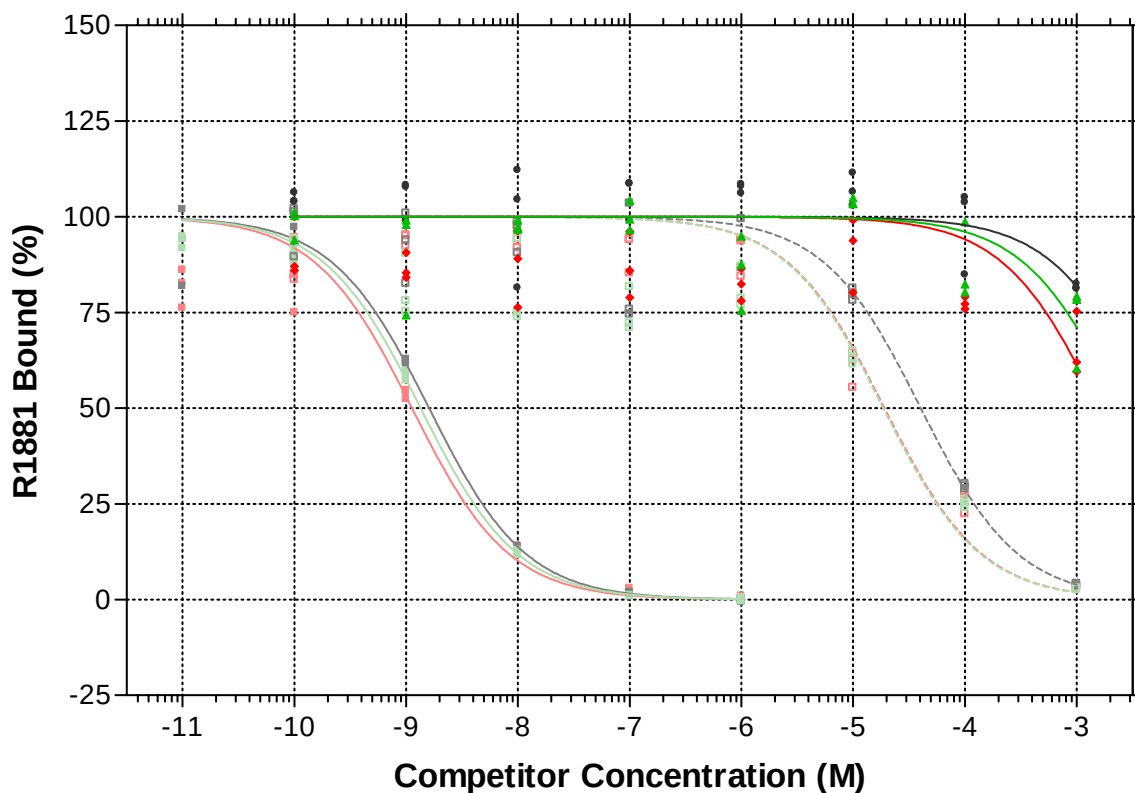
	CR42358	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-511-10/06/05	E-511-10/06/05	0.000	0.000	100.000	0.000	-2.764	0.570
◆ E-512-10/10/05	E-512-10/10/05	0.000	0.000	100.000	0.000	-3.163	0.097
● E-513-10/13/05	E-513-10/13/05	0.000	0.000	100.000	0.000	-3.226	0.081

WA 4-11-7 Competitive

Lab E CR42359

Protein: 1.0 mg per tube

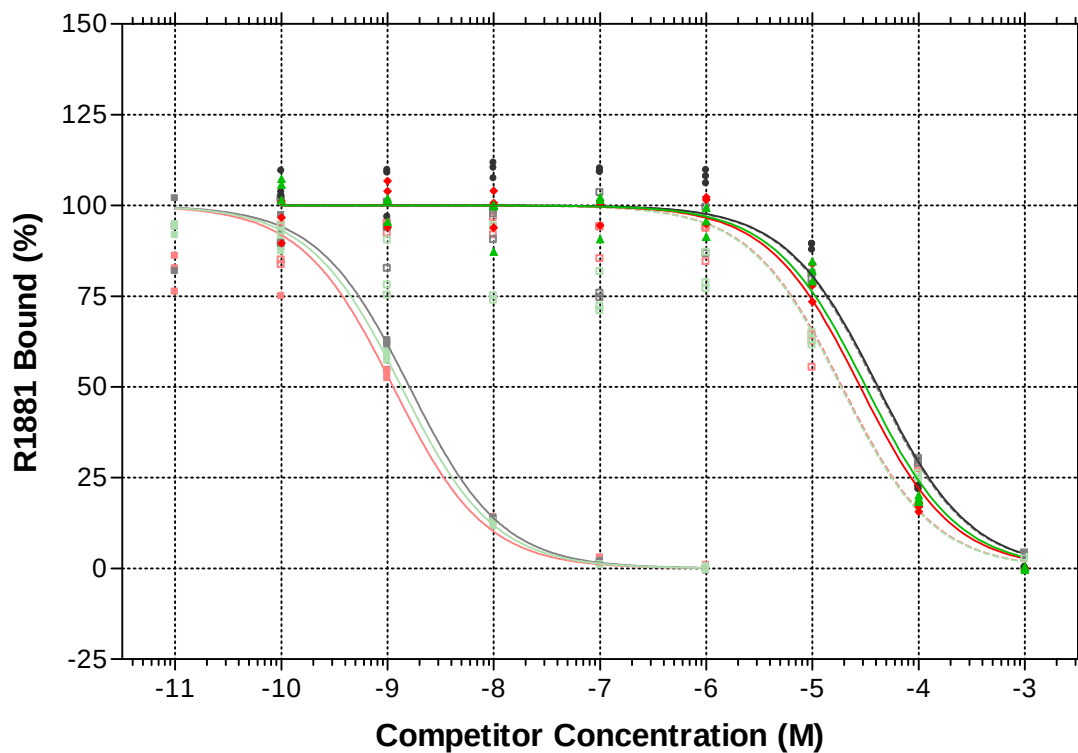
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42359	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
♦ E-504-9/20/05	E-504-9/20/05	0.000	0.000	100.000	0.000	-2.797	0.147
• E-509-10/03/05	E-509-10/03/05	0.000	0.000	100.000	0.000	-2.347	0.134
▲ E-510-10/04/05	E-510-10/04/05	0.000	0.000	100.000	0.000	-2.608	0.119

WA 4-11-7 Competitive

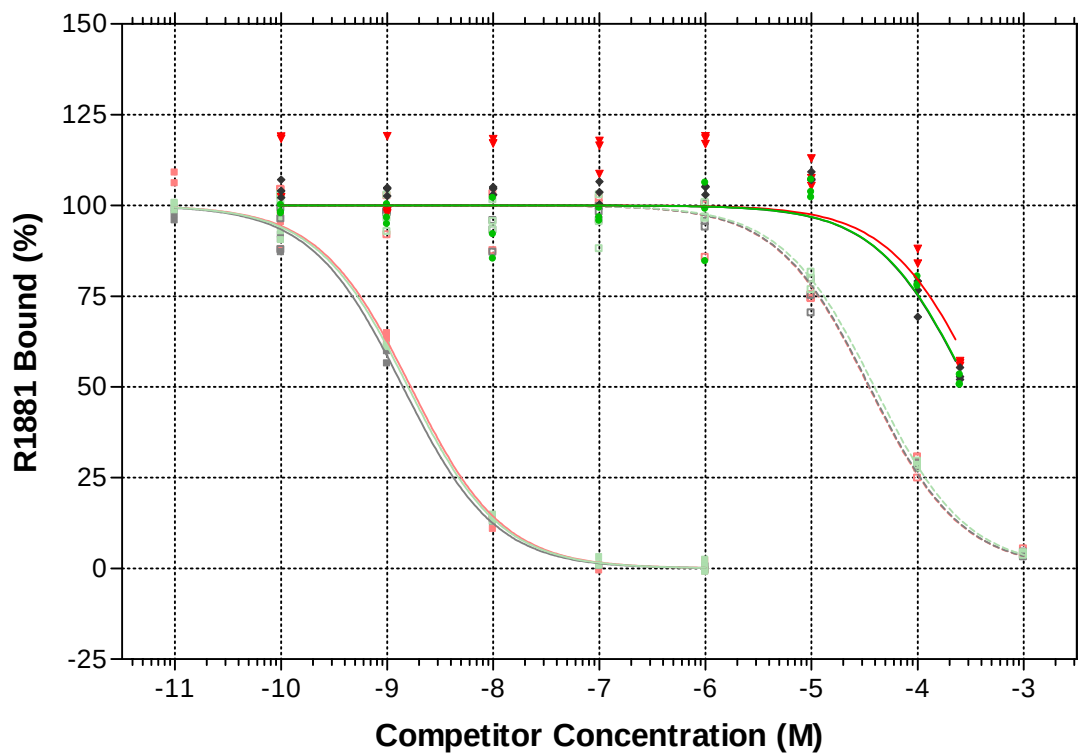
Lab E CR42360
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42360	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
♦ E-504-9/20/05	E-504-9/20/05	0.000	0.000	100.000	0.000	-4.548	0.049
• E-509-10/03/05	E-509-10/03/05	0.000	0.000	100.000	0.000	-4.381	0.081
▲ E-510-10/04/05	E-510-10/04/05	0.000	0.000	100.000	0.000	-4.496	0.050

WA 4-11-7 Competitive

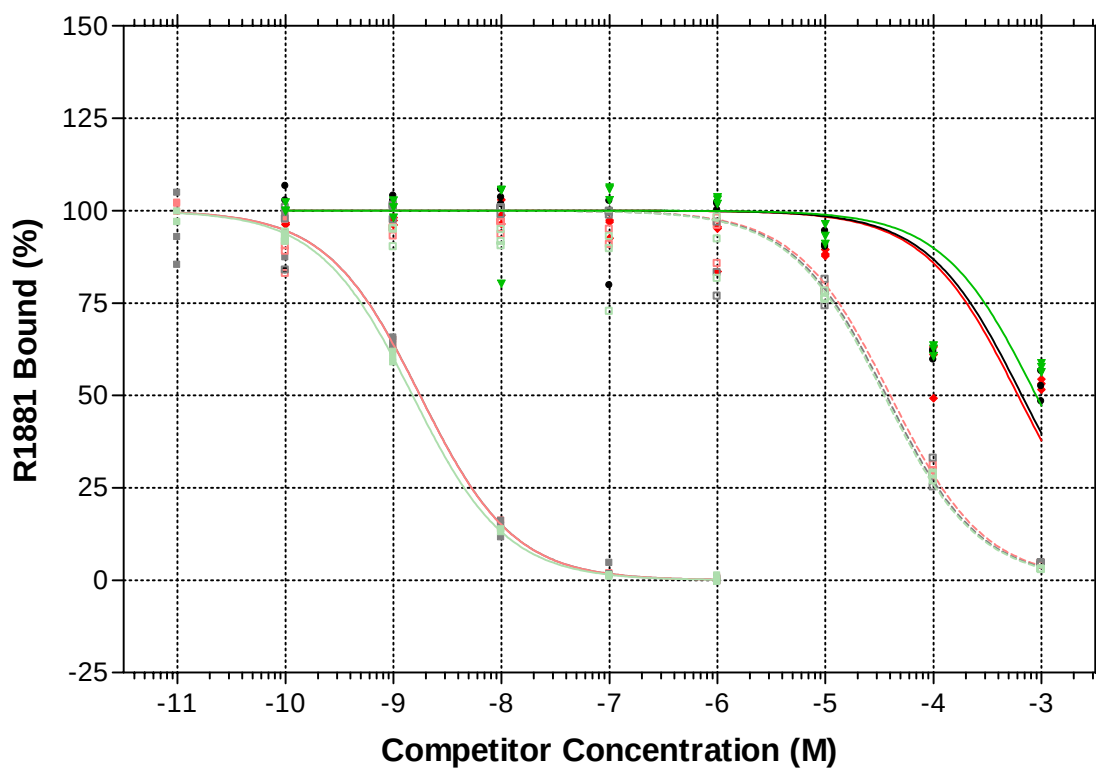
Lab E CR42361
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



CR42361		BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-511-10/06/05	E-511-10/06/05	0.000	0.000	100.000	0.000	-3.410	0.125
♦ E-512-10/10/05	E-512-10/10/05	0.000	0.000	100.000	0.000	-3.518	0.046
● E-513-10/13/05	E-513-10/13/05	0.000	0.000	100.000	0.000	-3.513	0.050

WA 4-11-7 Competitive

Lab E CR42362
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



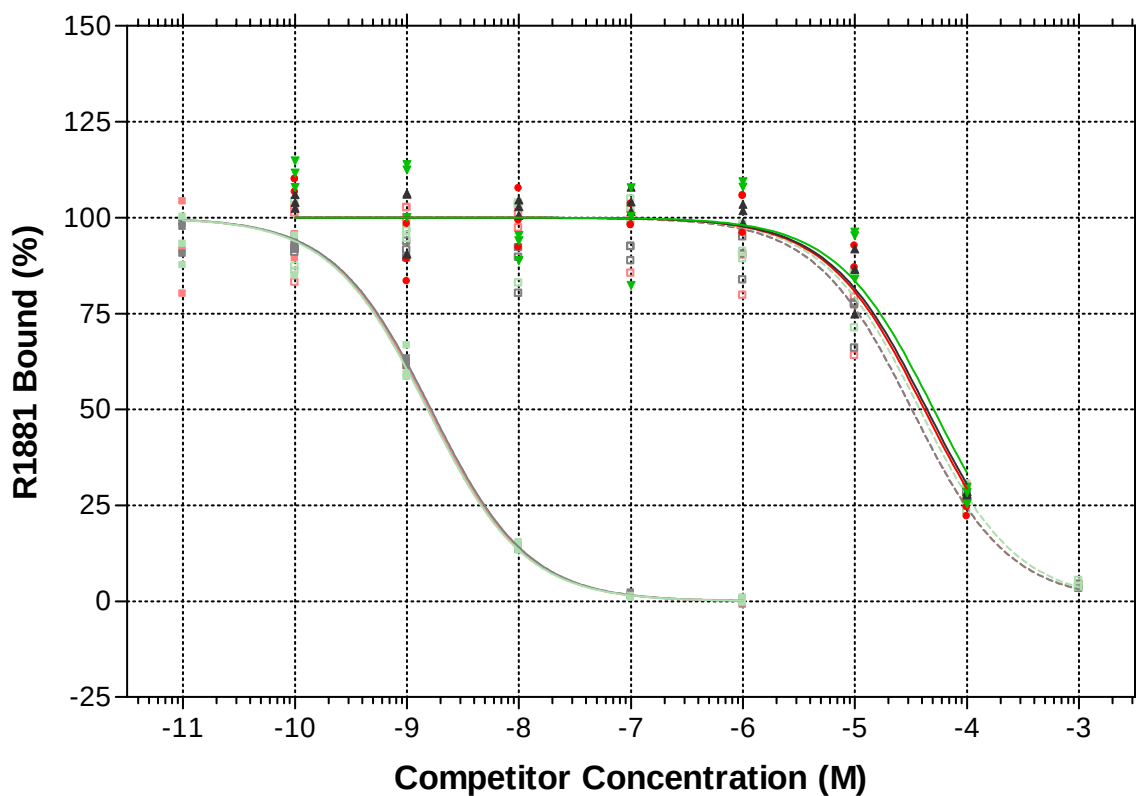
CR42362	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
♦ E-489-8/9/05	0.000	0.000	100.000	0.000	-3.216	0.124
• E-490-8/11/05	0.000	0.000	100.000	0.000	-3.180	0.116
▼ E-491-8/15/05	0.000	0.000	100.000	0.000	-3.048	0.113

WA 4-11-7 Competitive

Lab E CR42363

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



• E-506-9/26/05

▲ E-507-9/27/05

▼ E-508-9/28/05

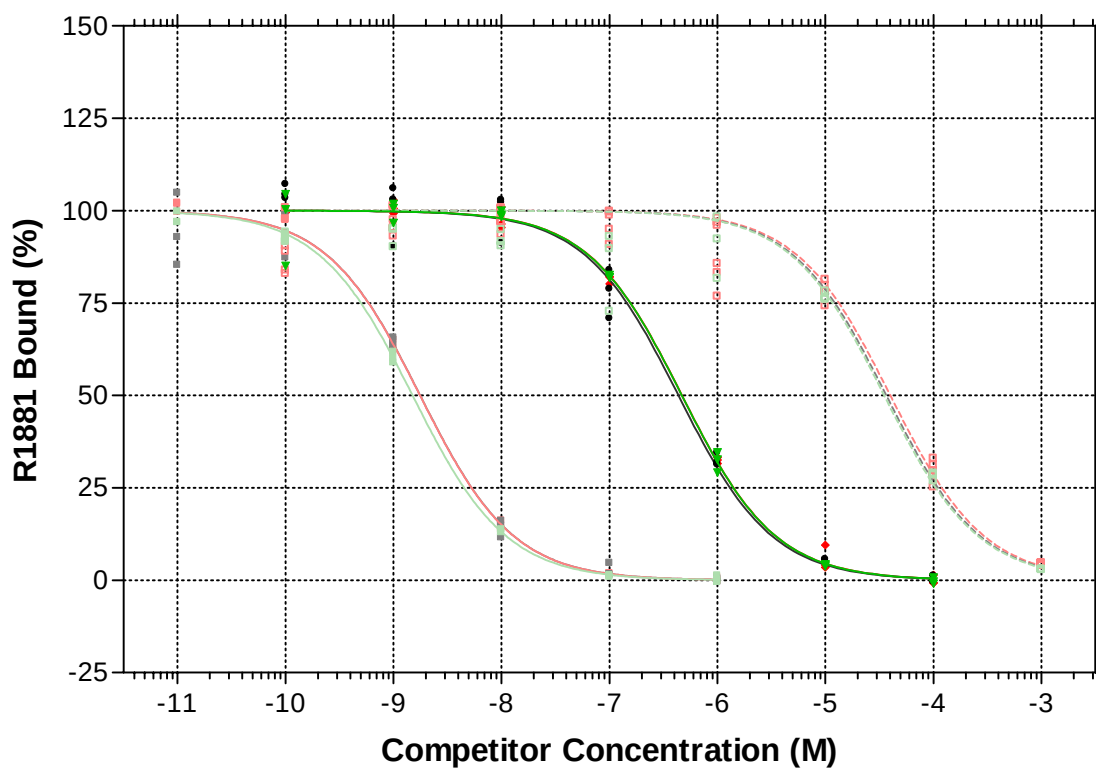
CR42363	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-506-9/26/05	0.000	0.000	100.000	0.000	-4.380	0.081
E-507-9/27/05	0.000	0.000	100.000	0.000	-4.356	0.052
E-508-9/28/05	0.000	0.000	100.000	0.000	-4.297	0.097

WA 4-11-7 Competitive

Lab E CR42365

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



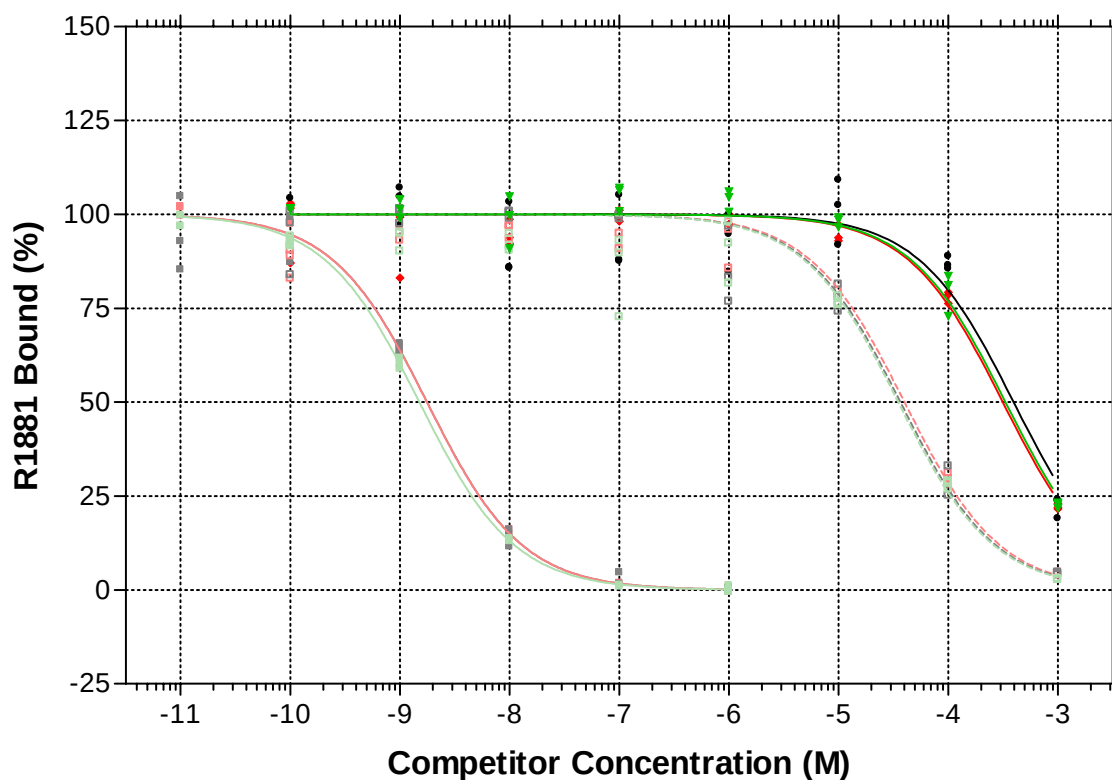
	CR42365	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
♦ E-489-8/9/05	E-489-8/9/05	0.000	0.000	100.000	0.000	-6.328	0.017
• E-490-8/11/05	E-490-8/11/05	0.000	0.000	100.000	0.000	-6.361	0.045
▼ E-491-8/15/05	E-491-8/15/05	0.000	0.000	100.000	0.000	-6.329	0.035

WA 4-11-7 Competitive

Lab E CR42367

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive



- ♦ E-489-8/9/05
- E-490-8/11/05
- ▼ E-491-8/15/05

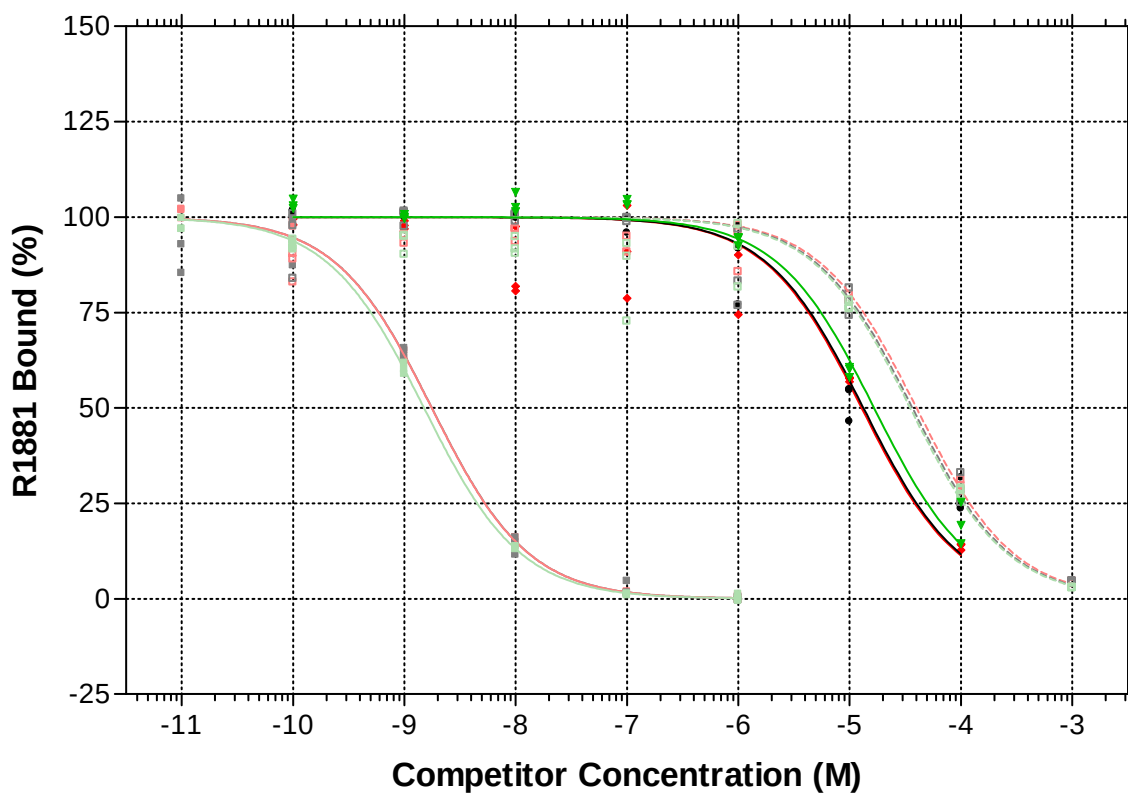
CR42367	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-489-8/9/05	0.000	0.000	100.000	0.000	-3.502	0.051
E-490-8/11/05	0.000	0.000	100.000	0.000	-3.404	0.081
E-491-8/15/05	0.000	0.000	100.000	0.000	-3.478	0.040

WA 4-11-7 Competitive

Lab E CR42368

Protein: 1.0 mg per tube

Solid squares = Standard Curve, Open squares = Weak Positive

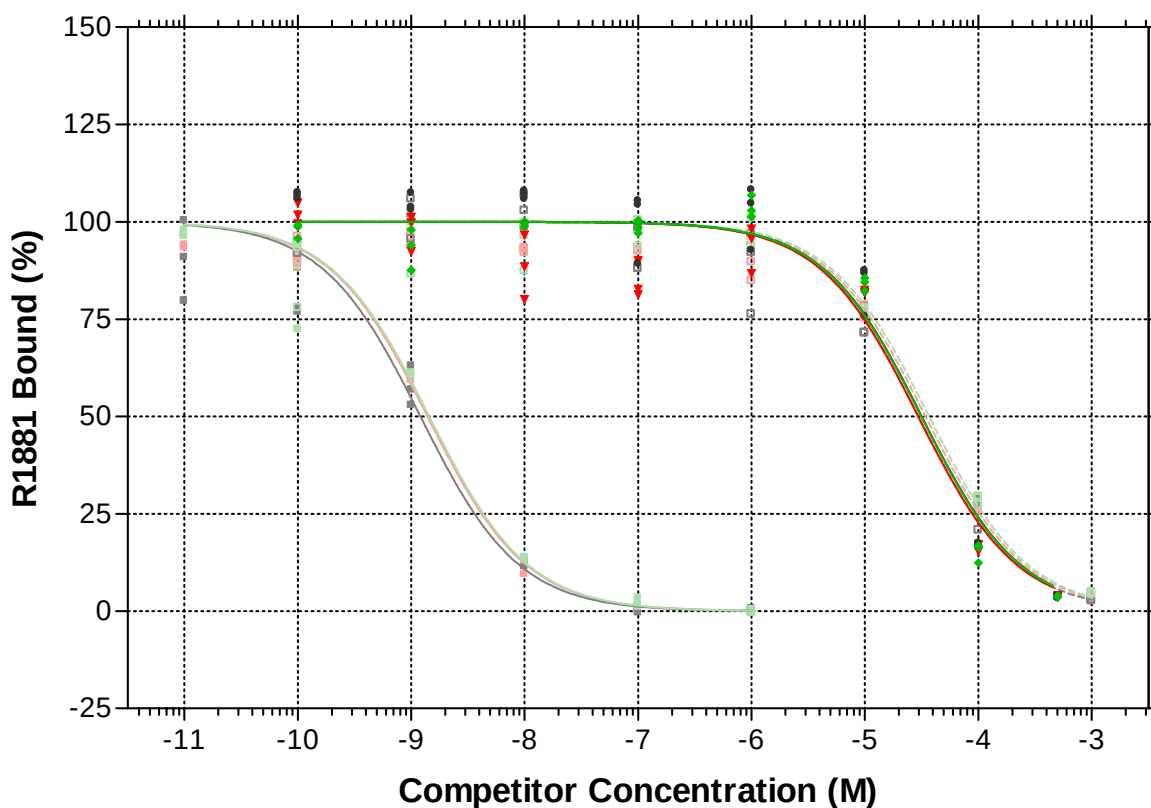


- ♦ E-489-8/9/05
- E-490-8/11/05
- ▼ E-491-8/15/05

CR42367	BOTTOM		TOP		LOGEC50	
	Y	SEM	Y	SEM	Y	SEM
E-489-8/9/05	0.000	0.000	100.000	0.000	-3.502	0.051
E-490-8/11/05	0.000	0.000	100.000	0.000	-3.404	0.081
E-491-8/15/05	0.000	0.000	100.000	0.000	-3.478	0.040

WA 4-11-7 Competitive

Lab E CR42369
Protein: 1.0 mg per tube
Solid squares = Standard Curve, Open squares = Weak Positive



	CR42369	BOTTOM		TOP		LOGEC50	
		Y	SEM	Y	SEM	Y	SEM
▼ E-514-10/18/05	E-514-10/18/05	0.000	0.000	100.000	0.000	-4.529	0.082
• E-515-10/19/05	E-515-10/19/05	0.000	0.000	100.000	0.000	-4.498	0.067
◆ E-516-10/27/05	E-516-10/27/05	0.000	0.000	100.000	0.000	-4.503	0.057

Appendix 5: Excel Files for Competitive Binding Experiments

Competitive Assay of a known Weak Positive**177 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed

by nonlinear regression software

Provide information in all blue cells in
this column

Laboratory Code:		
Run identification:	489	
Assay start date:	8/9/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.59	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.76E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	4.00E-05	M
RBA:	4.4061E-05	
Max Concentration, Unknown 1:	3.00E-02	M (example 5e-3)
IC50, Unknown 1:	9.67E-03	CR42357
RBA, Unknown 1:	0.00002%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	6.08E-04	CR42362
RBA, Unknown 2:	0.00029%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	4.70E-07	CR42365
RBA, Unknown 3:	0.37473%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	3.15E-04	CR42367
RBA, Unknown 4:	0.00056%	
Max Concentration, Unknown 5:	3.00E-02	M (example 5e-3)
IC50, Unknown 5:	1.28E-05	CR43268
RBA, Unknown 5:	0.01372%	
volume of ethanol counted:	2	mL
multitply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10870.1	282.26	Total Binding, solvent control, tubes
Hot	6	44724.8	214.54	Total hot R1881 added to each tube
NSB	6	508.2	44.08	Nonspecific Binding
Specific EtOH	6	10361.9	282.26	

Assay Characterization Values	
EtOH / Hot	0.24 less than 0.1?
NSB / EtOH	0.05 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.30%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3608.70	11186.97	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3353.10	10394.61	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3575.10	11082.81	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	166.83	500.49	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	155.34	466.02	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	154.91	464.73	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	220.62	683.92	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	223.74	693.59	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	210.00	651.00	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	702.02	2176.26	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	627.20	1944.32	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	641.36	1988.22	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2241.80	6949.58	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2340.10	7254.31	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2271.90	7042.89	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3466.60	10746.46	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3296.70	10219.77	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3420.00	10602.00	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3494.80	10833.88	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3566.50	11056.15	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3575.10	11082.81	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	324.21	972.63	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	329.39	988.17	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	304.79	914.37	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1141.20	3423.60	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1190.90	3572.70	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1244.60	3733.80	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2868.60	8605.80	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2921.80	8765.40	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	1700.40	5101.20	FALSE	spill
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3552.10	10656.30	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3483.90	10451.70	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3127.70	9383.10	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2761.00	8283.00	FALSE	spill
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3305.40	9916.20	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3448.30	10344.90	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3511.30	10533.90	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3521.50	10564.50	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3400.60	10201.80	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3454.40	10363.20	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3463.00	10389.00	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3383.50	10150.50	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3293.70	9881.10	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3243.10	9729.30	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3032.40	9097.20	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
1	1	—	103.1	11186.97	10678.8	-825.0	103.1	25.01288					
2	2	—	95.4	10394.61	9886.4	-32.7	95.4	23.24125					
3	3	—	102.1	11082.81	10574.6	-720.9	102.1	24.77999					
4	1	-6.00	-0.1	500.49	-7.7	9861.4	-0.1	1.119043					
5	2	-6.00	-0.4	466.02	-42.2	9895.9	-0.4	1.041971					
6	3	-6.00	0.0	464.73	-43.4	9897.2	-0.4	1.039087					
7	1	cold R1881	-7.01	1.7	683.922	175.7	1.7	1.529177					
8	2	cold R1881	-7.01	1.8	693.594	185.4	1.8	1.550803					
9	3	cold R1881	-7.01	1.4	651	142.8	1.4	1.455567					
10	1	cold R1881	-8.01	16.1	2176.262	1668.1	16.1	4.865892					
11	2	cold R1881	-8.01	13.9	1944.32	1436.1	13.9	4.347294					
12	3	cold R1881	-8.01	14.3	1988.216	1480.0	14.3	4.445441					
13	1	cold R1881	-9.01	62.2	6949.58	6441.4	62.2	15.53853					
14	2	cold R1881	-9.01	65.1	7254.31	6746.1	65.1	16.21987					
15	3	cold R1881	-9.01	63.1	7042.89	6534.7	63.1	15.74716					
16	1	cold R1881	-10.01	98.8	10746.46	10238.3	98.8	24.02795					
17	2	cold R1881	-10.01	93.7	10219.77	9711.6	93.7	22.85033					
18	3	cold R1881	-10.01	97.4	10602	10093.8	97.4	23.70495					
19	1	cold R1881	-11.01	99.7	10833.88	10325.7	99.7	24.22341					
20	2	cold R1881	-11.01	101.8	11056.15	10548.0	101.8	24.72038					
21	3	cold R1881	-11.01	102.1	11082.81	10574.6	102.1	24.77999					
22	1	Weak Positive	-3	4.5	972.63	464.5	4.5	2.174698					
23	2	Weak Positive	-3	4.6	988.17	480.0	4.6	2.209444					
24	3	Weak Positive	-3	3.9	914.37	406.2	3.9	2.044435					
25	1	Weak Positive	-4	28.1	3423.6	2915.4	28.1	7.654808					
26	2	Weak Positive	-4	29.6	3572.7	3064.5	29.6	7.98818					
27	3	Weak Positive	-4	31.1	3733.8	3225.6	31.1	8.348382					
28	1	Weak Positive	-5	78.1	8605.8	8097.6	78.1	19.24166					
29	2	Weak Positive	-5	79.7	8765.4	8257.2	79.7	19.59851					
30	3	Weak Positive	-5										
31	1	Weak Positive	-6	97.9	10656.3	10148.1	97.9	23.82636					
32	2	Weak Positive	-6	96.0	10451.7	9943.5	96.0	23.3689					
33	3	Weak Positive	-6	85.6	9383.1	8874.9	85.6	20.97962					
34	1	Weak Positive	-7										
35	2	Weak Positive	-7	90.8	9916.2	9408.0	90.8	22.17158					
36	3	Weak Positive	-7	94.9	10344.9	9836.7	94.9	23.1301					
37	1	Weak Positive	-8	96.8	10533.9	10025.7	96.8	23.55269					
38	2	Weak Positive	-8	97.1	10564.5	10056.3	97.1	23.62111					
39	3	Weak Positive	-8	93.6	10201.8	9693.6	93.6	22.81015					
40	1	Weak Positive	-9	95.1	10363.2	9855.0	95.1	23.17102					
41	2	Weak Positive	-9	95.4	10389	9880.8	95.4	23.22871					
42	3	Weak Positive	-9	93.1	10150.5	9642.3	93.1	22.69545					
43	1	Weak Positive	-10	90.5	9881.1	9372.9	90.5	22.0931					
44	2	Weak Positive	-10	89.0	9729.3	9221.1	89.0	21.75369					
45	3	Weak Positive	-10	82.9	9097.2	8589.0	82.9	20.34038					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

											Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100

DPM as sampled

corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
3198.90	TRUE	
3148.50	TRUE	
3285.60	TRUE	
3526.20	TRUE	
3549.60	TRUE	
2901.80	TRUE	
3398.20	TRUE	
3509.70	TRUE	
3508.90	TRUE	
3492.70	TRUE	
3457.40	TRUE	
3543.80	TRUE	
3431.90	TRUE	
2862.10	TRUE	
3574.50	TRUE	
3432.60	TRUE	
3088.30	TRUE	
3593.40	TRUE	
3437.10	TRUE	
3485.90	TRUE	
2911.10	TRUE	
2965.00	TRUE	
3441.40	TRUE	
3127.90	TRUE	
1940.60	TRUE	
1983.20	TRUE	
1888.60	TRUE	
1810.50	TRUE	
2203.50	TRUE	
2276.20	TRUE	
3115.60	TRUE	
3095.60	TRUE	
3154.30	TRUE	
3358.80	TRUE	
3346.10	TRUE	
2957.80	TRUE	
3422.00	TRUE	
3256.70	TRUE	
3405.00	TRUE	
3465.70	TRUE	
3385.80	TRUE	
3605.50	TRUE	
3417.40	TRUE	
3377.90	TRUE	
3445.80	TRUE	
3381.30	TRUE	
3396.60	TRUE	
3382.20	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	90.8	9916.59	9408.4	445.3	90.8	22.17245
47	2	Unknown 1	-3.01424	89.3	9760.35	9252.2	601.6	89.3	21.82311
48	3	Unknown 1	-3.01424	93.4	10185.36	9677.2	176.6	93.4	22.77339
49	1	Unknown 1	-4.01424	100.6	10931.22	10423.0	-569.3	100.6	24.44105
50	2	Unknown 1	-4.01424	101.3	11003.76	10495.6	-641.8	101.3	24.60324
51	3	Unknown 1	-4.01424	81.9	8995.58	8487.4	1366.3	81.9	20.11317
52	1	Unknown 1	-5.01424	96.8	10534.42	10026.2	-172.5	96.8	23.55385
53	2	Unknown 1	-5.01424	100.1	10880.07	10371.9	-518.1	100.1	24.32669
54	3	Unknown 1	-5.01424	100.1	10877.59	10369.4	-515.7	100.1	24.32114
55	1	Unknown 1	-6.01424	99.6	10827.37	10319.2	-465.4	99.6	24.20885
56	2	Unknown 1	-6.01424	98.5	10717.94	10209.8	-356.0	98.5	23.96418
57	3	Unknown 1	-6.01424	101.1	10985.78	10477.6	-623.9	101.1	24.56304
58	1	Unknown 1	-7.01424	97.8	10638.89	10130.7	-277.0	97.8	23.78743
59	2	Unknown 1	-7.01424	80.7	8872.51	8364.3	1489.4	80.7	19.83799
60	3	Unknown 1	-7.01424	102.0	11080.95	10572.8	-719.0	102.0	24.77583
61	1	Unknown 1	-8.01424	97.8	10641.06	10132.9	-279.1	97.8	23.79229
62	2	Unknown 1	-8.01424	87.5	9573.73	9065.6	788.2	87.5	21.40585
63	3	Unknown 1	-8.01424	102.6	11139.54	10631.4	-777.6	102.6	24.90683
64	1	Unknown 1	-9.01424	97.9	10655.01	10146.8	-293.1	97.9	23.82348
65	2	Unknown 1	-9.01424	99.4	10806.29	10298.1	-444.4	99.4	24.16172
66	3	Unknown 1	-9.01424	82.2	9024.41	8516.2	1337.5	82.2	20.17763
67	1	Unknown 1	-10.01424	83.8	9191.5	8683.3	1170.4	83.8	20.55122
68	2	Unknown 1	-10.01424	98.1	10668.34	10160.2	-306.4	98.1	23.85328
69	3	Unknown 1	-10.01424	88.7	9696.49	9188.3	665.4	88.7	21.68033
70	1	Unknown 2	-3.01424	53.2	6015.86	5507.7	4346.1	53.2	13.45083
71	2	Unknown 2	-3.01424	54.4	6147.92	5639.7	4214.0	54.4	13.7461
72	3	Unknown 2	-3.01424	51.6	5854.66	5346.5	4507.3	51.6	13.0904
73	1	Unknown 2	-4.01424	49.3	5612.55	5104.4	4749.4	49.3	12.54907
74	2	Unknown 2	-4.01424	61.0	6830.85	6322.7	3531.1	61.0	15.27306
75	3	Unknown 2	-4.01424	63.2	7056.22	6548.0	3305.7	63.2	15.77696
76	1	Unknown 2	-5.01424	88.3	9658.36	9150.2	703.6	88.3	21.59507
77	2	Unknown 2	-5.01424	87.7	9596.36	9088.2	765.6	87.7	21.45645
78	3	Unknown 2	-5.01424	89.5	9778.33	9270.2	583.6	89.5	21.86331
79	1	Unknown 2	-6.01424	95.6	10412.28	9904.1	-50.4	95.6	23.28076
80	2	Unknown 2	-6.01424	95.2	10372.91	9864.7	-11.0	95.2	23.19273
81	3	Unknown 2	-6.01424	83.6	9169.18	8661.0	1192.7	83.6	20.50132
82	1	Unknown 2	-7.01424	97.5	10608.2	10100.0	-246.3	97.5	23.71881
83	2	Unknown 2	-7.01424	92.5	10095.77	9587.6	266.2	92.5	22.57307
84	3	Unknown 2	-7.01424	97.0	10555.5	10047.3	-193.6	97.0	23.60098
85	1	Unknown 2	-8.01424	98.8	10743.67	10235.5	-381.7	98.8	24.02171
86	2	Unknown 2	-8.01424	96.4	10495.98	9987.8	-134.1	96.4	23.4679
87	3	Unknown 2	-8.01424	103.0	11177.05	10668.9	-815.1	103.0	24.9907
88	1	Unknown 2	-9.01424	97.3	10593.94	10085.8	-232.0	97.3	23.68693
89	2	Unknown 2	-9.01424	96.2	10471.49	9963.3	-109.6	96.2	23.41314
90	3	Unknown 2	-9.01424	98.2	10681.98	10173.8	-320.1	98.2	23.88378
91	1	Unknown 2	-10.01424	96.3	10482.03	9973.9	-120.1	96.3	23.43671
92	2	Unknown 2	-10.01424	96.7	10529.46	10021.3	-167.5	96.7	23.54276
93	3	Unknown 2	-10.01424	96.3	10484.82	9976.6	-122.9	96.3	23.44295

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.30%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	415.37	1287.65	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	896.58	2779.40	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	287.30	890.63	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	139.71	433.10	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	211.08	654.35	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	139.27	431.74	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	279.03	864.99	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	480.96	1490.98	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	301.28	933.97	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1250.20	3875.62	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1275.30	3953.43	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1219.80	3781.38	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2905.30	9006.43	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2910.50	9022.55	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2844.30	8817.33	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3386.10	10496.91	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3540.90	10976.79	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3354.30	10398.33	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3483.00	10797.30	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3603.70	11171.47	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3525.30	10928.43	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3490.60	10820.86	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3505.10	10865.81	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3492.20	10825.82	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	896.81	2780.11	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	932.60	2891.06	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	885.27	2744.34	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2791.70	8654.27	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2712.60	8409.06	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2812.40	8718.44	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3298.70	10225.97	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3271.90	10142.89	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3414.70	10585.57	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3509.00	10877.90	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3418.30	10596.73	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3411.80	10576.58	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3445.20	10680.12	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3497.50	10842.25	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3545.40	10990.74	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3461.00	10729.10	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3248.90	10071.59	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3300.70	10232.17	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3482.20	10794.82	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3506.60	10870.46	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	2940.50	9115.55	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3560.50	11037.55	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3607.00	11181.70	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3073.90	9529.09	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ELOH)	Ratio Total binding/ Hot	
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	-0.7	433.101	-75.1	9928.8	-0.7	
98	2	Unknown 3	-4.01424	1.4	654.348	146.2	9707.6	1.4	
99	3	Unknown 3	-4.01424	-0.7	431.737	-76.4	9930.2	-0.7	
100	1	Unknown 3	-5.01424	3.4	864.993	356.8	9496.9	3.4	
101	2	Unknown 3	-5.01424	9.5	1490.976	982.8	8870.9	9.5	
102	3	Unknown 3	-5.01424	4.1	933.968	425.8	9428.0	4.1	
103	1	Unknown 3	-6.01424	32.5	3875.62	3367.4	6486.3	32.5	
104	2	Unknown 3	-6.01424	33.2	3953.43	3445.3	6408.5	33.2	
105	3	Unknown 3	-6.01424	31.6	3781.38	3273.2	6580.5	31.6	
106	1	Unknown 3	-7.01424	82.0	9006.43	8498.3	1355.5	82.0	
107	2	Unknown 3	-7.01424	82.2	9022.55	8514.4	1339.4	82.2	
108	3	Unknown 3	-7.01424	80.2	8817.33	8309.2	1544.6	80.2	
109	1	Unknown 3	-8.01424	96.4	10496.91	9988.7	-135.0	96.4	
110	2	Unknown 3	-8.01424	101.0	10976.79	10468.6	-614.9	101.0	
111	3	Unknown 3	-8.01424	95.4	10398.33	9890.2	-36.4	95.4	
112	1	Unknown 3	-9.01424	99.3	10797.3	10289.1	-435.4	99.3	
113	2	Unknown 3	-9.01424	102.9	11171.47	10663.3	-809.5	102.9	
114	3	Unknown 3	-9.01424	100.6	10928.43	10420.3	-566.5	100.6	
115	1	Unknown 3	-10.01424	99.5	10820.86	10312.7	-458.9	99.5	
116	2	Unknown 3	-10.01424	100.0	10865.81	10357.6	-503.9	100.0	
117	3	Unknown 3	-10.01424	99.6	10825.82	10317.6	-463.9	99.6	
118	1	Unknown 4	-3.01424	21.9	2780.111	2271.9	7581.8	21.9	
119	2	Unknown 4	-3.01424	23.0	2891.06	2382.9	7470.9	23.0	
120	3	Unknown 4	-3.01424	21.6	2744.337	2236.2	7617.6	21.6	
121	1	Unknown 4	-4.01424	78.6	8654.27	8146.1	1707.7	78.6	
122	2	Unknown 4	-4.01424	76.2	8409.06	7900.9	1952.9	76.2	
123	3	Unknown 4	-4.01424	79.2	8718.44	8210.3	1643.5	79.2	
124	1	Unknown 4	-5.01424	93.8	10225.97	9717.8	136.0	93.8	
125	2	Unknown 4	-5.01424	93.0	10142.89	9634.7	219.0	93.0	
126	3	Unknown 4	-5.01424	97.3	10585.57	10077.4	-223.6	97.3	
127	1	Unknown 4	-6.01424	100.1	10877.9	10369.7	-516.0	100.1	
128	2	Unknown 4	-6.01424	97.4	10596.73	10088.6	-234.8	97.4	
129	3	Unknown 4	-6.01424	97.2	10576.58	10068.4	-214.7	97.2	
130	1	Unknown 4	-7.01424	98.2	10680.12	10171.9	-318.2	98.2	
131	2	Unknown 4	-7.01424	99.7	10842.25	10334.1	-480.3	99.7	
132	3	Unknown 4	-7.01424	101.2	10990.74	10482.6	-628.8	101.2	
133	1	Unknown 4	-8.01424	98.6	10729.1	10220.9	-367.2	98.6	
134	2	Unknown 4	-8.01424	92.3	10071.59	9563.4	290.3	92.3	
135	3	Unknown 4	-8.01424	93.8	10232.17	9724.0	129.8	93.8	
136	1	Unknown 4	-9.01424	99.3	10794.82	10286.6	-432.9	99.3	
137	2	Unknown 4	-9.01424	100.0	10870.46	10362.3	-508.5	100.0	
138	3	Unknown 4	-9.01424	83.1	9115.55	8607.4	1246.4	83.1	
139	1	Unknown 4	-10.01424	101.6	11037.55	10529.4	-675.6	101.6	
140	2	Unknown 4	-10.01424	103.0	11181.7	10673.5	-819.8	103.0	
141	3	Unknown 4	-10.01424	87.1	9529.09	9020.9	832.8	87.1	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	3981.20	12341.72	FALSE	precipitate in tube
143	2	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	3924.10	12164.71	FALSE	precipitate in tube
144	3	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	3704.00	11482.40	FALSE	precipitate in tube
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	589.58	1827.70	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	641.65	1989.12	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	638.29	1978.70	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2093.50	6489.85	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2102.00	6516.20	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2064.60	6400.26	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3236.40	10032.84	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	2652.60	8223.06	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3176.00	9845.60	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	2795.10	8664.81	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3608.60	11186.66	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3204.00	9932.40	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	2901.60	8994.96	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	2861.20	8869.72	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3423.40	10612.54	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3433.70	10644.47	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3474.30	10770.33	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3403.40	10550.54	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3491.40	10823.34	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3438.20	10658.42	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3494.80	10833.88	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3539.80	10973.38	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3467.50	10749.25	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3494.70	10833.57	TRUE	
169	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	169.46	508.38	TRUE		
170	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	194.51	583.53	TRUE		
171	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	175.30	525.90	TRUE		
172	1	none	Hot	—	—	—	30	—	—	—	—	—	44971.00	44971.00	TRUE		
173	2	none	Hot	—	—	—	30	—	—	—	—	—	44653.00	44653.00	TRUE		
174	3	none	Hot	—	—	—	30	—	—	—	—	—	44741.00	44741.00	TRUE		
175	1	none	Hot	—	—	—	30	—	—	—	—	—	44434.00	44434.00	TRUE		
176	2	none	Hot	—	—	—	30	—	—	—	—	—	44968.00	44968.00	TRUE		
177	3	none	Hot	—	—	—	30	—	—	—	—	—	44582.00	44582.00	TRUE		

Check the 10% rule: **24.30%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression						
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EOH)	Ratio Total binding/ Hot
142	1	Unknown 5	-3.01424					
143	2	Unknown 5	-3.01424					
144	3	Unknown 5	-3.01424					
145	1	Unknown 5	-4.01424	12.7	1827.698	1319.5	8534.2	12.7
146	2	Unknown 5	-4.01424	14.3	1989.115	1480.9	8372.8	14.3
147	3	Unknown 5	-4.01424	14.2	1978.699	1470.5	8383.2	14.2
148	1	Unknown 5	-5.01424	57.7	6489.85	5981.7	3872.1	57.7
149	2	Unknown 5	-5.01424	58.0	6516.2	6008.0	3845.7	58.0
150	3	Unknown 5	-5.01424	56.9	6400.26	5892.1	3961.7	56.9
151	1	Unknown 5	-6.01424	91.9	10032.84	9524.7	329.1	91.9
152	2	Unknown 5	-6.01424	74.5	8223.06	7714.9	2138.9	74.5
153	3	Unknown 5	-6.01424	90.1	9845.6	9337.4	516.3	90.1
154	1	Unknown 5	-7.01424	78.7	8664.81	8156.6	1697.1	78.7
155	2	Unknown 5	-7.01424	103.1	11186.66	10678.5	-824.7	103.1
156	3	Unknown 5	-7.01424	91.0	9932.4	9424.2	429.5	91.0
157	1	Unknown 5	-8.01424	81.9	8994.96	8486.8	1367.0	81.9
158	2	Unknown 5	-8.01424	80.7	8869.72	8361.5	1492.2	80.7
159	3	Unknown 5	-8.01424	97.5	10612.54	10104.4	-250.6	97.5
160	1	Unknown 5	-9.01424	97.8	10644.47	10136.3	-282.5	97.8
161	2	Unknown 5	-9.01424	99.0	10770.33	10262.2	-408.4	99.0
162	3	Unknown 5	-9.01424	96.9	10550.54	10042.4	-188.6	96.9
163	1	Unknown 5	-10.01424	99.5	10823.34	10315.2	-461.4	99.5
164	2	Unknown 5	-10.01424	98.0	10658.42	10150.2	-296.5	98.0
165	3	Unknown 5	-10.01424	99.7	10833.88	10325.7	-472.0	99.7
166	1	—	—	101.0	10973.38	10465.2	-611.5	101.0
167	2	—	—	98.8	10749.25	10241.1	-387.3	98.8
168	3	—	—	99.6	10833.57	10325.4	-471.6	99.6
169	1	-6.00	0.0	508.38	0.2	9853.5	0.0	1.136684
170	2	-6.00	0.7	583.53	75.4	9778.4	0.7	1.304711
171	3	-6.00	0.2	525.9	17.7	9836.0	0.2	1.175857
172	1			44971	44462.8			
173	2			44653	44144.8			
174	3			44741	44232.8			
175	1			44434	43925.8			
176	2			44968	44459.8			
177	3			44582	44073.8			

Prism data

<i>standard curve</i>				<i>weak positive</i>				<i>CR42357</i>				<i>CR42362</i>			
<i>conce ntratio n (log)</i>	Y1-SC	Y2-SC	Y3-SC	<i>conce ntratio n (log)</i>	y1-PC	y2-PC	y3-PC	<i>conce ntratio n (log)</i>	y1-U1	y2-U1	y3-U1	<i>conce ntratio n (log)</i>	y1-U1	y2-U1	y3-U1
-6.0	-0.07417	-0.40683	-0.41928	-3	4.4823	4.6323	3.9201	-3.0	90.7980	89.2901	93.3918	-3.0	53.1531	54.4276	51.5974
-6.0	0.00198	0.72723	0.17106	-4	28.1359	29.5749	31.1296	-4.0	100.5899	101.2899	81.9096	-4.0	49.2609	61.0184	63.1933
-7.0	1.69608	1.78943	1.37836	-5	78.1479	79.6881		-5.0	96.7605	100.0962	100.0723	-5.0	88.3059	87.7075	89.4637
-8.0	16.09824	13.85983	14.28346	-6	97.9367	95.9622	85.6494	-6.0	99.5876	98.5316	101.1164	-6.0	95.5817	95.2018	83.5849
-9.0	62.16418	65.10505	63.06469	-7		90.7942	94.9315	-7.0	97.7687	80.7218	102.0349	-7.0	97.4725	92.5272	96.9639
-10.0	98.80680	93.72386	97.41266	-8	96.7554	97.0508	93.5504	-8.0	97.7896	87.4891	102.6003	-8.0	98.7799	96.3895	102.9623
-11.0	99.65047	101.79553	102.05282	-9	95.1081	95.3571	93.0554	-9.0	97.9242	99.3842	82.1878	-9.0	97.3349	96.1531	98.1845
				-10	90.4555	88.9905	82.8903	-10.0	83.8003	98.0529	88.6738	-10.0	96.2549	96.7126	96.2818

CR42365				CR42367				CR43268			
concentration (log)	y1-U1	y2-U1	y3-U1	concentration (log)	y1-U1	y2-U1	y3-U1	concentration (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0	21.9258	22.9966	21.5806	-3.0			
-4.0	-0.7245	1.4107	-0.7377	-4.0	78.6157	76.2492	79.2350	-4.0	12.7343	14.2921	14.1916
-5.0	3.4435	9.4847	4.1092	-5.0	93.7837	92.9819	97.2541	-5.0	57.7275	57.9818	56.8629
-6.0	32.4983	33.2492	31.5888	-6.0	100.0753	97.3618	97.1673	-6.0	91.9199	74.4542	90.1129
-7.0	82.0143	82.1698	80.1893	-7.0	98.1666	99.7312	101.1643	-7.0	78.7174	103.0550	90.9505
-8.0	96.3985	101.0297	95.4471	-8.0	98.6393	92.2938	93.8435	-8.0	81.9036	80.6949	97.5144
-9.0	99.2974	102.9085	100.5629	-9.0	99.2735	100.0035	83.0673	-9.0	97.8225	99.0372	96.9160
-10.0	99.5248	99.9586	99.5727	-10.0	101.6160	103.0072	87.0583	-10.0	99.5487	97.9572	99.6505

Competitive Assay of a known Weak Positive**177 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	490	
Assay start date:	8/11/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.56	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.77E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.67E-05	M
RBA:	4.82279E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	2.21E-02	CR42357
RBA, Unknown 1:	0.00001%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	6.61E-04	CR42362
RBA, Unknown 2:	0.00027%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	4.36E-07	CR42365
RBA, Unknown 3:	0.40601%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	3.95E-04	CR42367
RBA, Unknown 4:	0.00045%	
Max Concentration, Unknown 5:	3.00E-02	M (example 5e-3)
IC50, Unknown 5:	1.33E-05	CR43268
RBA, Unknown 5:	0.01329%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

working volume**3.1E+02** uL

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10793.9	671.18	Total Binding, solvent control, tubes
Hot	6	43407.5	975.44	Total hot R1881 added to each tube
NSB	6	467.3	46.11	Nonspecific Binding
Specific EtOH	6	10326.7	671.18	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	Corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3564.40	11049.64	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3053.90	9467.09	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3642.80	11292.68	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	173.09	519.27	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	165.98	497.94	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	169.57	508.71	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	201.34	624.15	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	194.54	603.07	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	305.93	948.38	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	534.58	1657.20	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	682.09	2114.48	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	641.35	1988.19	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2337.30	7245.63	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2266.10	7024.91	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2316.90	7182.39	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3058.50	9481.35	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3279.60	10166.76	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3466.20	10745.22	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2991.70	9274.27	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3641.20	11287.72	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3242.10	10050.51	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	312.19	936.57	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	314.01	942.03	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	292.16	876.48	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1291.00	3873.00	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1022.38	3067.14	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1137.10	3411.30	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2839.50	8518.50	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2709.40	8128.20	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2955.60	8866.80	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3488.50	10465.50	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2798.30	8394.90	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3018.90	9056.70	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3592.70	10778.10	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3556.70	10670.10	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3584.10	10752.30	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3560.40	10681.20	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3615.50	10846.50	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3625.70	10877.10	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3650.10	10950.30	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3513.10	10539.30	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3633.90	10901.70	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3520.90	10562.70	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3044.00	9132.00	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3624.70	10874.10	TRUE	

Check the 10% rule: 24.87% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
11049.64	TRUE	
9467.09	TRUE	
11292.68	TRUE	
519.27	TRUE	
497.94	TRUE	
508.71	TRUE	
624.15	TRUE	
603.07	TRUE	
948.38	TRUE	
1657.20	TRUE	
682.09	TRUE	
2114.48	TRUE	
1988.19	TRUE	
7245.63	TRUE	
7024.91	TRUE	
7182.39	TRUE	
9481.35	TRUE	
10166.76	TRUE	
10745.22	TRUE	
9274.27	TRUE	
11287.72	TRUE	
10050.51	TRUE	
936.57	TRUE	
942.03	TRUE	
876.48	TRUE	
3873.00	TRUE	
3067.14	TRUE	
3411.30	TRUE	
8518.50	TRUE	
8128.20	TRUE	
8866.80	TRUE	
10465.50	TRUE	
8394.90	TRUE	
9056.70	TRUE	
10778.10	TRUE	
10670.10	TRUE	
10752.30	TRUE	
10681.20	TRUE	
10846.50	TRUE	
10877.10	TRUE	
10950.30	TRUE	
10539.30	TRUE	
10901.70	TRUE	
10562.70	TRUE	
9132.00	TRUE	
10874.10	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EIOH)	Ratio Total binding/ Hot					
1	1	—	102.5	11049.64	10582.4	-723.0	102.5	25.4556					
2	2	—	87.2	9467.09	8999.8	859.6	87.2	21.8098					
3	3	—	104.8	11292.68	10825.4	-966.0	104.8	26.0155					
4	1	-6.00	0.5	519.27	52.0	9807.4	0.5	1.196268					
5	2	-6.00	0.3	497.94	30.7	9828.7	0.3	1.147129					
6	3	-6.00	0.0	508.71	41.5	9818.0	0.4	1.17194					
7	1	cold R1881	-7.01	1.5	624.154	156.9	1.5	1.437894					
8	2	cold R1881	-7.01	1.3	603.074	135.8	1.3	1.389331					
9	3	cold R1881	-7.01	4.7	948.383	481.1	4.7	2.184837					
10	1	cold R1881	-8.01	11.5	1657.198	1189.9	11.5	3.817769					
11	2	cold R1881	-8.01	16.0	2114.479	1647.2	16.0	4.87123					
12	3	cold R1881	-8.01	14.7	1988.185	1520.9	14.7	4.58028					
13	1	cold R1881	-9.01	65.6	7245.63	6778.4	65.6	16.69212					
14	2	cold R1881	-9.01	63.5	7024.91	6557.7	63.5	16.18363					
15	3	cold R1881	-9.01	65.0	7182.39	6715.1	65.0	16.54643					
16	1	cold R1881	-10.01	87.3	9481.35	9014.1	87.3	21.84265					
17	2	cold R1881	-10.01	93.9	10166.76	9699.5	93.9	23.42167					
18	3	cold R1881	-10.01	99.5	10745.22	10278.0	99.5	24.75429					
19	1	cold R1881	-11.01	85.3	9274.27	8807.0	85.3	21.36559					
20	2	cold R1881	-11.01	104.8	11287.72	10820.5	104.8	26.00408					
21	3	cold R1881	-11.01	92.8	10050.51	9583.3	92.8	23.15386					
22	1	Weak Positive	-3	4.5	936.57	469.3	4.5	2.157623					
23	2	Weak Positive	-3	4.6	942.03	474.8	4.6	2.170201					
24	3	Weak Positive	-3	4.0	876.48	409.2	4.0	2.01919					
25	1	Weak Positive	-4	33.0	3873	3405.7	33.0	8.922421					
26	2	Weak Positive	-4	25.2	3067.14	2599.9	25.2	7.065922					
27	3	Weak Positive	-4	28.5	3411.3	2944.0	28.5	7.85878					
28	1	Weak Positive	-5	78.0	8518.5	8051.2	78.0	19.62449					
29	2	Weak Positive	-5	74.2	8128.2	7660.9	74.2	18.72534					
30	3	Weak Positive	-5	81.3	8866.8	8399.5	81.3	20.42688					
31	1	Weak Positive	-6	96.8	10465.5	9998.2	96.8	24.10989					
32	2	Weak Positive	-6	76.8	8394.9	7927.6	76.8	19.33975					
33	3	Weak Positive	-6	83.2	9056.7	8589.4	83.2	20.86437					
34	1	Weak Positive	-7	99.8	10778.1	10310.8	99.8	24.83004					
35	2	Weak Positive	-7	98.8	10670.1	10202.8	98.8	24.58124					
36	3	Weak Positive	-7	99.6	10752.3	10285.0	99.6	24.7706					
37	1	Weak Positive	-8	98.9	10681.2	10213.9	98.9	24.60681					
38	2	Weak Positive	-8	100.5	10846.5	10379.2	100.5	24.98762					
39	3	Weak Positive	-8	100.8	10877.1	10409.8	100.8	25.05811					
40	1	Weak Positive	-9	101.5	10950.3	10483.0	101.5	25.22675					
41	2	Weak Positive	-9	97.5	10539.3	10072.0	97.5	24.27991					
42	3	Weak Positive	-9	101.0	10901.7	10434.4	101.0	25.11478					
43	1	Weak Positive	-10	97.8	10562.7	10095.4	97.8	24.33381					
44	2	Weak Positive	-10	83.9	9132	8664.7	83.9	21.03784					
45	3	Weak Positive	-10	100.8	10874.1	10406.8	100.8	25.0512					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	3226.20	10001.22	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	3376.30	10466.53	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	3357.50	10408.25	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3571.50	11071.65	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3618.20	11216.42	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3652.60	11323.06	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3541.60	10978.96	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3618.90	11218.59	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3675.20	11393.12	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3666.40	11365.84	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3533.40	10953.54	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3649.90	11314.69	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3635.40	11269.74	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3475.80	10774.98	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3700.80	11472.48	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3649.80	11314.38	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3591.90	11134.89	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3797.80	11773.18	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3696.80	11460.08	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3675.00	11392.50	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3503.90	10862.09	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3022.70	9370.37	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	2919.40	9050.14	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	2974.20	9220.02	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1898.70	5885.97	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1760.80	5458.48	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	2034.60	6307.26	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2207.10	6842.01	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2138.10	6628.11	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2224.00	6894.40	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3154.00	9777.40	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3171.80	9832.58	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3299.30	10227.83	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3487.10	10810.01	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3555.10	11020.81	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3542.50	10981.75	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3460.40	10727.24	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	2808.90	8707.59	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3569.60	11065.76	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3669.80	11376.38	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3540.50	10975.55	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3602.10	11166.51	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3615.30	11207.43	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3571.60	11071.96	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3556.10	11023.91	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3570.80	11069.48	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3702.20	11476.82	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	2943.50	9124.85	TRUE	

Values for analysis by nonlinear regression

Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
46	1	Unknown 1	-3.01424	92.3	10001.22	9534.0	325.5	92.3	23.0403
47	2	Unknown 1	-3.01424	96.8	10466.53	9999.3	-139.8	96.8	24.11226
48	3	Unknown 1	-3.01424	96.3	10408.25	9941.0	-81.6	96.3	23.978
49	1	Unknown 1	-4.01424	102.7	11071.65	10604.4	-745.0	102.7	25.50631
50	2	Unknown 1	-4.01424	104.1	11216.42	10749.2	-889.7	104.1	25.83982
51	3	Unknown 1	-4.01424	105.1	11323.06	10855.8	-996.4	105.1	26.08549
52	1	Unknown 1	-5.01424	101.8	10978.96	10511.7	-652.3	101.8	25.29277
53	2	Unknown 1	-5.01424	104.1	11218.59	10751.3	-891.9	104.1	25.84482
54	3	Unknown 1	-5.01424	105.8	11393.12	10925.9	-1066.4	105.8	26.24689
55	1	Unknown 1	-6.01424	105.5	11365.84	10898.6	-1039.2	105.5	26.18405
56	2	Unknown 1	-6.01424	101.5	10953.54	10486.3	-626.9	101.5	25.23421
57	3	Unknown 1	-6.01424	105.0	11314.69	10847.4	-988.0	105.0	26.06621
58	1	Unknown 1	-7.01424	104.6	11269.74	10802.5	-943.1	104.6	25.96266
59	2	Unknown 1	-7.01424	99.8	10774.98	10307.7	-448.3	99.8	24.82285
60	3	Unknown 1	-7.01424	106.6	11472.48	11005.2	-1145.8	106.6	26.42972
61	1	Unknown 1	-8.01424	105.0	11314.38	10847.1	-987.7	105.0	26.0655
62	2	Unknown 1	-8.01424	103.3	11134.89	10667.6	-808.2	103.3	25.652
63	3	Unknown 1	-8.01424	109.5	11773.18	11305.9	-1446.5	109.5	27.12246
64	1	Unknown 1	-9.01424	106.5	11460.08	10992.8	-1133.4	106.5	26.40115
65	2	Unknown 1	-9.01424	105.8	11392.5	10925.2	-1065.8	105.8	26.24546
66	3	Unknown 1	-9.01424	100.7	10862.09	10394.8	-535.4	100.7	25.02353
67	1	Unknown 1	-10.01424	86.2	9370.37	8903.1	956.3	86.2	21.58698
68	2	Unknown 1	-10.01424	83.1	9050.14	8582.9	1276.5	83.1	20.84925
69	3	Unknown 1	-10.01424	84.8	9220.02	8752.8	1106.7	84.8	21.24062
70	1	Unknown 2	-3.01424	52.5	5885.97	5418.7	4440.7	52.5	13.5598
71	2	Unknown 2	-3.01424	48.3	5458.48	4991.2	4868.2	48.3	12.57497
72	3	Unknown 2	-3.01424	56.6	6307.26	5840.0	4019.4	56.6	14.53035
73	1	Unknown 2	-4.01424	61.7	6842.01	6374.8	3484.7	61.7	15.76228
74	2	Unknown 2	-4.01424	59.7	6628.11	6160.9	3698.6	59.7	15.2695
75	3	Unknown 2	-4.01424	62.2	6894.4	6427.1	3432.3	62.2	15.88297
76	1	Unknown 2	-5.01424	90.2	9777.4	9310.1	549.3	90.2	22.52468
77	2	Unknown 2	-5.01424	90.7	9832.58	9365.3	494.1	90.7	22.6518
78	3	Unknown 2	-5.01424	94.5	10227.83	9760.6	98.9	94.5	23.56236
79	1	Unknown 2	-6.01424	100.2	10810.01	10342.8	-483.3	100.2	24.90355
80	2	Unknown 2	-6.01424	102.2	11020.81	10553.6	-694.1	102.2	25.38918
81	3	Unknown 2	-6.01424	101.8	10981.75	10514.5	-655.1	101.8	25.2992
82	1	Unknown 2	-7.01424	99.4	10727.24	10260.0	-400.6	99.4	24.71287
83	2	Unknown 2	-7.01424	79.8	8707.59	8240.3	1619.1	79.8	20.0601
84	3	Unknown 2	-7.01424	102.6	11065.76	10598.5	-739.1	102.6	25.49274
85	1	Unknown 2	-8.01424	105.6	11376.38	10909.1	-1049.7	105.6	26.20833
86	2	Unknown 2	-8.01424	101.8	10975.55	10508.3	-648.9	101.8	25.28492
87	3	Unknown 2	-8.01424	103.6	11166.51	10699.3	-839.8	103.6	25.72484
88	1	Unknown 2	-9.01424	104.0	11207.43	10740.2	-880.7	104.0	25.81911
89	2	Unknown 2	-9.01424	102.7	11071.96	10604.7	-745.3	102.7	25.50702
90	3	Unknown 2	-9.01424	102.2	11023.91	10556.7	-697.2	102.2	25.39633
91	1	Unknown 2	-10.01424	102.7	11069.48	10602.2	-742.8	102.7	25.50131
92	2	Unknown 2	-10.01424	106.6	11476.82	11009.6	-1150.1	106.6	26.43972
93	3	Unknown 2	-10.01424	83.8	9124.85	8657.6	1201.8	83.8	21.02137

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.87%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	1878.50	5823.35	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2431.70	7538.27	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2173.30	6737.23	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	135.56	420.24	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	189.98	588.94	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	141.27	437.94	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	338.29	1048.70	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	316.85	982.24	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	312.86	969.87	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1192.50	3696.75	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1211.90	3756.89	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1300.40	4031.24	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2511.10	7784.41	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2775.50	8604.05	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2946.10	9132.91	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3190.60	9890.86	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3579.30	11095.83	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3558.00	11029.80	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3581.00	11101.10	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3161.50	9800.65	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3681.40	11412.34	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3626.20	11241.22	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3721.40	11536.34	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3594.10	11141.71	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	785.52	2435.11	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	950.79	2947.45	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	939.71	2913.10	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3111.80	9646.58	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3030.00	9393.00	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3001.10	9303.41	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3564.50	11049.95	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3211.70	9956.27	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3786.40	11737.84	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3305.80	10247.98	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	2972.70	9215.37	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3478.30	10782.73	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3653.20	11324.92	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3066.50	9506.15	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3079.60	9546.76	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3013.70	9342.47	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3005.90	9318.29	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3593.40	11139.54	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3381.20	10481.72	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3716.40	11520.84	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3639.40	11282.14	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3406.90	10561.39	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3623.80	11233.78	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3261.40	10110.34	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICR)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	-0.5	420.236	-47.0	9906.5	-0.5	0.968118
98	2	Unknown 3	-4.01424	1.2	588.938	121.7	9737.7	1.2	1.356766
99	3	Unknown 3	-4.01424	-0.3	437.937	-29.3	9888.7	-0.3	1.008897
100	1	Unknown 3	-5.01424	5.6	1048.699	581.4	9278.0	5.6	2.41594
101	2	Unknown 3	-5.01424	5.0	982.235	515.0	9344.5	5.0	2.262823
102	3	Unknown 3	-5.01424	4.9	969.866	502.6	9356.8	4.9	2.234328
103	1	Unknown 3	-6.01424	31.3	3696.75	3229.5	6629.9	31.3	8.516385
104	2	Unknown 3	-6.01424	31.9	3756.89	3289.6	6569.8	31.9	8.654933
105	3	Unknown 3	-6.01424	34.5	4031.24	3564.0	6295.4	34.5	9.286967
106	1	Unknown 3	-7.01424	70.9	7784.41	7317.2	2542.3	70.9	17.93333
107	2	Unknown 3	-7.01424	78.8	8604.05	8136.8	1722.6	78.8	19.82157
108	3	Unknown 3	-7.01424	83.9	9132.91	8665.7	1193.8	83.9	21.03994
109	1	Unknown 3	-8.01424	91.3	9890.86	9423.6	435.8	91.3	22.78606
110	2	Unknown 3	-8.01424	102.9	11095.83	10628.6	-769.1	102.9	25.56201
111	3	Unknown 3	-8.01424	102.3	11029.8	10562.5	-703.1	102.3	25.40989
112	1	Unknown 3	-9.01424	103.0	11101.1	10633.8	-774.4	103.0	25.57415
113	2	Unknown 3	-9.01424	90.4	9800.65	9333.4	526.0	90.4	22.57824
114	3	Unknown 3	-9.01424	106.0	11412.34	10945.1	-1085.7	106.0	26.29117
115	1	Unknown 3	-10.01424	104.3	11241.22	10774.0	-914.5	104.3	25.89695
116	2	Unknown 3	-10.01424	107.2	11536.34	11069.1	-1209.7	107.2	26.57684
117	3	Unknown 3	-10.01424	103.4	11141.71	10674.5	-815.0	103.4	25.66771
118	1	Unknown 4	-3.01424	19.1	2435.112	1967.9	7891.6	19.1	5.609888
119	2	Unknown 4	-3.01424	24.0	2947.449	2480.2	7379.2	24.0	6.790184
120	3	Unknown 4	-3.01424	23.7	2913.101	2445.8	7413.6	23.7	6.711055
121	1	Unknown 4	-4.01424	88.9	9646.58	9179.3	680.1	88.9	22.2233
122	2	Unknown 4	-4.01424	86.4	9393	8925.7	933.7	86.4	21.63912
123	3	Unknown 4	-4.01424	85.6	9303.41	8836.2	1023.3	85.6	21.43272
124	1	Unknown 4	-5.01424	102.5	11049.95	10582.7	-723.3	102.5	25.45632
125	2	Unknown 4	-5.01424	91.9	9956.27	9489.0	370.4	91.9	22.93675
126	3	Unknown 4	-5.01424	109.1	11737.84	11270.6	-1411.2	109.1	27.04104
127	1	Unknown 4	-6.01424	94.7	10247.98	9780.7	78.7	94.7	23.60878
128	2	Unknown 4	-6.01424	84.7	9215.37	8748.1	1111.3	84.7	21.2299
129	3	Unknown 4	-6.01424	99.9	10782.73	10315.5	-456.0	99.9	24.84071
130	1	Unknown 4	-7.01424	105.1	11324.92	10857.7	-998.2	105.1	26.08978
131	2	Unknown 4	-7.01424	87.5	9506.15	9038.9	820.5	87.5	21.89979
132	3	Unknown 4	-7.01424	87.9	9546.76	9079.5	779.9	87.9	21.99334
133	1	Unknown 4	-8.01424	85.9	9342.47	8875.2	984.2	85.9	21.52271
134	2	Unknown 4	-8.01424	85.7	9318.29	8851.0	1008.4	85.7	21.467
135	3	Unknown 4	-8.01424	103.3	11139.54	10672.3	-812.9	103.3	25.66271
136	1	Unknown 4	-9.01424	97.0	10481.72	10014.5	-155.0	97.0	24.14726
137	2	Unknown 4	-9.01424	107.0	11520.84	11053.6	-1194.2	107.0	26.54113
138	3	Unknown 4	-9.01424	104.7	11282.14	10814.9	-955.5	104.7	25.99122
139	1	Unknown 4	-10.01424	97.7	10561.39	10094.1	-234.7	97.7	24.3308
140	2	Unknown 4	-10.01424	104.3	11233.78	10766.5	-907.1	104.3	25.87981
141	3	Unknown 4	-10.01424	93.4	10110.34	9643.1	216.3	93.4	23.29169

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-4-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)
142	1	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100
143	2	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100
144	3	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
169	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100
170	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100
171	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100
172	1	none	Hot		—	—	—	30	—	—	—	—	—
173	2	none	Hot		—	—	—	30	—	—	—	—	—
174	3	none	Hot		—	—	—	30	—	—	—	—	—
175	1	none	Hot		—	—	—	30	—	—	—	—	—
176	2	none	Hot		—	—	—	30	—	—	—	—	—
177	3	none	Hot		—	—	—	30	—	—	—	—	—

DPM as sampled

Check the 10% rule:	24.87%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	
3883.00	12037.30	FALSE	precipitate in tube
3805.60	11797.36	FALSE	precipitate in tube
3905.40	12106.74	FALSE	precipitate in tube
960.70	2978.17	TRUE	
1207.90	3744.49	TRUE	
938.18	2908.36	TRUE	
1977.50	6130.25	TRUE	
1969.00	6103.90	TRUE	
1696.40	5258.84	TRUE	
3411.50	10575.65	TRUE	
2717.80	8425.18	TRUE	
3208.10	9945.11	TRUE	
3343.90	10366.09	TRUE	
3469.90	10756.69	TRUE	
3482.10	10794.51	TRUE	
3511.60	10885.96	TRUE	
3475.30	10773.43	TRUE	
3523.20	10921.92	TRUE	
3480.70	10790.17	TRUE	
3518.10	10906.11	TRUE	
3526.70	10932.77	TRUE	
3489.70	10818.07	TRUE	
3536.70	10963.77	TRUE	
3541.10	10977.41	TRUE	
3553.40	11015.54	TRUE	
3479.40	10786.14	TRUE	
3597.60	11152.56	TRUE	
144.27	432.81	TRUE	
139.09	417.27	TRUE	
142.51	427.53	TRUE	
44477.00	44477.00	TRUE	
42559.00	42559.00	TRUE	
43200.00	43200.00	TRUE	
44711.00	44711.00	TRUE	
42372.00	42372.00	TRUE	
43126.00	43126.00	TRUE	

		Values for analysis by nonlinear regression						
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EOH)	Ratio Total binding/ Hot
142	1	Unknown 5	-3.01424					
143	2	Unknown 5	-3.01424					
144	3	Unknown 5	-3.01424					
145	1	Unknown 5	-4.01424	24.3	2978.17	2510.9	7348.5	24.3
146	2	Unknown 5	-4.01424	31.7	3744.49	3277.2	6582.2	31.7
147	3	Unknown 5	-4.01424	23.6	2908.358	2441.1	7418.3	23.6
148	1	Unknown 5	-5.01424	54.8	6130.25	5663.0	4196.4	54.8
149	2	Unknown 5	-5.01424	54.6	6103.9	5636.6	4222.8	54.6
150	3	Unknown 5	-5.01424	46.4	5258.84	4791.6	5067.8	46.4
151	1	Unknown 5	-6.01424	97.9	10575.65	10108.4	-249.0	97.9
152	2	Unknown 5	-6.01424	77.1	8425.18	7957.9	1901.5	77.1
153	3	Unknown 5	-6.01424	91.8	9945.11	9477.9	381.6	91.8
154	1	Unknown 5	-7.01424	95.9	10366.09	9898.8	-39.4	95.9
155	2	Unknown 5	-7.01424	99.6	10756.69	10289.4	-430.0	99.6
156	3	Unknown 5	-7.01424	100.0	10794.51	10327.3	-467.8	100.0
157	1	Unknown 5	-8.01424	100.9	10885.96	10418.7	-559.3	100.9
158	2	Unknown 5	-8.01424	99.8	10773.43	10306.2	-446.7	99.8
159	3	Unknown 5	-8.01424	101.2	10921.92	10454.7	-595.2	101.2
160	1	Unknown 5	-9.01424	100.0	10790.17	10322.9	-463.5	100.0
161	2	Unknown 5	-9.01424	101.1	10906.11	10438.9	-579.4	101.1
162	3	Unknown 5	-9.01424	101.3	10932.77	10465.5	-606.1	101.3
163	1	Unknown 5	-10.01424	100.2	10818.07	10350.8	-491.4	100.2
164	2	Unknown 5	-10.01424	101.6	10963.77	10496.5	-637.1	101.6
165	3	Unknown 5	-10.01424	101.8	10977.41	10510.2	-650.7	101.8
166	1	—	—	102.1	11015.54	10548.3	-688.9	102.1
167	2	—	—	99.9	10786.14	10318.9	-459.5	99.9
168	3	—	—	103.5	11152.56	10685.3	-825.9	103.5
169	1	-6.00	-0.3	432.81	-34.4	9893.9	-0.3	0.997086
170	2	-6.00	-0.5	417.27	-50.0	9909.4	-0.5	0.961285
171	3	-6.00	-0.4	427.53	-39.7	9899.2	-0.4	0.984922
172	1			44477	44009.7			
173	2			42559	42091.7			
174	3			43200	42732.7			
175	1			44711	44243.7			
176	2			42372	41904.7			
177	3			43126	42658.7			

Prism data

standard curve				weak positive				CR42357				CR42362			
concentration (log)	Y1-SC	Y2-SC	Y3-SC	concentration (log)	y1-PC	y2-PC	y3-PC	concentration (log)	y1-U1	y2-U1	y3-U1	concentration (log)	y1-U1	y2-U1	y3-U1
-6.0	0.50369	0.29714	0.40144	-3	4.5447	4.5976	3.9628	-3.0	92.3236	96.8295	96.2651	-3.0	52.4729	48.3333	56.5526
-6.0	-0.33355	-0.48404	-0.38468	-4	32.9800	25.1764	28.5091	-4.0	102.6892	104.0911	105.1238	-4.0	61.7309	59.6596	62.2382
-7.0	1.51935	1.31522	4.65907	-5	77.9654	74.1859	81.3382	-5.0	101.7917	104.1121	105.8022	-5.0	90.1562	90.6905	94.5180
-8.0	11.52299	15.95114	14.72815	-6	96.8195	76.7685	83.1772	-6.0	105.5381	101.5455	105.0427	-6.0	100.1556	102.1969	101.8187
-9.0	65.63940	63.50202	65.02700	-7	99.8466	98.8008	99.5968	-7.0	104.6075	99.8164	106.5707	-7.0	99.3541	79.7965	102.6322
-10.0	87.28932	93.92659	99.52820	-8	98.9082	100.5090	100.8053	-8.0	105.0397	103.3016	109.4826	-8.0	105.6401	101.7586	103.6078
-11.0	85.28403	104.78158	92.80087	-9	101.5141	97.5341	101.0435	-9.0	106.4506	105.7962	100.6599	-9.0	104.0041	102.6922	102.2269
				-10	97.7607	83.9063	100.7762	-10.0	86.2146	83.1136	84.7587	-10.0	102.6682	106.6128	83.8371

CR42365					CR42367					CR43268				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.0					-3.0	19.0560	24.0173	23.6847		-3.0				
-4.0	-0.4553	1.1783	-0.2839		-4.0	88.8894	86.4338	85.5662		-4.0	24.3148	31.7356	23.6388	
-5.0	5.6305	4.9869	4.8671		-5.0	102.4791	91.8883	109.1404		-5.0	54.8385	54.5833	46.4000	
-6.0	31.2733	31.8557	34.5124		-6.0	94.7131	84.7137	99.8914		-6.0	97.8861	77.0617	91.7802	
-7.0	70.8568	78.7939	83.9152		-7.0	105.1418	87.5295	87.9227		-7.0	95.8568	99.6393	100.0055	
-8.0	91.2549	102.9234	102.2840		-8.0	85.9445	85.7103	103.3467		-8.0	100.8911	99.8014	101.2393	
-9.0	102.9744	90.3813	105.9884		-9.0	96.9766	107.0390	104.7275		-9.0	99.9635	101.0862	101.3444	
-10.0	104.3313	107.1891	103.3677		-10.0	97.7481	104.2592	93.3802		-10.0	100.2337	101.6446	101.7766	

Competitive Assay of a known Weak Positive**177 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	491	
Assay start date:	8/15/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.51	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.50E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.51E-05	M
RBA:	4.28408E-05	
Max Concentration, Unknown 1:	3.00E-02	M (example 5e-3)
IC50, Unknown 1:	5.45E-03	CR42357
RBA, Unknown 1:	0.00003%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	8.96E-04	CR42362
RBA, Unknown 2:	0.00017%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	4.69E-07	CR42365
RBA, Unknown 3:	0.32032%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	3.33E-04	CR42367
RBA, Unknown 4:	0.00045%	
Max Concentration, Unknown 5:	3.00E-02	M (example 5e-3)
IC50, Unknown 5:	1.66E-05	CR43268
RBA, Unknown 5:	0.00905%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

working volume**3.1E+02** uL

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11206.2	556.15	Total Binding, solvent control, tubes
Hot	6	45070.7	1025.27	Total hot R1881 added to each tube
NSB	6	451.9	67.81	Nonspecific Binding
Specific EtOH	6	10754.3	556.15	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3564.10	11048.71	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3405.20	10556.12	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3411.30	10575.03	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	146.30	438.90	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	135.82	407.46	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	149.07	447.21	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	176.06	545.79	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	191.24	592.84	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	184.20	571.02	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	595.27	1845.34	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	619.84	1921.50	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	617.61	1914.59	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2286.80	7089.08	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2228.60	6908.66	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2186.90	6779.39	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3332.40	10330.44	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3395.90	10527.29	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3358.10	10410.11	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3505.80	10867.98	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3606.40	11179.84	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3509.50	10879.45	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	251.10	753.30	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	257.27	771.81	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	252.54	757.62	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1168.00	3504.00	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1187.10	3561.30	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1113.00	3339.00	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2872.50	8617.50	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2954.70	8864.10	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2889.70	8669.10	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3671.30	11013.90	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3075.40	9226.20	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3459.10	10377.30	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3364.00	10092.00	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3483.60	10450.80	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2757.00	8271.00	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3433.70	10301.10	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3550.20	10650.60	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3393.40	10180.20	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3554.00	10662.00	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3385.00	10155.00	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3563.80	10691.40	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3525.40	10576.20	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3434.90	10304.70	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3459.20	10377.60	TRUE	

Check the 10% rule: 24.86% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
1	1	—	98.5	11048.71	10596.8	-294.4	98.5	24.51419					
2	2	—	94.0	10556.12	10104.2	198.1	94.0	23.42126					
3	3	—	94.1	10575.03	10123.1	179.2	94.1	23.46322					
4	1	-6.00	-0.1	438.9	-13.0	10315.4	-0.1	0.973804					
5	2	-6.00	-0.4	407.46	-44.5	10346.8	-0.4	0.904047					
6	3	-6.00	0.0	447.21	-4.7	10307.1	0.0	0.992242					
7	1	cold R1881	-7.01	0.9	545.786	93.9	0.9	1.210956					
8	2	cold R1881	-7.01	1.3	592.844	140.9	1.3	1.315366					
9	3	cold R1881	-7.01	1.1	571.02	119.1	1.1	1.266944					
10	1	cold R1881	-8.01	13.0	1845.337	1393.4	13.0	4.094319					
11	2	cold R1881	-8.01	13.7	1921.504	1469.6	13.7	4.263314					
12	3	cold R1881	-8.01	13.6	1914.591	1462.7	13.6	4.247976					
13	1	cold R1881	-9.01	61.7	7089.08	6637.2	61.7	15.72881					
14	2	cold R1881	-9.01	60.0	6908.66	6456.7	60.0	15.32851					
15	3	cold R1881	-9.01	58.8	6779.39	6327.5	58.8	15.04169					
16	1	cold R1881	-10.01	91.9	10330.44	9878.5	91.9	22.92054					
17	2	cold R1881	-10.01	93.7	10527.29	10075.4	93.7	23.3573					
18	3	cold R1881	-10.01	92.6	10410.11	9958.2	92.6	23.09731					
19	1	cold R1881	-11.01	96.9	10867.98	10416.1	96.9	24.1132					
20	2	cold R1881	-11.01	99.8	11179.84	10727.9	99.8	24.80514					
21	3	cold R1881	-11.01	97.0	10879.45	10427.5	97.0	24.13865					
22	1	Weak Positive	-3	2.8	753.3	301.4	2.8	1.671375					
23	2	Weak Positive	-3	3.0	771.81	319.9	3.0	1.712444					
24	3	Weak Positive	-3	2.8	757.62	305.7	2.8	1.68096					
25	1	Weak Positive	-4	28.4	3504	3052.1	28.4	7.774458					
26	2	Weak Positive	-4	28.9	3561.3	3109.4	28.9	7.901592					
27	3	Weak Positive	-4	26.8	3339	2887.1	26.8	7.408366					
28	1	Weak Positive	-5	75.9	8617.5	8165.6	75.9	19.11997					
29	2	Weak Positive	-5	78.2	8864.1	8412.2	78.2	19.66712					
30	3	Weak Positive	-5	76.4	8669.1	8217.2	76.4	19.23446					
31	1	Weak Positive	-6	98.2	11013.9	10562.0	98.2	24.43696					
32	2	Weak Positive	-6	81.6	9226.2	8774.3	81.6	20.47052					
33	3	Weak Positive	-6	92.3	10377.3	9925.4	92.3	23.02451					
34	1	Weak Positive	-7	89.6	10092	9640.1	89.6	22.3915					
35	2	Weak Positive	-7	93.0	10450.8	9998.9	93.0	23.18759					
36	3	Weak Positive	-7	72.7	8271	7819.1	72.7	18.35118					
37	1	Weak Positive	-8	91.6	10301.1	9849.2	91.6	22.85544					
38	2	Weak Positive	-8	94.8	10650.6	10198.7	94.8	23.63089					
39	3	Weak Positive	-8	90.5	10180.2	9728.3	90.5	22.5872					
40	1	Weak Positive	-9	94.9	10662	10210.1	94.9	23.65618					
41	2	Weak Positive	-9	90.2	10155	9703.1	90.2	22.53128					
42	3	Weak Positive	-9	95.2	10691.4	10239.5	95.2	23.72142					
43	1	Weak Positive	-10	94.1	10576.2	10124.3	94.1	23.46582					
44	2	Weak Positive	-10	91.6	10304.7	9852.8	91.6	22.86343					
45	3	Weak Positive	-10	92.3	10377.6	9925.7	92.3	23.02518					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.86%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	3351.60	10389.96	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	2682.00	8314.20	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	3215.10	9966.81	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3481.40	10792.34	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3548.50	11000.35	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	3513.60	10892.16	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3501.30	10854.03	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3561.10	11039.41	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3618.00	11215.80	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3634.80	11267.88	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3570.00	11067.00	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3524.30	10925.33	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3469.20	10754.52	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3534.50	10956.95	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3629.20	11250.52	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3734.70	11577.57	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3025.90	9380.29	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3744.10	11606.71	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2953.50	9155.85	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3707.40	11492.94	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2864.90	8881.19	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3513.00	10890.30	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3654.30	11328.33	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3805.40	11796.74	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	2095.80	6496.98	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	2181.70	6763.27	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	2146.70	6654.77	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2250.00	6975.00	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2348.10	7279.11	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	2319.00	7188.90	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3303.30	10240.23	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3377.50	10470.25	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3487.30	10810.63	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3677.20	11399.32	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3739.80	11593.38	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3717.90	11525.49	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3814.90	11826.19	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3830.60	11874.86	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3710.30	11501.93	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3809.10	11808.21	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3810.10	11811.31	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	2927.90	9076.49	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3707.40	11492.94	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3548.60	11000.66	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3645.80	11301.98	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3609.30	11188.83	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3614.40	11204.64	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3689.80	11438.38	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
46	1	Unknown 1	-3.01424	92.4	10389.96	9938.0	364.3	92.4	23.0526				
47	2	Unknown 1	-3.01424	73.1	8314.2	7862.3	2440.1	73.1	18.44703				
48	3	Unknown 1	-3.01424	88.5	9966.81	9514.9	787.5	88.5	22.11374				
49	1	Unknown 1	-4.01424	96.2	10792.34	10340.4	-38.1	96.2	23.94537				
50	2	Unknown 1	-4.01424	98.1	11000.35	10548.4	-246.1	98.1	24.40689				
51	3	Unknown 1	-4.01424	97.1	10892.16	10440.2	-137.9	97.1	24.16685				
52	1	Unknown 1	-5.01424	96.7	10854.03	10402.1	-99.8	96.7	24.08225				
53	2	Unknown 1	-5.01424	98.4	11039.41	10587.5	-285.1	98.4	24.49356				
54	3	Unknown 1	-5.01424	100.1	11215.8	10763.9	-461.5	100.1	24.88492				
55	1	Unknown 1	-6.01424	100.6	11267.88	10816.0	-513.6	100.6	25.00047				
56	2	Unknown 1	-6.01424	98.7	11067	10615.1	-312.7	98.7	24.55477				
57	3	Unknown 1	-6.01424	97.4	10925.33	10473.4	-171.1	97.4	24.24044				
58	1	Unknown 1	-7.01424	95.8	10754.52	10302.6	-0.3	95.8	23.86146				
59	2	Unknown 1	-7.01424	97.7	10956.95	10505.0	-202.7	97.7	24.3106				
60	3	Unknown 1	-7.01424	100.4	11250.52	10798.6	-496.3	100.4	24.96196				
61	1	Unknown 1	-8.01424	103.5	11577.57	11125.6	-823.3	103.5	25.68759				
62	2	Unknown 1	-8.01424	83.0	9380.29	8928.4	1374.0	83.0	20.81241				
63	3	Unknown 1	-8.01424	103.7	11606.71	11154.8	-852.4	103.7	25.75225				
64	1	Unknown 1	-9.01424	80.9	9155.85	8703.9	1598.4	80.9	20.31443				
65	2	Unknown 1	-9.01424	102.7	11492.94	11041.0	-738.7	102.7	25.49982				
66	3	Unknown 1	-9.01424	78.4	8881.19	8429.3	1873.1	78.4	19.70503				
67	1	Unknown 1	-10.01424	97.1	10890.3	10438.4	-136.0	97.1	24.16272				
68	2	Unknown 1	-10.01424	101.1	11328.33	10876.4	-574.1	101.1	25.1346				
69	3	Unknown 1	-10.01424	105.5	11796.74	11344.8	-1042.5	105.5	26.17388				
70	1	Unknown 2	-3.01424	56.2	6496.98	6045.1	4257.3	56.2	14.4151				
71	2	Unknown 2	-3.01424	58.7	6763.27	6311.3	3991.0	58.7	15.00592				
72	3	Unknown 2	-3.01424	57.7	6654.77	6202.8	4099.5	57.7	14.76519				
73	1	Unknown 2	-4.01424	60.7	6975	6523.1	3779.3	60.7	15.4757				
74	2	Unknown 2	-4.01424	63.5	7279.11	6827.2	3475.2	63.5	16.15044				
75	3	Unknown 2	-4.01424	62.6	7188.9	6737.0	3565.4	62.6	15.95029				
76	1	Unknown 2	-5.01424	91.0	10240.23	9788.3	514.0	91.0	22.72039				
77	2	Unknown 2	-5.01424	93.2	10470.25	10018.3	284.0	93.2	23.23074				
78	3	Unknown 2	-5.01424	96.3	10810.63	10358.7	-56.4	96.3	23.98596				
79	1	Unknown 2	-6.01424	101.8	11399.32	10947.4	-645.1	101.8	25.2921				
80	2	Unknown 2	-6.01424	103.6	11593.38	11141.5	-839.1	103.6	25.72267				
81	3	Unknown 2	-6.01424	103.0	11525.49	11073.6	-771.2	103.0	25.57204				
82	1	Unknown 2	-7.01424	105.8	11826.19	11374.3	-1071.9	105.8	26.23922				
83	2	Unknown 2	-7.01424	106.2	11874.86	11422.9	-1120.6	106.2	26.3472				
84	3	Unknown 2	-7.01424	102.7	11501.93	11050.0	-747.7	102.7	25.51977				
85	1	Unknown 2	-8.01424	105.6	11808.21	11356.3	-1053.9	105.6	26.19932				
86	2	Unknown 2	-8.01424	105.6	11811.31	11359.4	-1057.0	105.6	26.2062				
87	3	Unknown 2	-8.01424	80.2	9076.49	8624.6	1677.8	80.2	20.13835				
88	1	Unknown 2	-9.01424	102.7	11492.94	11041.0	-738.7	102.7	25.49982				
89	2	Unknown 2	-9.01424	98.1	11000.66	10548.7	-246.4	98.1	24.40758				
90	3	Unknown 2	-9.01424	100.9	11301.98	10850.1	-547.7	100.9	25.07613				
91	1	Unknown 2	-10.01424	99.8	11188.83	10736.9	-434.6	99.8	24.82508				
92	2	Unknown 2	-10.01424	100.0	11204.64	10752.7	-450.4	100.0	24.86016				
93	3	Unknown 2	-10.01424	102.2	11438.38	10986.5	-684.1	102.2	25.37877				

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.86%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	202.73	628.46	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	305.91	948.32	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	310.82	963.54	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	111.44	345.46	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	169.53	525.54	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	132.29	410.10	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	292.49	906.72	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	277.08	858.95	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	290.24	899.74	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1156.90	3586.39	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1278.70	3963.97	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	1342.90	4162.99	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3011.10	9334.41	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2988.00	9262.80	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2986.10	9256.91	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3559.50	11034.45	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3574.40	11080.64	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3614.40	11204.64	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3640.10	11284.31	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3500.50	10851.55	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3678.70	11403.97	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3096.30	9598.53	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3770.20	11687.62	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3625.40	11238.74	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	938.06	2907.99	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	949.61	2943.79	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	902.40	2797.44	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2672.50	8284.75	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3043.00	9433.30	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2960.50	9177.55	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3562.30	11043.13	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3585.50	11115.05	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3497.60	10842.56	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3771.20	11690.72	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3635.50	11270.05	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3823.30	11852.23	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3858.00	11959.80	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3837.30	11895.63	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3641.20	11287.72	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3606.40	11179.84	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3299.70	10229.07	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3778.00	11711.80	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3580.70	11100.17	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3663.20	11355.92	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3751.10	11628.41	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3670.00	11377.00	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3661.10	11349.41	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3670.60	11378.86	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	-1.0	345.464	-106.5	10408.8	-1.0	0.766494
98	2	Unknown 3	-4.01424	0.7	525.543	73.6	10228.7	0.7	1.166042
99	3	Unknown 3	-4.01424	-0.4	410.099	-41.8	10344.2	-0.4	0.909902
100	1	Unknown 3	-5.01424	4.2	906.719	454.8	9847.5	4.2	2.011772
101	2	Unknown 3	-5.01424	3.8	858.948	407.0	9895.3	3.8	1.905781
102	3	Unknown 3	-5.01424	4.2	899.744	447.8	9854.5	4.2	1.996296
103	1	Unknown 3	-6.01424	29.1	3586.39	3134.5	7167.9	29.1	7.95726
104	2	Unknown 3	-6.01424	32.7	3963.97	3512.0	6790.3	32.7	8.795011
105	3	Unknown 3	-6.01424	34.5	4162.99	3711.1	6591.3	34.5	9.236584
106	1	Unknown 3	-7.01424	82.6	9334.41	8882.5	1419.9	82.6	20.71061
107	2	Unknown 3	-7.01424	81.9	9262.8	8810.9	1491.5	81.9	20.55173
108	3	Unknown 3	-7.01424	81.9	9256.91	8805.0	1497.4	81.9	20.53866
109	1	Unknown 3	-8.01424	98.4	11034.45	10582.5	-280.2	98.4	24.48255
110	2	Unknown 3	-8.01424	98.8	11080.64	10628.7	-326.4	98.8	24.58504
111	3	Unknown 3	-8.01424	100.0	11204.64	10752.7	-450.4	100.0	24.86016
112	1	Unknown 3	-9.01424	100.7	11284.31	10832.4	-530.0	100.7	25.03693
113	2	Unknown 3	-9.01424	96.7	10851.55	10399.6	-97.3	96.7	24.07675
114	3	Unknown 3	-9.01424	101.8	11403.97	10952.0	-649.7	101.8	25.30242
115	1	Unknown 3	-10.01424	85.1	9598.53	9146.6	1155.7	85.1	21.29662
116	2	Unknown 3	-10.01424	104.5	11687.62	11235.7	-933.4	104.5	25.93177
117	3	Unknown 3	-10.01424	100.3	11238.74	10786.8	-484.5	100.3	24.93582
118	1	Unknown 4	-3.01424	22.8	2907.986	2456.1	7846.3	22.8	6.452059
119	2	Unknown 4	-3.01424	23.2	2943.791	2491.9	7810.5	23.2	6.531501
120	3	Unknown 4	-3.01424	21.8	2797.44	2345.5	7956.8	21.8	6.206786
121	1	Unknown 4	-4.01424	72.8	8284.75	7832.8	2469.5	72.8	18.38169
122	2	Unknown 4	-4.01424	83.5	9433.3	8981.4	1321.0	83.5	20.93002
123	3	Unknown 4	-4.01424	81.1	9177.55	8725.6	1576.7	81.1	20.36258
124	1	Unknown 4	-5.01424	98.5	11043.13	10591.2	-288.9	98.5	24.50181
125	2	Unknown 4	-5.01424	99.2	11115.05	10663.1	-360.8	99.2	24.66138
126	3	Unknown 4	-5.01424	96.6	10842.56	10390.6	-88.3	96.6	24.0568
127	1	Unknown 4	-6.01424	104.5	11690.72	11238.8	-936.5	104.5	25.93864
128	2	Unknown 4	-6.01424	100.6	11270.05	10818.1	-515.8	100.6	25.00529
129	3	Unknown 4	-6.01424	106.0	11852.23	11400.3	-1098.0	106.0	26.29699
130	1	Unknown 4	-7.01424	107.0	11959.8	11507.9	-1205.5	107.0	26.53566
131	2	Unknown 4	-7.01424	106.4	11895.63	11443.7	-1141.4	106.4	26.39329
132	3	Unknown 4	-7.01424	100.8	11287.72	10835.8	-533.5	100.8	25.04449
133	1	Unknown 4	-8.01424	99.8	11179.84	10727.9	-425.6	99.8	24.80514
134	2	Unknown 4	-8.01424	90.9	10229.07	9777.1	525.2	90.9	22.69563
135	3	Unknown 4	-8.01424	104.7	11711.8	11259.9	-957.5	104.7	25.98542
136	1	Unknown 4	-9.01424	99.0	11100.17	10648.2	-345.9	99.0	24.62837
137	2	Unknown 4	-9.01424	101.4	11355.92	10904.0	-601.7	101.4	25.19581
138	3	Unknown 4	-9.01424	103.9	11628.41	11176.5	-874.1	103.9	25.80039
139	1	Unknown 4	-10.01424	101.6	11377	10925.1	-622.7	101.6	25.24258
140	2	Unknown 4	-10.01424	101.3	11349.41	10897.5	-595.1	101.3	25.18137
141	3	Unknown 4	-10.01424	101.6	11378.86	10926.9	-624.6	101.6	25.24671

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	3520.10	10912.31	FALSE	precipitate in tube
143	2	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	3463.20	10735.92	FALSE	precipitate in tube
144	3	Unknown 5	U5	1	E-1-U5	3.00E-02	300	30	10	50	310	9.7E-04	100	2819.90	8741.69	FALSE	precipitate in tube
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	813.20	2520.92	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	1021.57	3166.87	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	646.29	2003.50	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2232.50	6920.75	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2247.60	6967.56	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2157.90	6689.49	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3353.40	10395.54	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3420.80	10604.48	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3430.60	10634.86	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3775.80	11704.98	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3726.10	11550.91	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3727.80	11556.18	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3839.20	11901.52	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3662.70	11354.37	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3703.20	11479.92	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3600.30	11160.93	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3638.80	11280.28	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3613.40	11201.54	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3779.40	11716.14	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3716.90	11522.39	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3694.70	11453.57	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3794.00	11761.40	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3746.70	11614.77	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3768.10	11681.11	TRUE	
169	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	194.78	584.34	TRUE		
170	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.19	396.57	TRUE		
171	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	145.69	437.07	TRUE		
172	1	none	Hot	—	—	—	—	30	—	—	—	—	44896.00	44896.00	TRUE		
173	2	none	Hot	—	—	—	—	30	—	—	—	—	44496.00	44496.00	TRUE		
174	3	none	Hot	—	—	—	—	30	—	—	—	—	44882.00	44882.00	TRUE		
175	1	none	Hot	—	—	—	—	30	—	—	—	—	47053.00	47053.00	TRUE		
176	2	none	Hot	—	—	—	—	30	—	—	—	—	44987.00	44987.00	TRUE		
177	3	none	Hot	—	—	—	—	30	—	—	—	—	44110.00	44110.00	TRUE		

Check the 10% rule: **24.86%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

			Values for analysis by nonlinear regression						
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EOH)	Ratio Total binding/ Hot
142	1	Unknown 5	-3.01424						
143	2	Unknown 5	-3.01424						
144	3	Unknown 5	-3.01424						
145	1	Unknown 5	-4.01424	19.2	2520.92	2069.0	8233.3	19.2	5.593261
146	2	Unknown 5	-4.01424	25.2	3166.867	2714.9	7587.4	25.2	7.026448
147	3	Unknown 5	-4.01424	14.4	2003.499	1551.6	8750.8	14.4	4.445239
148	1	Unknown 5	-5.01424	60.2	6920.75	6468.8	3833.5	60.2	15.35533
149	2	Unknown 5	-5.01424	60.6	6967.56	6515.6	3786.7	60.6	15.45919
150	3	Unknown 5	-5.01424	58.0	6689.49	6237.6	4064.8	58.0	14.84223
151	1	Unknown 5	-6.01424	92.5	10395.54	9943.6	358.7	92.5	23.06498
152	2	Unknown 5	-6.01424	94.4	10604.48	10152.6	149.8	94.4	23.52856
153	3	Unknown 5	-6.01424	94.7	10634.86	10182.9	119.4	94.7	23.59597
154	1	Unknown 5	-7.01424	104.6	11704.98	11253.1	-950.7	104.6	25.97028
155	2	Unknown 5	-7.01424	103.2	11550.91	11099.0	-796.6	103.2	25.62844
156	3	Unknown 5	-7.01424	103.3	11556.18	11104.3	-801.9	103.3	25.64014
157	1	Unknown 5	-8.01424	106.5	11901.52	11449.6	-1147.3	106.5	26.40635
158	2	Unknown 5	-8.01424	101.4	11354.37	10902.4	-600.1	101.4	25.19237
159	3	Unknown 5	-8.01424	102.5	11479.92	11028.0	-725.7	102.5	25.47093
160	1	Unknown 5	-9.01424	99.6	11160.93	10709.0	-406.7	99.6	24.76318
161	2	Unknown 5	-9.01424	100.7	11280.28	10828.4	-526.0	100.7	25.02799
162	3	Unknown 5	-9.01424	100.0	11201.54	10749.6	-447.3	100.0	24.85328
163	1	Unknown 5	-10.01424	104.7	11716.14	11264.2	-961.9	104.7	25.99504
164	2	Unknown 5	-10.01424	102.9	11522.39	11070.5	-768.1	102.9	25.56516
165	3	Unknown 5	-10.01424	102.3	11453.57	11001.6	-699.3	102.3	25.41247
166	1	—	—	105.2	11761.4	11309.5	-1007.1	105.2	26.09546
167	2	—	—	103.8	11614.77	11162.8	-860.5	103.8	25.77013
168	3	—	—	104.4	11681.11	11229.2	-926.8	104.4	25.91732
169	1		-6.00	1.2	584.34	132.4	10169.9	1.2	1.296497
170	2		-6.00	-0.5	396.57	-55.4	10357.7	-0.5	0.879885
171	3		-6.00	-0.1	437.07	-14.9	10317.2	-0.1	0.969744
172	1				44896	44444.1			
173	2				44496	44044.1			
174	3				44882	44430.1			
175	1				47053	46601.1			
176	2				44987	44535.1			
177	3				44110	43658.1			

Prism data															
standard curve				weak positive				CR42357				CR42362			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-6.0	-0.12111	-0.41346	-0.04384	-3	2.8024	2.9745	2.8425	-3.0	92.4102	73.1084	88.4755	-3.0	56.2108	58.6869	57.6780
-6.0	1.23128	-0.51473	-0.13813	-4	28.3801	28.9129	26.8459	-4.0	96.1518	98.0860	97.0799	-4.0	60.6557	63.4835	62.6447
-7.0	0.87278	1.31035	1.10742	-5	75.9287	78.2218	76.4085	-5.0	96.7254	98.4492	100.0894	-5.0	91.0179	93.1568	96.3218
-8.0	12.95683	13.66508	13.60080	-6	98.2120	81.5888	92.2925	-6.0	100.5736	98.7057	97.3884	-6.0	101.7958	103.6003	102.9691
-9.0	61.71649	60.03883	58.83680	-7	89.6396	92.9759	72.7067	-7.0	95.8001	97.6824	100.4122	-7.0	105.7652	106.2177	102.7500
-10.0	91.85672	93.68716	92.59754	-8	91.5839	94.8338	90.4597	-8.0	103.4533	83.0216	103.7243	-8.0	105.5980	105.6268	80.1967
-11.0	96.85511	99.75498	96.96176	-9	94.9398	90.2254	95.2132	-9.0	80.9346	102.6664	78.3807	-9.0	102.6664	98.0889	100.8907
				-10	94.1420	91.6174	92.2952	-10.0	97.0627	101.1357	105.4913	-10.0	99.8386	99.9856	102.1591

CR42365				CR42367				CR43268			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0	22.8380	23.1710	21.8101	-3.0			
-4.0	-0.9899	0.6845	-0.3889	-4.0	72.8346	83.5145	81.1364	-4.0	19.2388	25.2453	14.4275
-5.0	4.2290	3.7848	4.1641	-5.0	98.4838	99.1525	96.6187	-5.0	60.1513	60.5865	58.0008
-6.0	29.1463	32.6572	34.5078	-6.0	104.5055	100.5938	106.0073	-6.0	92.4621	94.4049	94.6874
-7.0	82.5950	81.9291	81.8744	-7.0	107.0075	106.4109	100.7581	-7.0	104.6381	103.2054	103.2544
-8.0	98.4031	98.8326	99.9856	-8.0	99.7550	90.9141	104.7015	-8.0	106.4656	101.3779	102.5453
-9.0	100.7264	96.7023	101.8391	-9.0	99.0142	101.3923	103.9261	-9.0	99.5791	100.6889	99.9568
-10.0	85.0510	104.4766	100.3027	-10.0	101.5883	101.3318	101.6056	-10.0	104.7418	102.9402	102.3003

Competitive Assay of a known Weak Positive
153 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
 Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:		
Run identification:	499	
Assay start date:	9/12/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.17	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.50E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.30E-05	M
RBA:	4.54821E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	2.38E-06	CR42343
RBA, Unknown 1:	0.06295%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	3.51E-06	CR42344
RBA, Unknown 2:	0.04276%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	3.15E-05	CR42348
RBA, Unknown 3:	0.00476%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	2.70E-05	CR42349
RBA, Unknown 4:	0.00555%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	

protocol calls for counting decanted EtOH supernate
 reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

working volume

3.1E+02 uL

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10340.8	782.46	Total Binding, solvent control, tubes
Hot	6	44682.5	781.73	Total hot R1881 added to each tube
NSB	6	449.9	63.53	Nonspecific Binding
Specific EtOH	6	9890.9	782.46	

Assay Characterization Values	
EtOH / Hot	0.23 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)													Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay		
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—			3515.90	10899.29
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	3494.20	10832.02	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	3275.90	10155.29	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	169.66	508.98	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	163.02	489.06	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	134.39	403.17	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	245.23	760.21	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	204.55	634.11	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	187.82	582.24	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	630.84	1955.60	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	587.42	1821.00	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	649.45	2013.30	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	2130.20	6603.62	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	2107.50	6533.25	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	1987.50	6161.25	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	3181.20	9861.72	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	2843.90	8816.09	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	2788.50	8644.35	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	3401.20	10543.72	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	3512.90	10889.99	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	2329.40	7221.14	FALSE	spill
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	270.27	810.81	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	272.81	818.43	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	321.88	965.64	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	1100.40	3301.20	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	944.32	2832.96	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	1241.20	3723.60	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	2868.00	8604.00	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	2486.30	7458.90	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	2462.80	7388.40	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	3003.60	9010.80	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	3001.40	9004.20	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	3024.90	9074.70	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	2808.20	8424.60	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	2431.60	7294.80	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	3187.30	9561.90	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	3409.90	10229.70	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	3618.60	10855.80	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	3520.80	10562.40	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	2983.00	8949.00	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	3106.50	9319.50	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	3380.70	10142.10	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	3011.30	9033.90	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	3077.10	9231.30	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	3298.20	9894.60	TRUE	

Values for analysis by nonlinear regression										
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot		
1	1	—	105.6	10899.29	10449.4	-1008.4	105.6	24.39275		
2	2	—	105.0	10832.02	10382.1	-941.1	105.0	24.2422		
3	3	—	98.1	10155.29	9705.4	-264.4	98.1	22.72767		
4	1	-6.00	0.6	508.98	59.1	9381.9	0.6	1.139104		
5	2	-6.00	0.4	489.06	39.2	9401.8	0.4	1.094522		
6	3	-6.00	0.0	403.17	-46.7	9487.7	-0.5	0.9023		
7	1	cold R1881	-7.01	3.1	760.213	310.3	9130.7	3.1	1.701366	
8	2	cold R1881	-7.01	1.9	634.105	184.2	9256.8	1.9	1.419135	
9	3	cold R1881	-7.01	1.3	582.242	132.4	9308.7	1.3	1.303065	
10	1	cold R1881	-8.01	15.2	1955.604	1505.7	7935.3	15.2	4.376666	
11	2	cold R1881	-8.01	13.9	1821.002	1371.1	8069.9	13.9	4.075426	
12	3	cold R1881	-8.01	15.8	2013.295	1563.4	7877.6	15.8	4.50578	
13	1	cold R1881	-9.01	62.2	6603.62	6153.7	3287.3	62.2	14.77899	
14	2	cold R1881	-9.01	61.5	6533.25	6083.4	3357.6	61.5	14.6215	
15	3	cold R1881	-9.01	57.7	6161.25	5711.4	3729.6	57.7	13.78896	
16	1	cold R1881	-10.01	95.2	9861.72	9411.8	29.2	95.2	22.07065	
17	2	cold R1881	-10.01	84.6	8816.09	8366.2	1074.8	84.6	19.73052	
18	3	cold R1881	-10.01	82.8	8644.35	8194.5	1246.5	82.8	19.34616	
19	1	cold R1881	-11.01	102.1	10543.72	10093.8	-652.8	102.1	23.59698	
20	2	cold R1881	-11.01	105.6	10889.99	10440.1	-999.1	105.6	24.37194	
21	3	cold R1881	-11.01							
22	1	Weak Positive	-3	3.6	810.81	360.9	9080.1	3.6	1.814603	
23	2	Weak Positive	-3	3.7	818.43	368.6	9072.5	3.7	1.831657	
24	3	Weak Positive	-3	5.2	965.64	515.8	8925.3	5.2	2.161115	
25	1	Weak Positive	-4	28.8	3301.2	2851.3	6589.7	28.8	7.388127	
26	2	Weak Positive	-4	24.1	2832.96	2383.1	7057.9	24.1	6.3402	
27	3	Weak Positive	-4	33.1	3723.6	3273.7	6167.3	33.1	8.333464	
28	1	Weak Positive	-5	82.4	8604	8154.1	1286.9	82.4	19.25586	
29	2	Weak Positive	-5	70.9	7458.9	7009.0	2432.0	70.9	16.69311	
30	3	Weak Positive	-5	70.2	7388.4	6938.5	2502.5	70.2	16.53533	
31	1	Weak Positive	-6	86.6	9010.8	8560.9	880.1	86.6	20.16628	
32	2	Weak Positive	-6	86.5	9004.2	8554.3	886.7	86.5	20.15151	
33	3	Weak Positive	-6	87.2	9074.7	8624.8	816.2	87.2	20.30929	
34	1	Weak Positive	-7	80.6	8424.6	7974.7	1466.3	80.6	18.85436	
35	2	Weak Positive	-7	69.2	7294.8	6844.9	2596.1	69.2	16.32585	
36	3	Weak Positive	-7	92.1	9561.9	9112.0	329.0	92.1	21.39965	
37	1	Weak Positive	-8	98.9	10229.7	9779.8	-338.8	98.9	22.8942	
38	2	Weak Positive	-8	105.2	10855.8	10405.9	-964.9	105.2	24.29542	
39	3	Weak Positive	-8	102.2	10562.4	10112.5	-671.5	102.2	23.63878	
40	1	Weak Positive	-9	85.9	8949	8499.1	941.9	85.9	20.02798	
41	2	Weak Positive	-9	89.7	9319.5	8869.6	571.4	89.7	20.85716	
42	3	Weak Positive	-9	98.0	10142.1	9692.2	-251.2	98.0	22.69815	
43	1	Weak Positive	-10	86.8	9033.9	8584.0	857.0	86.8	20.21798	
44	2	Weak Positive	-10	88.8	9231.3	8781.4	659.6	88.8	20.65977	
45	3	Weak Positive	-10	95.5	9894.6	9444.7	-3.7	95.5	22.14424	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay		
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	119.22	369.58	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	123.63	383.25	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	129.24	400.64	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	207.64	643.68	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	390.08	1209.25	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	211.04	654.22	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	932.98	2892.24	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	987.67	3061.78	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	957.80	2969.18	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2132.80	6611.68	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2264.30	7019.33	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2334.30	7236.33	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3163.20	9805.92	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3045.40	9440.74	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3318.50	10287.35	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3153.90	9777.09	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3541.70	10979.27	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3323.60	10303.16	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3301.60	10234.96	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3145.60	9751.36	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3214.00	9963.40	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	2848.80	8831.28	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3262.40	10113.44	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3256.50	10095.15	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	178.53	553.44	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	172.56	534.94	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	156.97	486.61	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	223.73	693.56	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	201.14	623.53	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	201.69	625.24	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	873.62	2708.22	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	851.86	2640.77	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	859.65	2664.92	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2632.30	8160.13	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2754.20	8538.02	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2773.20	8596.92	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3633.90	11265.09	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3423.60	10613.16	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3406.00	10558.60	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3677.00	11398.70	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3317.30	10283.63	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3561.30	11040.03	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3611.40	11195.34	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3617.30	11213.63	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3712.10	11507.51	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3233.50	10023.85	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3613.40	11201.54	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3232.50	10020.75	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-0.8	369.582	-80.3	9521.3	-0.8	0.827129
47	2	Unknown 1	-3.01424	-0.7	383.253	-66.6	9507.6	-0.7	0.857725
48	3	Unknown 1	-3.01424	-0.5	400.644	-49.2	9490.2	-0.5	0.896646
49	1	Unknown 1	-4.01424	2.0	643.684	193.8	9247.2	2.0	1.440573
50	2	Unknown 1	-4.01424	7.7	1209.248	759.4	8681.6	7.7	2.706312
51	3	Unknown 1	-4.01424	2.1	654.224	204.3	9236.7	2.1	1.464162
52	1	Unknown 1	-5.01424	24.7	2892.238	2442.4	6998.7	24.7	6.472865
53	2	Unknown 1	-5.01424	26.4	3061.777	2611.9	6829.1	26.4	6.852296
54	3	Unknown 1	-5.01424	25.5	2969.18	2519.3	6921.7	25.5	6.645062
55	1	Unknown 1	-6.01424	62.3	6611.68	6161.8	3279.2	62.3	14.79702
56	2	Unknown 1	-6.01424	66.4	7019.33	6569.5	2871.6	66.4	15.70935
57	3	Unknown 1	-6.01424	68.6	7236.33	6786.5	2654.6	68.6	16.195
58	1	Unknown 1	-7.01424	94.6	9805.92	9356.0	85.0	94.6	21.94577
59	2	Unknown 1	-7.01424	90.9	9440.74	8990.9	450.2	90.9	21.1285
60	3	Unknown 1	-7.01424	99.5	10287.35	9837.5	-396.5	99.5	23.02322
61	1	Unknown 1	-8.01424	94.3	9777.09	9327.2	113.8	94.3	21.88125
62	2	Unknown 1	-8.01424	106.5	10979.27	10529.4	-1088.4	106.5	24.57175
63	3	Unknown 1	-8.01424	99.6	10303.16	9853.3	-412.3	99.6	23.0586
64	1	Unknown 1	-9.01424	98.9	10234.96	9785.1	-344.1	98.9	22.90597
65	2	Unknown 1	-9.01424	94.0	9751.36	9301.5	139.5	94.0	21.82367
66	3	Unknown 1	-9.01424	96.2	9963.4	9513.5	-72.5	96.2	22.29822
67	1	Unknown 1	-10.01424	84.7	8831.28	8381.4	1059.6	84.7	19.76452
68	2	Unknown 1	-10.01424	97.7	10113.44	9663.6	-222.5	97.7	22.63401
69	3	Unknown 1	-10.01424	97.5	10095.15	9645.3	-204.3	97.5	22.59307
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	2.5	693.563	243.7	9197.3	2.5	1.552203
74	2	Unknown 2	-4.01424	1.8	623.534	173.7	9267.4	1.8	1.395477
75	3	Unknown 2	-4.01424	1.8	625.239	175.4	9265.7	1.8	1.399293
76	1	Unknown 2	-5.01424	22.8	2708.222	2258.3	7182.7	22.8	6.061035
77	2	Unknown 2	-5.01424	22.2	2640.766	2190.9	7250.1	22.2	5.910068
78	3	Unknown 2	-5.01424	22.4	2664.915	2215.0	7226.0	22.4	5.964113
79	1	Unknown 2	-6.01424	78.0	8160.13	7710.3	1730.8	78.0	18.26247
80	2	Unknown 2	-6.01424	81.8	8538.02	8088.1	1352.9	81.8	19.1082
81	3	Unknown 2	-6.01424	82.4	8596.92	8147.0	1294.0	82.4	19.24002
82	1	Unknown 2	-7.01424	109.3	11265.09	10815.2	-1374.2	109.3	25.21141
83	2	Unknown 2	-7.01424	102.8	10613.16	10163.3	-722.3	102.8	23.75239
84	3	Unknown 2	-7.01424	102.2	10558.6	10108.7	-667.7	102.2	23.63028
85	1	Unknown 2	-8.01424	110.7	11398.7	10948.8	-1507.8	110.7	25.51043
86	2	Unknown 2	-8.01424	99.4	10283.63	9833.8	-392.7	99.4	23.01489
87	3	Unknown 2	-8.01424	107.1	11040.03	10590.2	-1149.1	107.1	24.70773
88	1	Unknown 2	-9.01424	108.6	11195.34	10745.5	-1304.4	108.6	25.05531
89	2	Unknown 2	-9.01424	108.8	11213.63	10763.8	-1322.7	108.8	25.09625
90	3	Unknown 2	-9.01424	111.8	11507.51	11057.6	-1616.6	111.8	25.75395
91	1	Unknown 2	-10.01424	96.8	10023.85	9574.0	-133.0	96.8	22.4335
92	2	Unknown 2	-10.01424	108.7	11201.54	10751.7	-1310.6	108.7	25.06919
93	3	Unknown 2	-10.01424	96.8	10020.75	9570.9	-129.9	96.8	22.42657

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	Corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	587.98	1822.74	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	628.45	1948.20	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	484.94	1503.31	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	832.92	2582.05	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	980.35	3039.09	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	933.52	2893.91	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2424.10	7514.71	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2723.10	8441.61	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2374.60	7361.26	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3648.60	11310.66	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3441.60	10668.96	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3553.90	11017.09	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3644.10	11296.71	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3660.90	11348.79	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3285.80	10185.98	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3211.40	9955.34	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3088.30	9573.73	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3285.10	10183.81	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3697.40	11461.94	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3433.50	10643.85	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3789.30	11746.83	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3239.70	10043.07	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3210.70	9953.17	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	2692.30	8346.13	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	353.22	1094.98	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	427.18	1324.26	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	421.04	1305.22	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	514.09	1593.68	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	626.88	1943.33	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	498.31	1544.76	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2513.50	7791.85	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2641.20	8187.72	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2904.88	9004.88	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3691.20	11442.72	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3127.00	9693.70	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3306.20	10249.22	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3281.60	10172.96	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3194.00	9901.40	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	2960.60	9177.86	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3271.00	10140.10	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3905.70	12107.67	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3198.10	9914.11	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3076.30	9536.53	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3984.20	12351.02	FALSE	contamination
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3000.50	9301.55	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3719.40	11530.14	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3086.40	9567.84	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	2978.60	9233.66	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3453.20	10704.92	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2850.30	8835.93	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3424.90	10617.19	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	122.83	368.49	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	173.04	519.12	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	136.82	410.46	TRUE	
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44200.00	44200.00	TRUE	
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	44953.00	44953.00	TRUE	
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45018.00	45018.00	TRUE	
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	43352.00	43352.00	TRUE	
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	45549.00	45549.00	TRUE	
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45023.00	45023.00	TRUE	

Check the 10% rule: **23.14%** if the ratio of EtOH / Hot is > 10% then there are problems with the assay

corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1822.74	FALSE	precipitate in tube
1948.20	FALSE	precipitate in tube
1503.31	FALSE	precipitate in tube
2582.05	TRUE	
3039.09	TRUE	
2893.91	TRUE	
7514.71	TRUE	
8441.61	TRUE	
7361.26	TRUE	
11310.66	TRUE	
10668.96	TRUE	
11017.09	TRUE	
11296.71	TRUE	
11348.79	TRUE	
10185.98	TRUE	
9955.34	TRUE	
9573.73	TRUE	
10183.81	TRUE	
11461.94	TRUE	
10643.85	TRUE	
11746.83	TRUE	
10043.07	TRUE	
9953.17	TRUE	
8346.13	TRUE	
1094.98	FALSE	precipitate in tube
1324.26	FALSE	precipitate in tube
1305.22	FALSE	precipitate in tube
1593.68	TRUE	
1943.33	TRUE	
1544.76	TRUE	
7791.85	TRUE	
8187.72	TRUE	
9004.88	TRUE	
11442.72	TRUE	
9693.70	TRUE	
10249.22	TRUE	
10172.96	TRUE	
9901.40	TRUE	
9177.86	TRUE	
10140.10	TRUE	
12107.67	TRUE	
9914.11	TRUE	
9536.53	TRUE	
12351.02	FALSE	contamination
9301.55	TRUE	
11530.14	TRUE	
9567.84	TRUE	
9233.66	TRUE	
10704.92	TRUE	
8835.93	TRUE	
10617.19	TRUE	
368.49	TRUE	
519.12	TRUE	
410.46	TRUE	
44200.00	TRUE	
44953.00	TRUE	
45018.00	TRUE	
43352.00	TRUE	
45549.00	TRUE	
45023.00	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EOH)	Ratio Total binding/ Hot	
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	21.6	2582.052	2132.2	7308.8	21.6 5.778665	
98	2	Unknown 3	-4.01424	26.2	3039.085	2589.2	6851.8	26.2 6.801511	
99	3	Unknown 3	-4.01424	24.7	2893.912	2444.0	6997.0	24.7 6.476612	
100	1	Unknown 3	-5.01424	71.4	7514.71	7064.8	2376.2	71.4 16.81802	
101	2	Unknown 3	-5.01424	80.8	8441.61	7991.7	1449.3	80.8 18.89243	
102	3	Unknown 3	-5.01424	69.9	7361.26	6911.4	2529.6	69.9 16.47459	
103	1	Unknown 3	-6.01424	109.8	11310.66	10860.8	-1419.8	109.8 25.3134	
104	2	Unknown 3	-6.01424	103.3	10668.96	10219.1	-778.1	103.3 23.87727	
105	3	Unknown 3	-6.01424	106.8	11017.09	10567.2	-1126.2	106.8 24.65639	
106	1	Unknown 3	-7.01424	109.7	11296.71	10846.8	-1405.8	109.7 25.28218	
107	2	Unknown 3	-7.01424	110.2	11348.79	10898.9	-1457.9	110.2 25.39874	
108	3	Unknown 3	-7.01424	98.4	10185.98	9736.1	-295.1	98.4 22.79635	
109	1	Unknown 3	-8.01424	96.1	9955.34	9505.5	-64.4	96.1 22.28018	
110	2	Unknown 3	-8.01424	92.2	9573.73	9123.9	317.2	92.2 21.42613	
111	3	Unknown 3	-8.01424	98.4	10183.81	9733.9	-292.9	98.4 22.7915	
112	1	Unknown 3	-9.01424	111.3	11461.94	11012.1	-1571.0	111.3 25.65197	
113	2	Unknown 3	-9.01424	103.1	10643.85	10194.0	-753.0	103.1 23.82107	
114	3	Unknown 3	-9.01424	114.2	11746.83	11297.0	-1855.9	114.2 26.28955	
115	1	Unknown 3	-10.01424	97.0	10043.07	9593.2	-152.2	97.0 22.47652	
116	2	Unknown 3	-10.01424	96.1	9953.17	9503.3	-62.3	96.1 22.27532	
117	3	Unknown 3	-10.01424	79.8	8346.13	7896.3	1544.8	79.8 18.67874	
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	11.6	1593.679	1143.8	8297.2	11.6 3.566674	
122	2	Unknown 4	-4.01424	15.1	1943.328	1493.4	7947.6	15.1 4.349193	
123	3	Unknown 4	-4.01424	11.1	1544.761	1094.9	8346.1	11.1 3.457195	
124	1	Unknown 4	-5.01424	74.2	7791.85	7342.0	2099.0	74.2 17.43826	
125	2	Unknown 4	-5.01424	78.2	8187.72	7737.8	1703.2	78.2 18.32422	
126	3	Unknown 4	-5.01424	86.5	9004.88	8555.0	886.0	86.5 20.15304	
127	1	Unknown 4	-6.01424	111.1	11442.72	10992.8	-1551.8	111.1 25.60895	
128	2	Unknown 4	-6.01424	93.5	9693.7	9243.8	197.2	93.5 21.69462	
129	3	Unknown 4	-6.01424	99.1	10249.22	9799.3	-358.3	99.1 22.93788	
130	1	Unknown 4	-7.01424	98.3	10172.96	9723.1	-282.1	98.3 22.76721	
131	2	Unknown 4	-7.01424	95.6	9901.4	9451.5	-10.5	95.6 22.15946	
132	3	Unknown 4	-7.01424	88.2	9177.86	8728.0	713.0	88.2 20.54017	
133	1	Unknown 4	-8.01424	98.0	10140.1	9690.2	-249.2	98.0 22.69367	
134	2	Unknown 4	-8.01424	117.9	12107.67	11657.8	-2216.8	117.9 27.09712	
135	3	Unknown 4	-8.01424	95.7	9914.11	9464.2	-23.2	95.7 22.1879	
136	1	Unknown 4	-9.01424	91.9	9536.53	9086.7	354.4	91.9 21.34287	
137	2	Unknown 4	-9.01424						
138	3	Unknown 4	-9.01424	89.5	9301.55	8851.7	589.3	89.5 20.81699	
139	1	Unknown 4	-10.01424	112.0	11530.14	11080.3	-1639.2	112.0 25.8046	
140	2	Unknown 4	-10.01424	92.2	9567.84	9118.0	323.1	92.2 21.41295	
141	3	Unknown 4	-10.01424	88.8	9233.66	8783.8	657.2	88.8 20.66505	
142	1	—	—	103.7	10704.92	10255.0	-814.0	103.7 23.95775	
143	2	—	—	84.8	8835.93	8386.1	1055.0	84.8 19.77492	
144	3	—	—	102.8	10617.19	10167.3	-726.3	102.8 23.76141	
145	1	-6.00	-0.8	368.49	-81.4	9522.4	-0.8	0.824685	
146	2	-6.00	0.7	519.12	69.2	9371.8	0.7	1.161797	
147	3	-6.00	-0.4	410.46	-39.4	9480.4	-0.4	0.918615	
148	1			44200	43750.1				
149	2			44953	44503.1				
150	3			45018	44568.1				
151	1			43352	42902.1				
152	2			45549	45099.1				
153	3			45023	44573.1				

Prism data												
standard curve				weak positive				CR42343				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	0.59752	0.39612	-0.47225	-3	3.6491	3.7262	5.2145	-3.0	-0.8118	-0.6736	-0.4978	
-6.0	-0.82288	0.70004	-0.39855	-4	28.8277	24.0937	33.0983	-4.0	1.9594	7.6774	2.0660	
-7.0	3.13756	1.86257	1.33822	-5	82.4407	70.8634	70.1506	-5.0	24.6930	26.4071	25.4709	
-8.0	15.22334	13.86247	15.80661	-6	86.5536	86.4868	87.1996	-6.0	62.2977	66.4192	68.6131	
-9.0	62.21622	61.50476	57.74372	-7	80.6269	69.2043	92.1253	-7.0	94.5925	90.9004	99.4599	
-10.0	95.15662	84.58498	82.84863	-8	98.8770	105.2071	102.2407	-8.0	94.3010	106.4554	99.6197	
-11.0	102.05185	105.55275		-9	85.9287	89.6746	97.9914	-9.0	98.9302	94.0408	96.1846	
				-10	86.7871	88.7829	95.4890	-10.0	84.7386	97.7016	97.5167	

CR42344				CR42348				CR42349			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0				-3.0			
-4.0	2.4637	1.7557	1.7729	-4.0	21.5569	26.1777	24.7099	-4.0	11.5642	15.0992	11.0696
-5.0	22.8325	22.1505	22.3947	-5.0	71.4276	80.7989	69.8762	-5.0	74.2296	78.2320	86.4937
-6.0	77.9530	81.7736	82.3691	-6.0	109.8059	103.3181	106.8378	-6.0	111.1410	93.4579	99.0744
-7.0	109.3451	102.7539	102.2023	-7.0	109.6648	110.1914	98.4350	-7.0	98.3034	95.5578	88.2426
-8.0	110.6960	99.4223	107.0697	-8.0	96.1031	92.2450	98.4131	-8.0	97.9711	117.8639	95.6863
-9.0	108.6399	108.8249	111.7961	-9.0	111.3353	103.0642	114.2157	-9.0	91.8689		89.4931
-10.0	96.7958	108.7026	96.7645	-10.0	96.9901	96.0812	79.8335	-10.0	112.0249	92.1854	88.8067

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:			
Run identification:	501		
Assay start date:	9/13/2005		
Tracer lot number:	3559-507		
Specific activity on day of assay:	80.16	Ci/mmole	
Cytosol vial or lot identification:	051905		
Protein (cytosol):	1000	micro gram per tube	
Standard Curve IC50:	1.47E-09	M	
Weak Positive, Max Concentration:	3.00E-02	M	
Weak Positive IC50:	4.19E-05	M	
RBA:	3.51635E-05		
Max Concentration, Unknown 1:	3.00E-02	M	5e-3)
IC50, Unknown 1:	4.62E-06	CR42343	
RBA, Unknown 1:	0.03188%		
Max Concentration, Unknown 2:	3.00E-02	M	(example 5e-3)
IC50, Unknown 2:	4.73E-06	CR42344	
RBA, Unknown 2:	0.03117%		
Max Concentration, Unknown 3:	3.00E-02	M	(example 5e-3)
IC50, Unknown 3:	4.81E-05	CR42348	
RBA, Unknown 3:	0.00306%		
Max Concentration, Unknown 4:	3.00E-02	M	(example 5e-3)
IC50, Unknown 4:	2.93E-05	CR42349	
RBA, Unknown 4:	0.00502%		
volume of ethanol counted:	2	mL	protocol calls for counting decanted EtOH supernate
multiply DPM in sample by :	3.1		reflects 100ul of reaction mixture processed
working volume	3.1E+02	uL	

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	9167.7	790.80	Total Binding, solvent control, tubes
Hot	6	44245.0	812.24	Total hot R1881 added to each tube
NSB	6	431.1	57.54	Nonspecific Binding
Specific EtOH	6	8736.6	790.80	

Assay Characterization Values	
EtOH / Hot	0.21 less than 0.1?
NSB / EtOH	0.05 around 0.25 ?

ate

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	Triancelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2622.70	8130.37	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2777.70	8610.87	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2866.20	8885.22	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	140.33	420.99	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	134.99	404.97	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.90	398.70	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	174.70	541.57	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	196.30	608.53	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	157.19	487.29	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	526.37	1631.75	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	527.40	1634.94	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	473.69	1468.44	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	1920.10	5952.31	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	1750.00	5425.00	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	1918.00	5945.80	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2477.90	7681.49	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2599.90	8059.69	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2668.40	8272.04	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2645.80	8201.98	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3414.70	10585.57	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2728.90	8459.59	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	235.94	707.82	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	231.06	693.18	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	237.82	713.46	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1161.50	3484.50	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1024.26	3072.78	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1021.76	3065.28	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2459.20	7377.60	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2408.80	7226.40	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2400.30	7200.90	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2904.60	8713.80	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2970.50	8911.50	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2889.70	8669.10	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3001.70	9005.10	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2984.50	8953.50	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3124.60	9373.80	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3434.50	10303.50	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3537.00	10611.00	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2998.10	8994.30	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3534.30	10602.90	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3278.60	9835.80	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	2926.30	8778.90	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3157.60	9472.80	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3252.00	9756.00	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3002.00	9006.00	TRUE	

Check the 10% rule:	20.72%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EOH)	Ratio Total binding/ Hot	
1	1			88.1	8130.37	7699.3	88.1	18.37579	
2	2			93.6	8610.87	8179.8	93.6	19.46179	
3	3			96.8	8885.22	8454.1	96.8	20.08186	
4	1	-6.00	-0.1	420.99	-10.1	8315.6	-0.1	0.951497	
5	2	-6.00	-0.3	404.97	-26.1	8331.6	-0.3	0.91529	
6	3	-6.00	0.0	398.7	-32.4	8337.9	-0.4	0.901119	
7	1	cold R1881	-7.01	1.3	541.57	110.5	1.3	1.224025	
8	2	cold R1881	-7.01	2.0	608.53	177.4	2.0	1.375364	
9	3	cold R1881	-7.01	0.6	487.289	56.2	0.6	1.101343	
10	1	cold R1881	-8.01	13.7	1631.747	1200.7	13.7	3.687981	
11	2	cold R1881	-8.01	13.8	1634.94	1203.9	13.8	3.695197	
12	3	cold R1881	-8.01	11.9	1468.439	1037.3	11.9	3.318881	
13	1	cold R1881	-9.01	63.2	5952.31	5521.2	63.2	13.45307	
14	2	cold R1881	-9.01	57.2	5425	4993.9	57.2	12.26127	
15	3	cold R1881	-9.01	63.1	5945.8	5514.7	63.1	13.43835	
16	1	cold R1881	-10.01	83.0	7681.49	7250.4	83.0	17.36126	
17	2	cold R1881	-10.01	87.3	8059.69	7628.6	87.3	18.21605	
18	3	cold R1881	-10.01	89.7	8272.04	7841.0	89.7	18.69599	
19	1	cold R1881	-11.01	88.9	8201.98	7770.9	88.9	18.53764	
20	2	cold R1881	-11.01	116.2	10585.57	10154.5	116.2	23.9249	
21	3	cold R1881	-11.01	91.9	8459.59	8028.5	91.9	19.11988	
22	1	Weak Positive	-3	3.2	707.82	276.7	3.2	1.599774	
23	2	Weak Positive	-3	3.0	693.18	262.1	3.0	1.566686	
24	3	Weak Positive	-3	3.2	713.46	282.4	3.2	1.612521	
25	1	Weak Positive	-4	34.9	3484.5	3053.4	34.9	7.875466	
26	2	Weak Positive	-4	30.2	3072.78	2641.7	30.2	6.94492	
27	3	Weak Positive	-4	30.2	3065.28	2634.2	30.2	6.927969	
28	1	Weak Positive	-5	79.5	7377.6	6946.5	79.5	16.67443	
29	2	Weak Positive	-5	77.8	7226.4	6795.3	77.8	16.33269	
30	3	Weak Positive	-5	77.5	7200.9	6769.8	77.5	16.27506	
31	1	Weak Positive	-6	94.8	8713.8	8282.7	94.8	19.69443	
32	2	Weak Positive	-6	97.1	8911.5	8480.4	97.1	20.14126	
33	3	Weak Positive	-6	94.3	8669.1	8238.0	94.3	19.5934	
34	1	Weak Positive	-7	98.1	9005.1	8574.0	98.1	20.35281	
35	2	Weak Positive	-7	97.5	8953.5	8522.4	97.5	20.23618	
36	3	Weak Positive	-7	102.4	9373.8	8942.7	102.4	21.18612	
37	1	Weak Positive	-8	113.0	10303.5	9872.4	113.0	23.28738	
38	2	Weak Positive	-8	116.5	10611	10179.9	116.5	23.98237	
39	3	Weak Positive	-8	98.0	8994.3	8563.2	98.0	20.3284	
40	1	Weak Positive	-9	116.4	10602.9	10171.8	116.4	23.96406	
41	2	Weak Positive	-9	107.6	9835.8	9404.7	107.6	22.23031	
42	3	Weak Positive	-9	95.5	8778.9	8347.8	95.5	19.84156	
43	1	Weak Positive	-10	103.5	9472.8	9041.7	103.5	21.40988	
44	2	Weak Positive	-10	106.7	9756	9324.9	106.7	22.04995	
45	3	Weak Positive	-10	98.1	9006	8574.9	98.1	20.35484	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E Supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	Irradiation Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	111.87	346.80	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	118.45	367.20	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	121.28	375.97	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	257.55	798.41	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	230.03	713.09	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	234.70	727.57	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	1038.24	3218.54	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	974.89	3022.16	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	819.11	2539.24	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2637.80	8177.18	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2411.70	7476.27	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2459.80	7625.38	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3483.10	10797.61	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3295.40	10215.74	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3544.90	10989.19	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3756.30	11644.53	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3647.90	11308.49	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3345.20	10370.12	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3677.20	11399.32	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3287.30	10190.63	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3070.80	9519.48	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3559.50	11034.45	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3424.90	10617.19	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3023.90	9374.09	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	167.18	518.26	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	194.54	603.07	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	206.66	640.65	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	197.53	612.34	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	205.16	636.00	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	221.19	685.69	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	694.30	2152.33	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	763.19	2365.89	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	937.36	2905.82	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2522.90	7820.99	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2872.90	8905.99	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2918.50	9047.35	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3156.60	9785.46	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3366.30	10435.53	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3673.10	11386.61	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3654.90	11330.19	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3695.50	11456.05	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3683.80	11419.78	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3640.20	11284.62	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3745.90	11612.29	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3156.30	9784.53	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3147.70	9757.87	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3536.90	10964.39	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3643.30	11294.23	TRUE	

Check the 10% rule: 20.72% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Values for analysis by nonlinear regression

Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EIOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-1.0	346.797	-84.3	8389.8	-1.0	0.783811
47	2	Unknown 1	-3.01424	-0.7	367.195	-63.9	8369.4	-0.7	0.829913
48	3	Unknown 1	-3.01424	-0.6	375.968	-55.1	8360.6	-0.6	0.849741
49	1	Unknown 1	-4.01424	4.2	798.405	367.3	7938.2	4.2	1.804509
50	2	Unknown 1	-4.01424	3.2	713.093	282.0	8023.5	3.2	1.611692
51	3	Unknown 1	-4.01424	3.4	727.57	296.5	8009.0	3.4	1.644412
52	1	Unknown 1	-5.01424	31.9	3218.544	2787.5	5518.0	31.9	7.274368
53	2	Unknown 1	-5.01424	29.7	3022.159	2591.1	5714.4	29.7	6.83051
54	3	Unknown 1	-5.01424	24.1	2539.241	2108.2	6197.4	24.1	5.739046
55	1	Unknown 1	-6.01424	88.7	8177.18	7746.1	559.4	88.7	18.48159
56	2	Unknown 1	-6.01424	80.6	7476.27	7045.2	1260.3	80.6	16.89743
57	3	Unknown 1	-6.01424	82.3	7625.38	7194.3	1111.2	82.3	17.23444
58	1	Unknown 1	-7.01424	118.7	10797.61	10366.5	-2061.0	118.7	24.40414
59	2	Unknown 1	-7.01424	112.0	10215.74	9784.7	-1479.1	112.0	23.08903
60	3	Unknown 1	-7.01424	120.8	10989.19	10558.1	-2252.6	120.8	24.83713
61	1	Unknown 1	-8.01424	128.4	11644.53	11213.4	-2907.9	128.4	26.3183
62	2	Unknown 1	-8.01424	124.5	11308.49	10877.4	-2571.9	124.5	25.5588
63	3	Unknown 1	-8.01424	113.8	10370.12	9939.0	-1633.5	113.8	23.43795
64	1	Unknown 1	-9.01424	125.5	11399.32	10968.2	-2662.7	125.5	25.76409
65	2	Unknown 1	-9.01424	111.7	10190.63	9759.5	-1454.0	111.7	23.03227
66	3	Unknown 1	-9.01424	104.0	9519.48	9088.4	-782.9	104.0	21.51538
67	1	Unknown 1	-10.01424	121.4	11034.45	10603.4	-2297.9	121.4	24.93943
68	2	Unknown 1	-10.01424	116.6	10617.19	10186.1	-1880.6	116.6	23.99636
69	3	Unknown 1	-10.01424	102.4	9374.09	8943.0	-637.5	102.4	21.18678
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	2.1	612.343	181.3	8124.2	2.1	1.383982
74	2	Unknown 2	-4.01424	2.3	635.996	204.9	8100.6	2.3	1.437442
75	3	Unknown 2	-4.01424	2.9	685.689	254.6	8050.9	2.9	1.549755
76	1	Unknown 2	-5.01424	19.7	2152.33	1721.2	6584.3	19.7	4.864572
77	2	Unknown 2	-5.01424	22.1	2365.889	1934.8	6370.7	22.1	5.347246
78	3	Unknown 2	-5.01424	28.3	2905.816	2474.7	5830.8	28.3	6.567558
79	1	Unknown 2	-6.01424	84.6	7820.99	7389.9	915.6	84.6	17.67655
80	2	Unknown 2	-6.01424	97.0	8905.99	8474.9	-169.4	97.0	20.12881
81	3	Unknown 2	-6.01424	98.6	9047.35	8616.3	-310.8	98.6	20.4483
82	1	Unknown 2	-7.01424	107.1	9785.46	9354.4	-1048.9	107.1	22.11653
83	2	Unknown 2	-7.01424	114.5	10435.53	10004.4	-1698.9	114.5	23.58578
84	3	Unknown 2	-7.01424	125.4	11386.61	10955.5	-2650.0	125.4	25.73536
85	1	Unknown 2	-8.01424	124.8	11330.19	10899.1	-2593.6	124.8	25.60784
86	2	Unknown 2	-8.01424	126.2	11456.05	11025.0	-2719.5	126.2	25.8923
87	3	Unknown 2	-8.01424	125.8	11419.78	10988.7	-2683.2	125.8	25.81033
88	1	Unknown 2	-9.01424	124.2	11284.62	10853.5	-2548.0	124.2	25.50485
89	2	Unknown 2	-9.01424	128.0	11612.29	11181.2	-2875.7	128.0	26.24543
90	3	Unknown 2	-9.01424	107.1	9784.53	9353.4	-1047.9	107.1	22.11443
91	1	Unknown 2	-10.01424	106.8	9757.87	9326.8	-1021.3	106.8	22.05418
92	2	Unknown 2	-10.01424	120.6	10964.39	10533.3	-2227.8	120.6	24.78108
93	3	Unknown 2	-10.01424	124.3	11294.23	10863.1	-2557.6	124.3	25.52657

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	493.56	1530.04	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	490.89	1521.76	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	564.27	1749.24	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	847.49	2627.22	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	912.94	2830.11	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	879.21	2725.55	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2713.60	8412.16	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2783.10	8627.61	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2489.40	7717.14	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3544.00	10986.40	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3454.10	10707.71	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3149.20	9762.52	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3786.50	11738.15	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3776.30	11706.53	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3223.60	9993.16	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	1825.40	5658.74	FALSE	spill
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3308.40	10256.04	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3265.70	10123.67	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3320.30	10292.93	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2956.70	9165.77	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2902.60	8998.06	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3740.20	11594.62	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3811.60	11815.96	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3209.60	9949.76	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	350.11	1085.34	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	384.17	1190.93	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	433.44	1343.66	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	514.01	1593.43	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	418.81	1298.31	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	427.83	1326.27	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2877.60	8920.56	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2435.70	7550.67	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2339.40	7252.14	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3098.10	9604.11	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	2715.30	8417.43	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	2622.20	8128.82	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	2872.20	8903.82	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	2855.20	8851.12	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	2746.90	8515.39	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3770.40	11688.24	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3854.90	11950.19	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3109.00	9637.90	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3696.40	11458.84	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	2533.60	7854.16	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	2485.40	7704.74	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3778.50	11713.35	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3105.70	9627.67	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3190.50	9890.55	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3011.50	9335.65	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3138.00	9727.80	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3327.80	10316.18	TRUE	
145	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	182.20	546.60	TRUE		
146	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	131.95	395.85	TRUE		
147	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	139.81	419.43	TRUE		
148	1	none	Hot	—	—	—	30	—	—	—	—	—	44525.00	44525.00	TRUE		
149	2	none	Hot	—	—	—	30	—	—	—	—	—	43262.00	43262.00	TRUE		
150	3	none	Hot	—	—	—	30	—	—	—	—	—	44673.00	44673.00	TRUE		
151	1	none	Hot	—	—	—	30	—	—	—	—	—	44235.00	44235.00	TRUE		
152	2	none	Hot	—	—	—	30	—	—	—	—	—	45395.00	45395.00	TRUE		
153	3	none	Hot	—	—	—	30	—	—	—	—	—	43380.00	43380.00	TRUE		

		Values for analysis by nonlinear regression						
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424					
95	2	Unknown 3	-3.01424					
96	3	Unknown 3	-3.01424					
97	1	Unknown 3	-4.01424	25.1	2627.219	2196.1	6109.4	5.937889
98	2	Unknown 3	-4.01424	27.5	2830.114	2399.0	5906.5	6.396461
99	3	Unknown 3	-4.01424	26.3	2725.551	2294.5	6011.0	6.160133
100	1	Unknown 3	-5.01424	91.4	8412.16	7981.1	324.4	19.01268
101	2	Unknown 3	-5.01424	93.8	8627.61	8196.5	109.0	19.49963
102	3	Unknown 3	-5.01424	83.4	7717.14	7286.1	1019.5	17.44184
103	1	Unknown 3	-6.01424	120.8	10986.4	10555.3	-2249.8	120.8 24.83083
104	2	Unknown 3	-6.01424	117.6	10707.71	10276.6	-1971.1	117.6 24.20095
105	3	Unknown 3	-6.01424	106.8	9762.52	9331.4	-1025.9	106.8 22.06469
106	1	Unknown 3	-7.01424	129.4	11738.15	11307.1	-3001.6	129.4 26.52989
107	2	Unknown 3	-7.01424	129.1	11706.53	11275.4	-2969.9	129.1 26.45842
108	3	Unknown 3	-7.01424	109.4	9993.16	9562.1	-1256.6	109.4 22.58596
109	1	Unknown 3	-8.01424					
110	2	Unknown 3	-8.01424	112.5	10256.04	9825.0	-1519.4	112.5 23.18011
111	3	Unknown 3	-8.01424	110.9	10123.67	9692.6	-1387.1	110.9 22.88094
112	1	Unknown 3	-9.01424	112.9	10292.93	9861.8	-1556.3	112.9 23.26349
113	2	Unknown 3	-9.01424	100.0	9165.77	8734.7	-429.2	100.0 20.71595
114	3	Unknown 3	-9.01424	98.1	8998.06	8567.0	-261.5	98.1 20.3369
115	1	Unknown 3	-10.01424	127.8	11594.62	11163.5	-2858.0	127.8 26.20549
116	2	Unknown 3	-10.01424	130.3	11815.96	11384.9	-3079.4	130.3 26.70575
117	3	Unknown 3	-10.01424	109.0	9949.76	9518.7	-1213.2	109.0 22.48787
118	1	Unknown 4	-3.01424					
119	2	Unknown 4	-3.01424					
120	3	Unknown 4	-3.01424					
121	1	Unknown 4	-4.01424	13.3	1593.431	1162.3	7143.2	3.601381
122	2	Unknown 4	-4.01424	9.9	1298.311	867.2	7438.3	2.934368
123	3	Unknown 4	-4.01424	10.2	1326.273	895.2	7410.3	2.997566
124	1	Unknown 4	-5.01424	97.2	8920.56	8489.5	-184.0	97.2 20.16174
125	2	Unknown 4	-5.01424	81.5	7550.67	7119.6	1185.9	81.5 17.06559
126	3	Unknown 4	-5.01424	78.1	7252.14	6821.1	1484.5	78.1 16.39087
127	1	Unknown 4	-6.01424	105.0	9604.11	9173.0	-867.5	105.0 21.70666
128	2	Unknown 4	-6.01424	91.4	8417.43	7986.3	319.2	91.4 19.02459
129	3	Unknown 4	-6.01424	88.1	8128.82	7697.7	607.8	88.1 18.37229
130	1	Unknown 4	-7.01424	97.0	8903.82	8472.7	-167.2	97.0 20.1239
131	2	Unknown 4	-7.01424	96.4	8851.12	8420.0	-114.5	96.4 20.00479
132	3	Unknown 4	-7.01424	92.5	8515.39	8084.3	221.2	92.5 19.24599
133	1	Unknown 4	-8.01424	128.9	11688.24	11257.2	-2951.6	128.9 26.41709
134	2	Unknown 4	-8.01424	131.8	11950.19	11519.1	-3213.6	131.8 27.00913
135	3	Unknown 4	-8.01424	105.4	9637.9	9206.8	-901.3	105.4 21.78303
136	1	Unknown 4	-9.01424	126.2	11458.84	11027.8	-2722.2	126.2 25.89861
137	2	Unknown 4	-9.01424	85.0	7854.16	7423.1	882.4	85.0 17.75152
138	3	Unknown 4	-9.01424	83.3	7704.74	7273.7	1031.9	83.3 17.41381
139	1	Unknown 4	-10.01424	129.1	11713.35	11282.3	-2976.8	129.1 26.47384
140	2	Unknown 4	-10.01424	105.3	9627.67	9196.6	-891.1	105.3 21.75991
141	3	Unknown 4	-10.01424	108.3	9890.55	9459.5	-1154.0	108.3 22.35405
142	1	—	—	101.9	9335.65	8904.6	-599.1	101.9 21.0999
143	2	—	—	106.4	9727.8	9296.7	-991.2	106.4 21.98621
144	3	—	—	113.1	10316.18	9885.1	-1579.6	113.1 23.31604
145	1	-6.00	1.3	546.6	115.5	8190.0	1.3	1.235394
146	2	-6.00	-0.4	395.85	-35.2	8340.7	-0.4	0.894677
147	3	-6.00	-0.1	419.43	-11.7	8317.2	-0.1	0.947972
148	1			44525	44093.9			
149	2			43262	42830.9			
150	3			44673	44241.9			
151	1			44235	43803.9			
152	2			45395	44963.9			
153	3			43380	42948.9			

Prism data												
standard curve				weak positive				CR42343				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	-0.11561	-0.29897	-0.37074	-3	3.1675	2.9999	3.2320	-3.0	-0.9648	-0.7313	-0.6309	
-6.0	1.32214	-0.40336	-0.13346	-4	34.9497	30.2371	30.1512	-4.0	4.2043	3.2278	3.3935	
-7.0	1.26457	2.03100	0.64326	-5	79.5105	77.7799	77.4880	-5.0	31.9055	29.6577	24.1301	
-8.0	13.74285	13.77940	11.87361	-6	94.8048	97.0677	94.2932	-6.0	88.6626	80.6399	82.3466	
-9.0	63.19650	57.16085	63.12198	-7	98.1391	97.5485	102.3593	-7.0	118.6563	111.9962	120.8492	
-10.0	82.98888	87.31780	89.74839	-8	113.0007	116.5204	98.0155	-8.0	128.3503	124.5039	113.7632	
-11.0	88.94647	116.22931	91.89510	-9	116.4277	107.6474	95.5500	-9.0	125.5436	111.7088	104.0267	
				-10	103.4924	106.7340	98.1494	-10.0	121.3672	116.5912	102.3626	

CR42344				CR42348				CR42349			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0				-3.0			
-4.0	2.0746	2.3454	2.9142	-4.0	25.1371	27.4595	26.2627	-4.0	13.3043	9.9263	10.2464
-5.0	19.7015	22.1459	28.3260	-5.0	91.3522	93.8183	83.3969	-5.0	97.1714	81.4915	78.0745
-6.0	84.5856	97.0046	98.6227	-6.0	120.8173	117.6273	106.8086	-6.0	104.9954	91.4125	88.1091
-7.0	107.0712	114.5119	125.3981	-7.0	129.4219	129.0599	109.4485	-7.0	96.9798	96.3766	92.5338
-8.0	124.7523	126.1929	125.7778	-8.0		112.4575	110.9423	-8.0	128.8506	131.8489	105.3822
-9.0	124.2307	127.9813	107.0605	-9.0	112.8797	99.9781	98.0585	-9.0	126.2249	84.9653	83.2550
-10.0	106.7554	120.5653	124.3407	-10.0	127.7790	130.3125	108.9518	-10.0	129.1380	105.2651	108.2740

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:	502	
Run identification:	9/14/2005	
Assay start date:	3559-507	
Tracer lot number:	80.14	Ci/mmole
Specific activity on day of assay:	051905	
Cytosol vial or lot identification:	1000	micro gram per tube
Protein (cytosol):		
Standard Curve IC50:	1.59E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.02E-05	M
RBA:	5.26455E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	2.21E-06	CR42343
RBA, Unknown 1:	0.07194%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	2.29E-06	CR42344
RBA, Unknown 2:	0.06955%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	2.25E-05	CR42348
RBA, Unknown 3:	0.00707%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	1.62E-05	CR42349
RBA, Unknown 4:	0.00983%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11075.2	983.86	Total Binding, solvent control, tubes
Hot	6	44928.2	1147.86	Total hot R1881 added to each tube
NSB	6	483.8	49.90	Nonspecific Binding
Specific EtOH	6	10591.3	983.86	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)											Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	100
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	100
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	100
7	1	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	100
8	2	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	100
9	3	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	100
10	1	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	100
11	2	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	100
12	3	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	100
13	1	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	100
14	2	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	100
15	3	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	100
16	1	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	100
17	2	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	100
18	3	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	100
19	1	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	100
20	2	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	100
21	3	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	100
22	1	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	100
23	2	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	100
24	3	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	100
25	1	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	100
26	2	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	100
27	3	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	100
28	1	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	100
29	2	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	100
30	3	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	100
31	1	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	100
32	2	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	100
33	3	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	100
34	1	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	100
35	2	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	100
36	3	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	100
37	1	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	100
38	2	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	100
39	3	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	100
40	1	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	100
41	2	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	100
42	3	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	100
43	1	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	100
44	2	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	100
45	3	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	100

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
1	1			99.3	11005.31	10521.5	-414.0	99.3	24.49535
2	2			82.9	9267.45	8783.6	1323.9	82.9	20.62726
3	3			98.2	10881.93	10398.1	-290.6	98.2	24.22073
4	1	-6.00	-0.3	453.15	-30.7	10138.2	-0.3	1.00861	
5	2	-6.00	-0.6	423.45	-60.4	10167.9	-0.6	0.942505	
6	3	-6.00	0.0	471.93	-11.9	10119.4	-0.1	1.05041	
7	1	cold R1881	-7.01	1.4	628.773	145.0	9962.6	1.4	1.399507
8	2	cold R1881	-7.01	1.3	626.634	142.8	9964.7	1.3	1.394746
9	3	cold R1881	-7.01	2.2	715.976	232.2	9875.4	2.2	1.593602
10	1	cold R1881	-8.01	12.7	1825.776	1342.0	8765.6	12.7	4.063767
11	2	cold R1881	-8.01	13.7	1935.919	1452.1	8655.4	13.7	4.308921
12	3	cold R1881	-8.01	13.3	1895.991	1412.2	8695.4	13.3	4.22005
13	1	cold R1881	-9.01	61.9	7036.38	6552.6	3555.0	61.9	15.6614
14	2	cold R1881	-9.01	59.9	6828.68	6344.9	3762.7	59.9	15.19911
15	3	cold R1881	-9.01	63.0	7159.76	6675.9	3431.6	63.0	15.93602
16	1	cold R1881	-10.01	94.0	10444.52	9960.7	146.8	94.0	23.24715
17	2	cold R1881	-10.01	92.7	10298.82	9815.0	292.5	92.7	22.92286
18	3	cold R1881	-10.01	95.4	10589.91	10106.1	1.4	95.4	23.57076
19	1	cold R1881	-11.01	104.9	11590.59	11106.8	-999.2	104.9	25.79805
20	2	cold R1881	-11.01	103.4	11434.04	10950.2	-842.7	103.4	25.4496
21	3	cold R1881	-11.01	99.0	10972.76	10488.9	-381.4	99.0	24.4229
22	1	Weak Positive	-3	3.6	860.73	376.9	9730.6	3.6	1.915792
23	2	Weak Positive	-3	2.7	767.73	283.9	9823.6	2.7	1.708794
24	3	Weak Positive	-3	3.7	878.16	394.3	9713.2	3.7	1.954587
25	1	Weak Positive	-4	29.7	3629.4	3145.6	6961.9	29.7	8.078229
26	2	Weak Positive	-4	28.0	3444.9	2961.1	7146.4	28.0	7.667573
27	3	Weak Positive	-4	29.0	3550.8	3067.0	7040.5	29.0	7.903283
28	1	Weak Positive	-5	68.7	7756.5	7272.7	2834.8	68.7	17.26423
29	2	Weak Positive	-5	78.5	8794.5	8310.7	1796.8	78.5	19.57458
30	3	Weak Positive	-5	62.8	7136.1	6652.3	3455.2	62.8	15.88335
31	1	Weak Positive	-6	99.1	10977.3	10493.5	-386.0	99.1	24.433
32	2	Weak Positive	-6	99.8	11056.2	10572.4	-464.9	99.8	24.60862
33	3	Weak Positive	-6	92.7	10302.3	9818.5	289.0	92.7	22.9306
34	1	Weak Positive	-7	84.3	9414.6	8930.8	1176.7	84.3	20.95478
35	2	Weak Positive	-7	83.7	9345.9	8862.1	1245.4	83.7	20.80187
36	3	Weak Positive	-7	74.6	8385.3	7901.5	2206.0	74.6	18.66379
37	1	Weak Positive	-8	93.5	10386.3	9902.5	205.0	93.5	23.11757
38	2	Weak Positive	-8	98.1	10877.1	10393.3	-285.8	98.1	24.20998
39	3	Weak Positive	-8	78.5	8798.7	8314.9	1792.6	78.5	19.58393
40	1	Weak Positive	-9	83.2	9296.7	8812.9	1294.6	83.2	20.69236
41	2	Weak Positive	-9	82.4	9206.1	8722.3	1385.2	82.4	20.49071
42	3	Weak Positive	-9	77.7	8710.5	8226.7	1880.8	77.7	19.38762
43	1	Weak Positive	-10	97.4	10801.5	10317.7	-210.2	97.4	24.04171
44	2	Weak Positive	-10	76.9	8633.4	8149.6	1957.9	76.9	19.21601
45	3	Weak Positive	-10	78.8	8825.4	8341.6	1765.9	78.8	19.64336

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay		
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	132.13	409.60	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	136.31	422.56	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	132.33	410.22	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	239.14	741.33	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	253.91	787.12	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	231.55	717.81	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	1007.41	3122.97	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	1039.02	3220.96	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	1002.51	3107.78	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2308.60	7156.66	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	21.00	65.10	FALSE	spill
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2268.10	7031.11	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3419.90	10601.69	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3523.20	10921.92	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3145.60	9751.36	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	2872.50	8904.75	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3646.20	11303.22	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3050.20	9455.62	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3174.60	9841.26	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3321.90	10297.89	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3126.90	9693.39	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3483.00	10797.30	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3554.40	11018.64	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3316.90	10282.39	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	212.52	658.81	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	169.55	525.61	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	155.47	481.96	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	223.63	693.25	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	241.04	747.22	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	191.12	592.47	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	865.51	2683.08	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	737.37	2285.85	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	665.98	2064.54	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2352.70	7293.37	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2456.60	7615.46	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2834.00	8785.40	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3708.30	11495.73	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3070.40	9518.24	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3739.60	11592.76	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3661.30	11350.03	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3430.80	10635.48	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3481.80	10793.58	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3294.70	10213.57	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3384.90	10493.19	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3342.50	10361.75	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3207.30	9942.63	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3201.10	9923.41	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3120.80	9674.48	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-0.7	409.603	-74.2	10181.7	-0.7	0.911684
47	2	Unknown 1	-3.01424	-0.6	422.561	-61.3	10168.8	-0.6	0.940526
48	3	Unknown 1	-3.01424	-0.7	410.223	-73.6	10181.1	-0.7	0.913064
49	1	Unknown 1	-4.01424	2.4	741.334	257.5	9850.0	2.4	1.650043
50	2	Unknown 1	-4.01424	2.9	787.121	303.3	9804.2	2.9	1.751954
51	3	Unknown 1	-4.01424	2.2	717.805	234.0	9873.5	2.2	1.597673
52	1	Unknown 1	-5.01424	24.9	3122.971	2639.2	7468.4	24.9	6.951031
53	2	Unknown 1	-5.01424	25.8	3220.962	2737.1	7370.4	25.8	7.169137
54	3	Unknown 1	-5.01424	24.8	3107.781	2624.0	7483.6	24.8	6.917222
55	1	Unknown 1	-6.01424	63.0	7156.66	6672.8	3434.7	63.0	15.92912
56	2	Unknown 1	-6.01424						
57	3	Unknown 1	-6.01424	61.8	7031.11	6547.3	3560.2	61.8	15.64967
58	1	Unknown 1	-7.01424	95.5	10601.69	10117.9	-10.3	95.5	23.59698
59	2	Unknown 1	-7.01424	98.6	10921.92	10438.1	-330.6	98.6	24.30974
60	3	Unknown 1	-7.01424	87.5	9751.36	9267.5	840.0	87.5	21.70434
61	1	Unknown 1	-8.01424	79.5	8904.75	8420.9	1686.6	79.5	19.81997
62	2	Unknown 1	-8.01424	102.2	11303.22	10819.4	-711.9	102.2	25.15843
63	3	Unknown 1	-8.01424	84.7	9455.62	8971.8	1135.7	84.7	21.04608
64	1	Unknown 1	-9.01424	88.3	9841.26	9357.4	750.1	88.3	21.90443
65	2	Unknown 1	-9.01424	92.7	10297.89	9814.1	293.5	92.7	22.92079
66	3	Unknown 1	-9.01424	87.0	9693.39	9209.6	898.0	87.0	21.57531
67	1	Unknown 1	-10.01424	97.4	10797.3	10313.5	-206.0	97.4	24.03236
68	2	Unknown 1	-10.01424	99.5	11018.64	10534.8	-427.3	99.5	24.52502
69	3	Unknown 1	-10.01424	92.5	10282.39	9798.6	309.0	92.5	22.88629
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	2.0	693.253	209.4	9898.1	2.0	1.543025
74	2	Unknown 2	-4.01424	2.5	747.224	263.4	9844.1	2.5	1.663153
75	3	Unknown 2	-4.01424	1.0	592.472	108.7	9998.9	1.0	1.318709
76	1	Unknown 2	-5.01424	20.8	2683.081	2199.3	7908.3	20.8	5.971935
77	2	Unknown 2	-5.01424	17.0	2285.847	1802.0	8305.5	17.0	5.087782
78	3	Unknown 2	-5.01424	14.9	2064.538	1580.7	8526.8	14.9	4.595198
79	1	Unknown 2	-6.01424	64.3	7293.37	6809.6	3298.0	64.3	16.2334
80	2	Unknown 2	-6.01424	67.3	7615.46	7131.6	2975.9	67.3	16.9503
81	3	Unknown 2	-6.01424	78.4	8785.4	8301.6	1805.9	78.4	19.55433
82	1	Unknown 2	-7.01424	104.0	11495.73	11011.9	-904.4	104.0	25.58691
83	2	Unknown 2	-7.01424	85.3	9518.24	9034.4	1073.1	85.3	21.18546
84	3	Unknown 2	-7.01424	104.9	11592.76	11108.9	-1001.4	104.9	25.80288
85	1	Unknown 2	-8.01424	102.6	11350.03	10866.2	-758.7	102.6	25.26262
86	2	Unknown 2	-8.01424	95.8	10635.48	10151.7	-44.1	95.8	23.67219
87	3	Unknown 2	-8.01424	97.3	10793.58	10309.8	-202.2	97.3	24.02408
88	1	Unknown 2	-9.01424	91.9	10213.57	9729.8	377.8	91.9	22.73311
89	2	Unknown 2	-9.01424	94.5	10493.19	10009.4	98.2	94.5	23.35548
90	3	Unknown 2	-9.01424	93.3	10361.75	9877.9	229.6	93.3	23.06293
91	1	Unknown 2	-10.01424	89.3	9942.63	9458.8	648.7	89.3	22.13006
92	2	Unknown 2	-10.01424	89.1	9923.41	9439.6	667.9	89.1	22.08728
93	3	Unknown 2	-10.01424	86.8	9674.48	9190.7	916.9	86.8	21.53322

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.65%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	transcelonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	472.89	1465.96	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	440.13	1364.40	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	533.33	1653.32	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	863.62	2677.22	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	772.46	2394.63	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	761.71	2361.30	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2551.20	7908.72	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2286.70	7088.77	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2703.30	8380.23	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3160.10	9796.31	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3600.20	11160.62	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3535.60	10960.36	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3652.40	11322.44	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3765.10	11671.81	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2943.00	9123.30	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3346.30	10373.53	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3210.20	9951.62	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	2846.90	8825.39	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2891.70	8964.27	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3225.80	9999.98	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3135.30	9719.43	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3254.10	10087.71	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3238.40	10039.04	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3118.10	9666.11	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	326.79	1013.05	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	344.67	1068.48	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	336.02	1041.66	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	540.39	1675.21	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	390.20	1209.62	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	473.67	1468.38	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2398.00	7433.80	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2438.40	7559.04	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2271.10	7040.41	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3737.60	11586.56	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3003.80	9311.78	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3282.60	10176.06	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3233.80	10024.78	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3093.40	9589.54	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3235.60	10030.36	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3612.80	11199.68	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3719.20	11529.52	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3428.20	10627.42	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3476.00	10775.60	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3233.30	10023.23	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3889.40	12057.14	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3724.30	11545.33	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	2971.70	9212.27	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3837.30	11895.63	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3793.00	11758.30	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3724.20	11545.02	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3868.70	11992.97	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	181.52	544.56	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	155.09	465.27	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	181.52	544.56	TRUE	
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44748.00	44748.00	TRUE	
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	43799.00	43799.00	TRUE	
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	43597.00	43597.00	TRUE	
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	45156.00	45156.00	TRUE	
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	46657.00	46657.00	TRUE	
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45612.00	45612.00	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICP)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	20.7	2677.222	2193.4	7914.1	20.7	5.958894
98	2	Unknown 3	-4.01424	18.0	2394.626	1910.8	8196.7	18.0	5.329899
99	3	Unknown 3	-4.01424	17.7	2361.301	1877.5	8230.0	17.7	5.255725
100	1	Unknown 3	-5.01424	70.1	7908.72	7424.9	2682.6	70.1	17.60303
101	2	Unknown 3	-5.01424	62.4	7088.77	6605.0	3502.6	62.4	15.77801
102	3	Unknown 3	-5.01424	74.6	8380.23	7896.4	2211.1	74.6	18.65251
103	1	Unknown 3	-6.01424	87.9	9796.31	9312.5	795.0	87.9	21.80438
104	2	Unknown 3	-6.01424	100.8	11160.62	10676.8	-569.3	100.8	24.84103
105	3	Unknown 3	-6.01424	98.9	10960.36	10476.5	-369.0	98.9	24.3953
106	1	Unknown 3	-7.01424	102.3	11322.44	10838.6	-731.1	102.3	25.20121
107	2	Unknown 3	-7.01424	105.6	11671.81	11188.0	-1080.5	105.6	25.97883
108	3	Unknown 3	-7.01424	81.6	9123.3	8639.5	1468.0	81.6	20.30642
109	1	Unknown 3	-8.01424	93.4	10373.53	9889.7	217.8	93.4	23.08915
110	2	Unknown 3	-8.01424	89.4	9951.62	9467.8	639.7	89.4	22.15007
111	3	Unknown 3	-8.01424	78.8	8825.39	8341.6	1766.0	78.8	19.64333
112	1	Unknown 3	-9.01424	80.1	8964.27	8480.5	1627.1	80.1	19.95245
113	2	Unknown 3	-9.01424	89.8	9999.98	9516.2	591.4	89.8	22.25771
114	3	Unknown 3	-9.01424	87.2	9719.43	9235.6	871.9	87.2	21.63327
115	1	Unknown 3	-10.01424	90.7	10087.71	9603.9	503.6	90.7	22.45297
116	2	Unknown 3	-10.01424	90.2	10039.04	9555.2	552.3	90.2	22.34465
117	3	Unknown 3	-10.01424	86.7	9666.11	9182.3	925.2	86.7	21.51459
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	11.2	1675.209	1191.4	8916.1	11.2	3.728639
122	2	Unknown 4	-4.01424	6.9	1209.62	725.8	9381.7	6.9	2.692342
123	3	Unknown 4	-4.01424	9.3	1468.377	984.6	9123.0	9.3	3.268277
124	1	Unknown 4	-5.01424	65.6	7433.8	6950.0	3157.5	65.6	16.54597
125	2	Unknown 4	-5.01424	66.8	7559.04	7075.2	3032.3	66.8	16.82472
126	3	Unknown 4	-5.01424	61.9	7040.41	6556.6	3550.9	61.9	15.67037
127	1	Unknown 4	-6.01424	104.8	11586.56	11102.7	-995.2	104.8	25.78908
128	2	Unknown 4	-6.01424	83.4	9311.78	8828.0	1279.6	83.4	20.72593
129	3	Unknown 4	-6.01424	91.5	10176.06	9692.2	415.3	91.5	22.64962
130	1	Unknown 4	-7.01424	90.1	10024.78	9541.0	566.6	90.1	22.31291
131	2	Unknown 4	-7.01424	86.0	9589.54	9105.7	1001.8	86.0	21.34416
132	3	Unknown 4	-7.01424	90.1	10030.36	9546.5	561.0	90.1	22.32533
133	1	Unknown 4	-8.01424	101.2	11199.68	10715.9	-608.3	101.2	24.92797
134	2	Unknown 4	-8.01424	104.3	11529.52	11045.7	-938.2	104.3	25.66212
135	3	Unknown 4	-8.01424	95.8	10627.42	10143.6	-36.1	95.8	23.65425
136	1	Unknown 4	-9.01424	97.2	10775.6	10291.8	-184.3	97.2	23.98406
137	2	Unknown 4	-9.01424	90.1	10023.23	9539.4	568.1	90.1	22.30946
138	3	Unknown 4	-9.01424	109.3	12057.14	11573.3	-1465.8	109.3	26.83648
139	1	Unknown 4	-10.01424	104.4	11545.33	11061.5	-954.0	104.4	25.69731
140	2	Unknown 4	-10.01424	82.4	9212.27	8728.5	1379.1	82.4	20.50444
141	3	Unknown 4	-10.01424	107.7	11895.63	11411.8	-1304.3	107.7	26.477
142	1	—	—	106.4	11758.3	11274.5	-1167.0	106.4	26.17133
143	2	—	—	104.4	11545.02	11061.2	-953.7	104.4	25.69662
144	3	—	—	108.7	11992.97	11509.2	-1401.6	108.7	26.69366
145	1	-6.00		0.6	544.56	60.7	10046.8	0.6	1.212068
146	2	-6.00		-0.2	465.27	-18.6	10126.1	-0.2	1.035586
147	3	-6.00		0.6	544.56	60.7	10046.8	0.6	1.212068
148	1				44748	44264.2			
149	2				43799	43315.2			
150	3				43597	43113.2			
151	1				45156	44672.2			
152	2				46657	46173.2			
153	3				45612	45128.2			

Prism data												
standard curve				weak positive				CR42343				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	-0.28958	-0.56999	-0.11226	-3	3.5587	2.6806	3.7232	-3.0	-0.7007	-0.5784	-0.6949	
-6.0	0.57349	-0.17514	0.57349	-4	29.6995	27.9575	28.9574	-4.0	2.4314	2.8637	2.2092	
-7.0	1.36860	1.34840	2.19194	-5	68.6663	78.4667	62.8087	-5.0	24.9180	25.8432	24.7746	
-8.0	12.67031	13.71024	13.33326	-6	99.0760	99.8210	92.7029	-6.0	63.0028		61.8174	
-9.0	61.86713	59.90609	63.03204	-7	84.3215	83.6729	74.6032	-7.0	95.5296	98.5531	87.5011	
-10.0	94.04567	92.67002	95.41840	-8	93.4960	98.1300	78.5064	-8.0	79.5077	102.1532	84.7088	
-11.0	104.86649	103.38840	99.03314	-9	83.2083	82.3529	77.6736	-9.0	88.3499	92.6612	86.9537	
				-10	97.4162	76.9457	78.7585	-10.0	97.3765	99.4663	92.5149	

CR42344					CR42348					CR42349				
conce	nitrate				conce	nitrate				conce	nitrate			
n (log)	y1-U1	y2-U1	y3-U1		n (log)	y1-U1	y2-U1	y3-U1		n (log)	y1-U1	y2-U1	y3-U1	
-3.0					-3.0					-3.0				
-4.0	1.9774	2.4870	1.0259		-4.0	20.7094	18.0412	17.7266		-4.0	11.2487	6.8528	9.2959	
-5.0	20.7647	17.0141	14.9246		-5.0	70.1035	62.3618	74.5553		-5.0	65.6194	66.8019	61.9052	
-6.0	64.2935	67.3346	78.3808		-6.0	87.9255	100.8069	98.9161		-6.0	104.8284	83.3507	91.5110	
-7.0	103.9709	85.3000	104.8870		-7.0	102.3347	105.6333	81.5711		-7.0	90.0826	85.9732	90.1353	
-8.0	102.5952	95.8487	97.3414		-8.0	93.3754	89.3919	78.7584		-8.0	101.1756	104.2899	95.7726	
-9.0	91.8651	94.5052	93.2642		-9.0	80.0696	89.8485	87.1996		-9.0	97.1716	90.0680	109.2715	
-10.0	89.3070	89.1255	86.7752		-10.0	90.6768	90.2173	86.6962		-10.0	104.4392	82.4112	107.7466	

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	504	
Assay start date:	9/20/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.07	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.13E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	1.91E-05	M
RBA:	5.89864E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3
IC50, Unknown 1:	2.71E-05	CR42352
RBA, Unknown 1:	0.00417%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	2.87E-05	CR42353
RBA, Unknown 2:	0.00394%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	1.60E-03	CR42359
RBA, Unknown 3:	0.00007%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	2.83E-05	CR42360
RBA, Unknown 4:	0.00399%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	4	11561.1	609.15	Total Binding, solvent control, tubes
Hot	6	45560.3	732.84	Total hot R1881 added to each tube
NSB	6	438.3	66.36	Nonspecific Binding
Specific EtOH	4	11122.8	609.15	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	transcenenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3706.50	11490.15	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2619.50	8120.45	FALSE	spill
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2696.60	8359.46	FALSE	spill
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	125.22	375.66	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.35	397.05	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	133.07	399.21	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	197.19	611.29	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	187.39	580.91	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	247.36	766.82	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	599.39	1858.11	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	646.80	2005.08	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	596.26	1848.41	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2104.20	6523.02	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2021.60	6266.96	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2091.10	6482.41	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3488.80	10815.28	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3523.40	10922.54	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2830.30	8773.93	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2874.00	8909.40	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3104.90	9625.19	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3228.50	10008.35	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	282.94	848.82	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	263.75	791.25	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	276.53	829.59	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1194.30	3582.90	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	975.73	2927.19	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1162.70	3488.10	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2530.10	7590.30	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2197.40	6592.20	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2463.50	7390.50	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3615.80	10847.40	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3631.50	10894.50	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3276.60	9829.80	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3629.40	10888.20	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3635.60	10906.80	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3307.80	9923.40	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3634.80	10904.40	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3551.20	10653.60	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3730.00	11190.00	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3569.30	10707.90	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3676.00	11028.00	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3668.30	11004.90	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3245.30	9735.90	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3294.00	9882.00	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3650.00	10950.00	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
1	1			99.4	11490.15	11051.9	-367.3	99.4	25.21964
2	2								
3	3								
4	1	-6.00	-0.6	375.66	-62.6	10747.1	-0.6	0.824533	
5	2	-6.00	-0.4	397.05	-41.2	10725.8	-0.4	0.871482	
6	3	-6.00	0.0	399.21	-39.1	10723.6	-0.4	0.876223	
7	1	cold R1881	-7.01	1.6	611.289	173.0	10511.5	1.6	1.341713
8	2	cold R1881	-7.01	1.3	580.909	142.6	10541.9	1.3	1.275032
9	3	cold R1881	-7.01	3.0	766.816	328.6	10356.0	3.0	1.683078
10	1	cold R1881	-8.01	12.8	1858.109	1419.8	9264.7	12.8	4.078348
11	2	cold R1881	-8.01	14.1	2005.08	1566.8	9117.7	14.1	4.400934
12	3	cold R1881	-8.01	12.7	1848.406	1410.1	9274.4	12.7	4.057051
13	1	cold R1881	-9.01	54.7	6523.02	6084.8	4599.8	54.7	14.31732
14	2	cold R1881	-9.01	52.4	6266.96	5828.7	4855.8	52.4	13.7553
15	3	cold R1881	-9.01	54.3	6482.41	6044.2	4640.4	54.3	14.22819
16	1	cold R1881	-10.01	93.3	10815.28	10377.0	307.5	93.3	23.73837
17	2	cold R1881	-10.01	94.3	10922.54	10484.3	200.3	94.3	23.97379
18	3	cold R1881	-10.01	74.9	8773.93	8335.7	2348.9	74.9	19.25783
19	1	cold R1881	-11.01	76.2	8909.4	8471.1	2213.4	76.2	19.55517
20	2	cold R1881	-11.01	82.6	9625.19	9186.9	1497.6	82.6	21.12625
21	3	cold R1881	-11.01	86.0	10008.35	9570.1	1114.5	86.0	21.96724
22	1	Weak Positive	-3	3.7	848.82	410.6	10274.0	3.7	1.863068
23	2	Weak Positive	-3	3.2	791.25	353.0	10331.6	3.2	1.736708
24	3	Weak Positive	-3	3.5	829.59	391.3	10293.2	3.5	1.82086
25	1	Weak Positive	-4	28.3	3582.9	3144.6	7539.9	28.3	7.864078
26	2	Weak Positive	-4	22.4	2927.19	2488.9	8195.6	22.4	6.424865
27	3	Weak Positive	-4	27.4	3488.1	3049.8	7634.7	27.4	7.656002
28	1	Weak Positive	-5	64.3	7590.3	7152.0	3532.5	64.3	16.65989
29	2	Weak Positive	-5	55.3	6592.2	6153.9	4530.6	55.3	14.46917
30	3	Weak Positive	-5	62.5	7390.5	6952.2	3732.3	62.5	16.22135
31	1	Weak Positive	-6	93.6	10847.4	10409.1	275.4	93.6	23.80887
32	2	Weak Positive	-6	94.0	10894.5	10456.2	228.3	94.0	23.91225
33	3	Weak Positive	-6	84.4	9829.8	9391.5	1293.0	84.4	21.57535
34	1	Weak Positive	-7	94.0	10888.2	10449.9	234.6	94.0	23.89842
35	2	Weak Positive	-7	94.1	10906.8	10468.5	216.0	94.1	23.93925
36	3	Weak Positive	-7	85.3	9923.4	9485.1	1199.4	85.3	21.78079
37	1	Weak Positive	-8	94.1	10904.4	10466.1	218.4	94.1	23.93398
38	2	Weak Positive	-8	91.8	10653.6	10215.3	469.2	91.8	23.3835
39	3	Weak Positive	-8	96.7	11190	10751.7	-67.2	96.7	24.56084
40	1	Weak Positive	-9	92.3	10707.9	10269.6	414.9	92.3	23.50268
41	2	Weak Positive	-9	95.2	11028	10589.7	94.8	95.2	24.20527
42	3	Weak Positive	-9	95.0	11004.9	10566.6	117.9	95.0	24.15456
43	1	Weak Positive	-10	83.6	9735.9	9297.6	1386.9	83.6	21.36925
44	2	Weak Positive	-10	84.9	9882	9443.7	1240.8	84.9	21.68992
45	3	Weak Positive	-10	94.5	10950	10511.7	172.8	94.5	24.03406

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay		
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	190.43	590.33	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	238.18	738.36	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	185.60	575.36	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1102.70	3418.37	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1111.10	3444.41	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1117.60	3464.56	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2790.00	8649.00	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2392.20	7415.82	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2762.90	8564.99	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3217.70	9974.87	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3718.40	11527.04	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3036.90	9414.39	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3392.60	10517.06	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	2939.50	9112.45	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3708.30	11495.73	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3208.30	9945.73	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3436.00	10651.60	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3731.70	11568.27	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3707.10	11492.01	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3410.70	10573.17	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3271.40	10141.34	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	2996.30	9288.53	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	2828.20	8767.42	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3737.80	11587.18	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1241.60	3848.96	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1226.90	3803.39	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1113.60	3452.16	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1039.86	3223.57	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1252.70	3883.37	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1189.20	3686.52	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2317.10	7183.01	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2852.40	8842.44	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2829.70	8772.07	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3356.50	10405.15	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2945.90	9132.29	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3596.40	11148.84	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3606.40	11179.84	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	2715.90	8419.29	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3119.40	9670.14	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3522.40	10919.44	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3257.40	10097.94	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3623.10	11231.61	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3654.20	11328.02	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3623.00	11231.30	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3005.90	9318.29	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3729.30	11560.83	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	2935.10	9098.81	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3183.90	9870.09	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	1.4	590.333	152.1	10532.5	1.4	1.295717
47	2	Unknown 1	-3.01424	2.7	738.358	300.1	10384.4	2.7	1.620616
48	3	Unknown 1	-3.01424	1.2	575.36	137.1	10547.4	1.2	1.262853
49	1	Unknown 1	-4.01424	26.8	3418.37	2980.1	7704.4	26.8	7.502952
50	2	Unknown 1	-4.01424	27.0	3444.41	3006.2	7678.4	27.0	7.560107
51	3	Unknown 1	-4.01424	27.2	3464.56	3026.3	7658.2	27.2	7.604334
52	1	Unknown 1	-5.01424	73.8	8649	8210.7	2473.8	73.8	18.98362
53	2	Unknown 1	-5.01424	62.7	7415.82	6977.6	3707.0	62.7	16.27692
54	3	Unknown 1	-5.01424	73.1	8564.99	8126.7	2557.8	73.1	18.79923
55	1	Unknown 1	-6.01424	85.7	9974.87	9536.6	1147.9	85.7	21.89376
56	2	Unknown 1	-6.01424	99.7	11527.04	11088.8	-404.2	99.7	25.30061
57	3	Unknown 1	-6.01424	80.7	9414.39	8976.1	1708.4	80.7	20.66357
58	1	Unknown 1	-7.01424	90.6	10517.06	10078.8	605.7	90.6	23.08381
59	2	Unknown 1	-7.01424	78.0	9112.45	8674.2	2010.4	78.0	20.00084
60	3	Unknown 1	-7.01424	99.4	11495.73	11057.5	-372.9	99.4	25.23188
61	1	Unknown 1	-8.01424	85.5	9945.73	9507.5	1177.1	85.5	21.8298
62	2	Unknown 1	-8.01424	91.8	10651.6	10213.3	471.2	91.8	23.37911
63	3	Unknown 1	-8.01424	100.1	11568.27	11130.0	-445.5	100.1	25.3911
64	1	Unknown 1	-9.01424	99.4	11492.01	11053.8	-369.2	99.4	25.22372
65	2	Unknown 1	-9.01424	91.1	10573.17	10134.9	549.6	91.1	23.20696
66	3	Unknown 1	-9.01424	87.2	10141.34	9703.1	981.5	87.2	22.25914
67	1	Unknown 1	-10.01424	79.6	9288.53	8850.3	1834.3	79.6	20.38732
68	2	Unknown 1	-10.01424	74.9	8767.42	8329.2	2355.4	74.9	19.24354
69	3	Unknown 1	-10.01424	100.2	11587.18	11148.9	-464.4	100.2	25.43261
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	25.0	3223.566	2785.3	7899.2	25.0	7.075378
74	2	Unknown 2	-4.01424	31.0	3883.37	3445.1	7239.4	31.0	8.523577
75	3	Unknown 2	-4.01424	29.2	3686.52	3248.3	7436.3	29.2	8.091512
76	1	Unknown 2	-5.01424	60.6	7183.01	6744.8	3939.8	60.6	15.76593
77	2	Unknown 2	-5.01424	75.6	8842.44	8404.2	2280.4	75.6	19.4082
78	3	Unknown 2	-5.01424	74.9	8772.07	8333.8	2350.7	74.9	19.25374
79	1	Unknown 2	-6.01424	89.6	10405.15	9966.9	717.7	89.6	22.83818
80	2	Unknown 2	-6.01424	78.2	9132.29	8694.0	1990.5	78.2	20.04439
81	3	Unknown 2	-6.01424	96.3	11148.84	10710.6	-26.0	96.3	24.4705
82	1	Unknown 2	-7.01424	96.6	11179.84	10741.6	-57.0	96.6	24.53854
83	2	Unknown 2	-7.01424	71.8	8419.29	7981.0	2703.5	71.8	18.47943
84	3	Unknown 2	-7.01424	83.0	9670.14	9231.9	1452.7	83.0	21.22491
85	1	Unknown 2	-8.01424	94.2	10919.44	10481.2	203.4	94.2	23.96699
86	2	Unknown 2	-8.01424	86.8	10097.94	9659.7	1024.9	86.8	22.16389
87	3	Unknown 2	-8.01424	97.0	11231.61	10793.4	-108.8	97.0	24.65217
88	1	Unknown 2	-9.01424	97.9	11328.02	10889.8	-205.2	97.9	24.86378
89	2	Unknown 2	-9.01424	97.0	11231.3	10793.0	-108.5	97.0	24.65149
90	3	Unknown 2	-9.01424	79.8	9318.29	8880.0	1804.5	79.8	20.45264
91	1	Unknown 2	-10.01424	100.0	11560.83	11122.6	-438.0	100.0	25.37477
92	2	Unknown 2	-10.01424	77.9	9098.81	8660.6	2024.0	77.9	19.9709
93	3	Unknown 2	-10.01424	84.8	9870.09	9431.8	1252.7	84.8	21.66378

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2368.00	7340.80	TRUE	
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2278.40	7063.04	TRUE	
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2843.40	8814.54	TRUE	
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2977.30	9229.63	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2913.50	9031.85	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2864.60	8880.26	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3699.00	11466.90	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3505.80	10867.98	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3020.70	9364.17	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3096.70	9599.77	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2940.30	9114.93	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3245.90	10062.29	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3222.90	9990.99	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3591.00	11132.10	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2971.10	9210.41	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	2881.80	8933.58	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3337.00	10344.70	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3595.80	11146.98	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3203.80	9931.78	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3161.40	9800.34	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3393.90	10521.09	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3265.80	10123.98	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3731.30	11567.03	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3228.30	10007.73	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	127.49	395.22	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	144.52	448.01	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	128.87	399.50	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	750.86	2327.67	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	780.61	2419.89	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	702.55	2177.91	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2941.80	9119.58	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3150.70	9767.17	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2777.40	8609.94	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3811.80	11816.58	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3544.60	10988.26	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3787.00	11739.70	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3741.80	11599.58	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3530.30	10943.93	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3772.60	11695.06	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3754.90	11640.19	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3510.50	10882.55	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3874.50	12010.95	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3970.90	12309.79	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3513.10	10890.61	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3869.30	11994.83	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3770.60	11688.86	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3355.30	10401.43	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3609.80	11190.38	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3900.90	12092.79	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3848.50	11930.35	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3461.60	10730.96	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	139.79	419.37	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	164.10	492.30	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	181.99	545.97	TRUE	
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	46778.00	46778.00	TRUE	
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	45761.00	45761.00	TRUE	
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45162.00	45162.00	TRUE	
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	45072.00	45072.00	TRUE	
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	45853.00	45853.00	TRUE	
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	44736.00	44736.00	TRUE	

			Values for analysis by nonlinear regression						
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424	62.1	7340.8	6902.5	3782.0	62.1	16.11226
95	2	Unknown 3	-3.01424	59.6	7063.04	6624.8	4059.8	59.6	15.50261
96	3	Unknown 3	-3.01424	75.3	8814.54	8376.3	2308.3	75.3	19.34696
97	1	Unknown 3	-4.01424	79.0	9229.63	8791.4	1893.2	79.0	20.25804
98	2	Unknown 3	-4.01424	77.3	9031.85	8593.6	2091.0	77.3	19.82393
99	3	Unknown 3	-4.01424	75.9	8880.26	8442.0	2242.5	75.9	19.49121
100	1	Unknown 3	-5.01424	99.2	11466.9	11028.6	-344.1	99.2	25.1686
101	2	Unknown 3	-5.01424	93.8	10867.98	10429.7	254.8	93.8	23.85404
102	3	Unknown 3	-5.01424	80.2	9364.17	8925.9	1758.6	80.2	20.55334
103	1	Unknown 3	-6.01424	82.4	9599.77	9161.5	1523.0	82.4	21.07046
104	2	Unknown 3	-6.01424	78.0	9114.93	8676.7	2007.9	78.0	20.00628
105	3	Unknown 3	-6.01424	86.5	10062.29	9624.0	1060.5	86.5	22.08564
106	1	Unknown 3	-7.01424	85.9	9990.99	9552.7	1131.8	85.9	21.92914
107	2	Unknown 3	-7.01424	96.1	11132.1	10693.8	-9.3	96.1	24.43375
108	3	Unknown 3	-7.01424	78.9	9210.41	8772.2	1912.4	78.9	20.21585
109	1	Unknown 3	-8.01424	76.4	8933.58	8495.3	2189.2	76.4	19.60824
110	2	Unknown 3	-8.01424	89.1	10344.7	9906.4	778.1	89.1	22.7055
111	3	Unknown 3	-8.01424	96.3	11146.98	10708.7	-24.2	96.3	24.46641
112	1	Unknown 3	-9.01424	85.4	9931.78	9493.5	1191.0	85.4	21.79918
113	2	Unknown 3	-9.01424	84.2	9800.34	9362.1	1322.5	84.2	21.51069
114	3	Unknown 3	-9.01424	90.7	10521.09	10082.8	601.7	90.7	23.09265
115	1	Unknown 3	-10.01424	87.1	10123.98	9685.7	998.8	87.1	22.22104
116	2	Unknown 3	-10.01424	100.1	11567.03	11128.8	-444.2	100.1	25.38838
117	3	Unknown 3	-10.01424	86.0	10007.73	9569.5	1115.1	86.0	21.96588
118	1	Unknown 4	-3.01424	-0.4	395.219	-43.0	10727.6	-0.4	0.867463
119	2	Unknown 4	-3.01424	0.1	448.012	9.8	10674.8	0.1	0.983338
120	3	Unknown 4	-3.01424	-0.3	399.497	-38.8	10723.3	-0.3	0.876853
121	1	Unknown 4	-4.01424	17.0	2327.666	1889.4	8795.1	17.0	5.108975
122	2	Unknown 4	-4.01424	17.8	2419.891	1981.6	8702.9	17.8	5.311399
123	3	Unknown 4	-4.01424	15.6	2177.905	1739.6	8944.9	15.6	4.780266
124	1	Unknown 4	-5.01424	78.0	9119.58	8681.3	2003.2	78.0	20.01649
125	2	Unknown 4	-5.01424	83.9	9767.17	9328.9	1355.6	83.9	21.43788
126	3	Unknown 4	-5.01424	73.5	8609.94	8171.7	2512.9	73.5	18.89789
127	1	Unknown 4	-6.01424	102.3	11816.58	11378.3	-693.8	102.3	25.93611
128	2	Unknown 4	-6.01424	94.9	10988.26	10550.0	134.5	94.9	24.11804
129	3	Unknown 4	-6.01424	101.6	11739.7	11301.4	-616.9	101.6	25.76737
130	1	Unknown 4	-7.01424	100.3	11599.58	11161.3	-476.8	100.3	25.45982
131	2	Unknown 4	-7.01424	94.5	10943.93	10505.7	178.9	94.5	24.02074
132	3	Unknown 4	-7.01424	101.2	11695.06	11256.8	-572.3	101.2	25.66939
133	1	Unknown 4	-8.01424	100.7	11640.19	11201.9	-517.4	100.7	25.54896
134	2	Unknown 4	-8.01424	93.9	10882.55	10444.3	240.3	93.9	23.88602
135	3	Unknown 4	-8.01424	104.0	12010.95	11572.7	-888.1	104.0	26.36274
136	1	Unknown 4	-9.01424	106.7	12309.79	11871.5	-1187.0	106.7	27.01866
137	2	Unknown 4	-9.01424	94.0	10890.61	10452.4	232.2	94.0	23.90371
138	3	Unknown 4	-9.01424	103.9	11994.83	11556.6	-872.0	103.9	26.32735
139	1	Unknown 4	-10.01424	101.1	11688.86	11250.6	-566.1	101.1	25.65578
140	2	Unknown 4	-10.01424	89.6	10401.43	9963.2	721.4	89.6	22.83001
141	3	Unknown 4	-10.01424	96.7	11190.38	10752.1	-67.6	96.7	24.56167
142	1	—	—	104.8	12092.79	11654.5	-970.0	104.8	26.54237
143	2	—	—	103.3	11930.35	11492.1	-807.5	103.3	26.18583
144	3	—	—	92.5	10730.96	10292.7	391.8	92.5	23.5533
145	1	-6.00	-0.2	419.37	46778	45322.7	10703.4	-0.2	0.920472
146	2	-6.00	0.5	492.3	45162	44723.7	10630.5	0.5	1.080545
147	3	-6.00	1.0	545.97	45072	44633.7	10576.8	1.0	1.198345
148	1				46778	46339.7			
149	2				45761	45322.7			
150	3				45162	44723.7			
151	1				45072	44633.7			
152	2				45853	45414.7			
153	3				44736	44297.7			

Prism data												
standard curve				weak positive				CR42352				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	-0.56281	-0.37050	-0.35108	-3	3.6912	3.1736	3.5183	-3.0	1.3672	2.6980	1.2326	
-6.0	-0.16983	0.48585	0.96837	-4	28.2720	22.3768	27.4197	-4.0	26.7928	27.0269	27.2081	
-7.0	1.55562	1.28249	2.95390	-5	64.3007	55.3272	62.5044	-5.0	73.8190	62.7320	73.0637	
-8.0	12.76521	14.08656	12.67797	-6	93.5838	94.0072	84.4350	-6.0	85.7393	99.6941	80.7003	
-9.0	54.70528	52.40316	54.34017	-7	93.9506	94.1178	85.2765	-7.0	90.6139	77.9857	99.4126	
-10.0	93.29501	94.25934	74.94217	-8	94.0962	91.8414	96.6639	-8.0	85.4773	91.8234	100.0648	
-11.0	76.16012	82.59546	86.04028	-9	92.3296	95.2075	94.9998	-9.0	99.3792	91.1183	87.2359	
				-10	83.5908	84.9043	94.5062	-10.0	79.5687	74.8836	100.2348	

CR42353					CR42359					CR42360				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.0					-3.0	62.0576	59.5603	75.3073		-3.0	-0.3870	0.0877	-0.3485	
-4.0	25.0414	30.9734	29.2036		-4.0	79.0392	77.2610	75.8981		-4.0	16.9868	17.8159	15.6403	
-5.0	60.6389	75.5581	74.9255		-5.0	99.1534	93.7688	80.2488		-5.0	78.0498	83.8719	73.4678	
-6.0	89.6077	78.1640	96.2939		-6.0	82.3669	78.0079	86.5252		-6.0	102.2972	94.8502	101.6060	
-7.0	96.5726	71.7538	82.9996		-7.0	85.8842	96.1434	78.8664		-7.0	100.3463	94.4516	101.2047	
-8.0	94.2315	86.8457	97.0380		-8.0	76.3775	89.0642	96.2772		-8.0	100.7114	93.8998	104.0447	
-9.0	97.9048	97.0353	79.8363		-9.0	85.3519	84.1702	90.6501		-9.0	106.7315	93.9723	103.8998	
-10.0	99.9979	77.8630	84.7972		-10.0	87.0799	100.0537	86.0347		-10.0	101.1490	89.5743	96.6674	

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	506	
Assay start date:	9/26/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	80.00	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.57E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.24E-05	M
RBA:	4.86094E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	1.85E-09	CR42340
RBA, Unknown 1:	85.21127%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	5.15E-05	CR42350
RBA, Unknown 2:	0.00305%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	1.76E-04	CR42354
RBA, Unknown 3:	0.00089%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	4.17E-05	CR42363
RBA, Unknown 4:	0.00377%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11264.8	1072.65	Total Binding, solvent control, tubes
Hot	6	45672.0	514.85	Total hot R1881 added to each tube
NSB	6	444.9	57.25	Nonspecific Binding
Specific EtOH	6	10819.9	1072.65	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)															Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	transcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3571.20	11070.72	TRUE		
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3212.00	9957.20	TRUE		
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3238.40	10039.04	TRUE		
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	151.87	455.61	TRUE			
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	140.52	421.56	TRUE			
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	113.39	340.17	TRUE			
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	209.90	650.69	TRUE		
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	195.56	606.24	TRUE		
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	188.13	583.20	TRUE		
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	625.61	1939.39	TRUE		
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	611.07	1894.32	TRUE		
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	443.03	1373.39	FALSE	spill	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2279.90	7067.69	TRUE		
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2292.80	7107.68	TRUE		
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2314.40	7174.64	TRUE		
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3265.40	10122.74	TRUE		
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3383.60	10489.16	TRUE		
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3479.70	10787.07	TRUE		
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2939.40	9112.14	TRUE		
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3780.50	11719.55	TRUE		
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3336.00	10341.60	TRUE		
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	276.45	829.35	TRUE		
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	308.55	925.65	TRUE		
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	305.17	915.51	TRUE		
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1199.80	3599.40	TRUE		
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1080.69	3242.07	TRUE		
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1243.80	3731.40	TRUE		
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2933.10	8799.30	TRUE		
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2456.40	7369.20	TRUE		
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3007.60	9022.80	TRUE		
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3402.40	10207.20	TRUE		
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3021.60	9064.80	TRUE		
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3635.30	10905.90	TRUE		
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3231.40	9694.20	TRUE		
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3830.60	11491.80	TRUE		
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3731.10	11193.30	TRUE		
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3868.20	11604.60	TRUE		
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3791.80	11375.40	TRUE		
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3655.90	10967.70	TRUE		
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3848.50	11545.50	TRUE		
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3844.90	11534.70	TRUE		
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3745.90	11237.70	TRUE		
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3794.50	11383.50	TRUE		
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3144.40	9433.20	TRUE		
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3862.60	11587.80	TRUE		

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
1	1			98.2	11070.72	10625.8	98.2	24.23962	
2	2			87.9	9957.2	9512.3	87.9	21.80154	
3	3			88.7	10039.04	9594.1	88.7	21.98073	
4	1	-6.00	0.1	455.61	10.7	10364.3	0.1	0.99757	
5	2	-6.00	-0.2	421.56	-23.4	10398.3	-0.2	0.923016	
6	3	-6.00	0.0	340.17	-104.8	10479.7	-1.0	0.744811	
7	1	cold R1881	-7.01	1.9	650.69	205.8	1.9	1.424702	
8	2	cold R1881	-7.01	1.5	606.236	161.3	1.5	1.327369	
9	3	cold R1881	-7.01	1.3	583.203	138.3	1.3	1.276938	
10	1	cold R1881	-8.01	13.8	1939.391	1494.5	13.8	4.246346	
11	2	cold R1881	-8.01	13.4	1894.317	1449.4	13.4	4.147655	
12	3	cold R1881	-8.01						
13	1	cold R1881	-9.01	61.2	7067.69	6622.8	61.2	15.47489	
14	2	cold R1881	-9.01	61.6	7107.68	6662.7	61.6	15.56245	
15	3	cold R1881	-9.01	62.2	7174.64	6729.7	62.2	15.70906	
16	1	cold R1881	-10.01	89.4	10122.74	9677.8	89.4	22.164	
17	2	cold R1881	-10.01	92.8	10489.16	10044.2	92.8	22.96628	
18	3	cold R1881	-10.01	95.6	10787.07	10342.1	95.6	23.61856	
19	1	cold R1881	-11.01	80.1	9112.14	8667.2	80.1	19.95126	
20	2	cold R1881	-11.01	104.2	11719.55	11274.6	104.2	25.66025	
21	3	cold R1881	-11.01	91.5	10341.6	9896.7	91.5	22.64319	
22	1	Weak Positive	-3	3.6	829.35	384.4	3.6	1.815883	
23	2	Weak Positive	-3	4.4	925.65	480.7	4.4	2.026734	
24	3	Weak Positive	-3	4.3	915.51	470.6	4.3	2.004532	
25	1	Weak Positive	-4	29.2	3599.4	3154.5	29.2	7.880977	
26	2	Weak Positive	-4	25.9	3242.07	2797.1	25.9	7.098594	
27	3	Weak Positive	-4	30.4	3731.4	3286.5	30.4	8.169995	
28	1	Weak Positive	-5	77.2	8799.3	8354.4	77.2	19.26629	
29	2	Weak Positive	-5	64.0	7369.2	6924.3	64.0	16.13505	
30	3	Weak Positive	-5	79.3	9022.8	8577.9	79.3	19.75565	
31	1	Weak Positive	-6	90.2	10207.2	9762.3	90.2	22.34892	
32	2	Weak Positive	-6	79.7	9064.8	8619.9	79.7	19.84761	
33	3	Weak Positive	-6	96.7	10905.9	10461.0	96.7	23.87874	
34	1	Weak Positive	-7	85.5	9694.2	9249.3	85.5	21.2257	
35	2	Weak Positive	-7	102.1	11491.8	11046.9	102.1	25.16159	
36	3	Weak Positive	-7	99.3	11193.3	10748.4	99.3	24.50801	
37	1	Weak Positive	-8	103.1	11604.6	11159.7	103.1	25.40857	
38	2	Weak Positive	-8	101.0	11375.4	10930.5	101.0	24.90673	
39	3	Weak Positive	-8	97.3	10967.7	10522.8	97.3	24.01406	
40	1	Weak Positive	-9	102.6	11545.5	11100.6	102.6	25.27916	
41	2	Weak Positive	-9	102.5	11534.7	11089.8	102.5	25.25552	
42	3	Weak Positive	-9	99.7	11237.7	10792.8	99.7	24.60523	
43	1	Weak Positive	-10	101.1	11383.5	10938.6	101.1	24.92446	
44	2	Weak Positive	-10	83.1	9433.2	8988.3	83.1	20.65423	
45	3	Weak Positive	-10	103.0	11587.8	11142.9	103.0	25.37178	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)															Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,3-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	134.64	417.38	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	150.17	465.53	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	140.84	436.60	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	148.81	461.31	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	147.50	457.25	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	167.59	519.53	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	157.52	488.31	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	190.61	590.89	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	164.05	508.56	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	190.86	591.67	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	167.40	518.94	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	140.00	434.00	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	237.85	737.34	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	194.43	602.73	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	197.46	612.13	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	769.02	2383.96	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	698.87	2166.50	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	788.65	2444.82	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2284.80	7082.88	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2633.40	8163.54	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2109.90	6540.69	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3549.90	11004.69	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3659.90	11345.69	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3533.50	10953.85	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1047.40	3246.94	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	810.54	2512.67	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	871.72	2702.33	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1270.90	3939.79	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1423.70	4413.47	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1245.10	3859.81	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3040.90	9426.79	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3150.30	9765.93	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2983.80	9249.78	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3790.40	11750.24	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3848.30	11929.73	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3802.10	11786.51	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3739.90	11593.69	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3820.20	11842.62	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3880.10	12028.31	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3845.00	11919.50	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3917.00	12142.70	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3652.10	11321.51	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3973.60	12318.16	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3863.80	11977.78	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3743.60	11605.16	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3770.80	11689.48	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3429.60	10631.76	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3810.10	11811.31	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-0.3	417.384	-27.6	10402.5	-0.3	0.913873
47	2	Unknown 1	-3.01424	0.2	465.527	20.6	10354.4	0.2	1.019283
48	3	Unknown 1	-3.01424	-0.1	436.604	-8.3	10383.3	-0.1	0.955956
49	1	Unknown 1	-4.01424	0.2	461.311	16.4	10358.6	0.2	1.010052
50	2	Unknown 1	-4.01424	0.1	457.25	12.3	10362.6	0.1	1.00116
51	3	Unknown 1	-4.01424	0.7	519.529	74.6	10300.4	0.7	1.137522
52	1	Unknown 1	-5.01424	0.4	488.312	43.4	10331.6	0.4	1.069171
53	2	Unknown 1	-5.01424	1.3	590.891	146.0	10229.0	1.3	1.293771
54	3	Unknown 1	-5.01424	0.6	508.555	63.6	10311.3	0.6	1.113494
55	1	Unknown 1	-6.01424	1.4	591.666	146.7	10228.2	1.4	1.295468
56	2	Unknown 1	-6.01424	0.7	518.94	74.0	10301.0	0.7	1.136232
57	3	Unknown 1	-6.01424	-0.1	434	-10.9	10385.9	-0.1	0.950254
58	1	Unknown 1	-7.01424	2.7	737.335	292.4	10082.6	2.7	1.614414
59	2	Unknown 1	-7.01424	1.5	602.733	157.8	10217.2	1.5	1.319699
60	3	Unknown 1	-7.01424	1.5	612.126	167.2	10207.8	1.5	1.340265
61	1	Unknown 1	-8.01424	17.9	2383.962	1939.0	8435.9	17.9	5.219745
62	2	Unknown 1	-8.01424	15.9	2166.497	1721.6	8653.4	15.9	4.7436
63	3	Unknown 1	-8.01424	18.5	2444.815	1999.9	8375.1	18.5	5.352984
64	1	Unknown 1	-9.01424	61.3	7082.88	6637.9	3737.0	61.3	15.50815
65	2	Unknown 1	-9.01424	71.3	8163.54	7718.6	2656.4	71.3	17.87428
66	3	Unknown 1	-9.01424	56.3	6540.69	6095.8	4279.2	56.3	14.32101
67	1	Unknown 1	-10.01424	97.6	11004.69	10559.8	-184.8	97.6	24.09505
68	2	Unknown 1	-10.01424	100.7	11345.69	10900.8	-525.8	100.7	24.84168
69	3	Unknown 1	-10.01424	97.1	10953.85	10508.9	-134.0	97.1	23.98373
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	32.3	3939.79	3494.9	6880.1	32.3	8.62627
74	2	Unknown 2	-4.01424	36.7	4413.47	3968.5	6406.4	36.7	9.663404
75	3	Unknown 2	-4.01424	31.6	3859.81	3414.9	6960.1	31.6	8.451152
76	1	Unknown 2	-5.01424	83.0	9426.79	8981.9	1393.1	83.0	20.6402
77	2	Unknown 2	-5.01424	86.1	9765.93	9321.0	1054.0	86.1	21.38275
78	3	Unknown 2	-5.01424	81.4	9249.78	8804.8	1570.1	81.4	20.25263
79	1	Unknown 2	-6.01424	104.5	11750.24	11305.3	-930.3	104.5	25.72745
80	2	Unknown 2	-6.01424	106.1	11929.73	11484.8	-1109.8	106.1	26.12045
81	3	Unknown 2	-6.01424	104.8	11786.51	11341.6	-966.6	104.8	25.80686
82	1	Unknown 2	-7.01424	103.0	11593.69	11148.8	-773.8	103.0	25.38468
83	2	Unknown 2	-7.01424	105.3	11842.62	11397.7	-1022.7	105.3	25.92972
84	3	Unknown 2	-7.01424	107.1	12028.31	11583.4	-1208.4	107.1	26.33629
85	1	Unknown 2	-8.01424	106.1	11919.5	11474.6	-1099.6	106.1	26.09805
86	2	Unknown 2	-8.01424	108.1	12142.7	11697.8	-1322.8	108.1	26.58675
87	3	Unknown 2	-8.01424	100.5	11321.51	10876.6	-501.6	100.5	24.78873
88	1	Unknown 2	-9.01424	109.7	12318.16	11873.2	-1498.3	109.7	26.97092
89	2	Unknown 2	-9.01424	106.6	11977.78	11532.8	-1157.9	106.6	26.22565
90	3	Unknown 2	-9.01424	103.1	11605.16	11160.2	-785.3	103.1	25.40979
91	1	Unknown 2	-10.01424	103.9	11689.48	11244.5	-869.6	103.9	25.59441
92	2	Unknown 2	-10.01424	94.1	10631.76	10186.8	188.1	94.1	23.27851
93	3	Unknown 2	-10.01424	105.1	11811.31	11366.4	-991.4	105.1	25.86116

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	292.32	906.19	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	261.56	810.84	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	283.45	878.70	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2318.00	7185.80	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2364.80	7330.88	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2301.50	7134.65	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3540.60	10975.86	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3605.20	11176.12	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3706.30	11489.53	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3919.00	12148.90	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3828.40	11868.04	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3479.10	10785.21	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3527.60	10935.56	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3651.60	11319.96	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	2825.90	8760.29	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3732.80	11571.68	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3644.90	11299.19	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3113.60	9652.16	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3567.90	11060.49	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3000.50	9301.55	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3146.40	9753.84	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3522.10	10918.51	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	2894.30	8972.33	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3075.80	9534.98	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1430.30	4433.93	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1173.60	3638.16	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1222.10	3788.51	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	916.48	2841.09	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1063.13	3295.70	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	997.53	3092.34	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2598.40	8055.04	FALSE	spill
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3377.60	10470.56	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3177.20	9849.32	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3493.40	10829.54	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3827.90	11866.49	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3835.20	11889.12	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3564.20	11049.02	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3570.10	11067.31	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3757.90	11649.49	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3607.20	11182.32	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3900.50	12091.55	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3361.70	10421.27	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3574.40	11080.64	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3053.60	9466.16	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3255.70	10092.67	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3981.50	12342.65	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3865.60	11983.36	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3984.30	12351.33	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3951.90	12250.89	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3887.60	12051.56	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3941.80	12219.58	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	164.10	492.30	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	158.33	474.99	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	161.66	484.98	TRUE	
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	45698.00	45698.00	TRUE	
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	45390.00	45390.00	TRUE	
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	46325.00	46325.00	TRUE	
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44935.00	44935.00	TRUE	
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	46172.00	46172.00	TRUE	
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45512.00	45512.00	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (Specific bound / mean specific EICOH)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	62.3	7185.8	6740.9	3634.1	62.3	15.73349
98	2	Unknown 3	-4.01424	63.6	7330.88	6885.9	3489.0	63.6	16.05115
99	3	Unknown 3	-4.01424	61.8	7134.65	6689.7	3685.2	61.8	15.6215
100	1	Unknown 3	-5.01424	97.3	10975.86	10530.9	-156.0	97.3	24.03192
101	2	Unknown 3	-5.01424	99.2	11176.12	10731.2	-356.2	99.2	24.4704
102	3	Unknown 3	-5.01424	102.1	11489.53	11044.6	-669.6	102.1	25.15662
103	1	Unknown 3	-6.01424	108.2	12148.9	11704.0	-1329.0	108.2	26.60032
104	2	Unknown 3	-6.01424	105.6	11868.04	11423.1	-1048.1	105.6	25.98537
105	3	Unknown 3	-6.01424	95.6	10785.21	10340.3	34.7	95.6	23.61449
106	1	Unknown 3	-7.01424	97.0	10935.56	10490.6	-115.7	97.0	23.94369
107	2	Unknown 3	-7.01424	100.5	11319.96	10875.0	-500.1	100.5	24.78534
108	3	Unknown 3	-7.01424	76.9	8760.29	8315.4	2059.6	76.9	19.18088
109	1	Unknown 3	-8.01424	102.8	11571.68	11126.7	-751.8	102.8	25.33649
110	2	Unknown 3	-8.01424	100.3	11299.19	10854.3	-479.3	100.3	24.73986
111	3	Unknown 3	-8.01424	85.1	9652.16	9207.2	1167.7	85.1	21.13365
112	1	Unknown 3	-9.01424	98.1	11060.49	10615.6	-240.6	98.1	24.21722
113	2	Unknown 3	-9.01424	81.9	9301.55	8856.6	1518.3	81.9	20.36598
114	3	Unknown 3	-9.01424	86.0	9753.84	9308.9	1066.1	86.0	21.35628
115	1	Unknown 3	-10.01424	96.8	10918.51	10473.6	-98.6	96.8	23.90635
116	2	Unknown 3	-10.01424	78.8	8972.33	8527.4	1847.6	78.8	19.64514
117	3	Unknown 3	-10.01424	84.0	9534.98	9090.0	1284.9	84.0	20.87708
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	22.1	2841.088	2396.2	7978.8	22.1	6.220634
122	2	Unknown 4	-4.01424	26.3	3295.703	2850.8	7524.2	26.3	7.216025
123	3	Unknown 4	-4.01424	24.5	3092.343	2647.4	7727.6	24.5	6.770763
124	1	Unknown 4	-5.01424						
125	2	Unknown 4	-5.01424	92.7	10470.56	10025.6	349.3	92.7	22.92556
126	3	Unknown 4	-5.01424	86.9	9849.32	9404.4	970.6	86.9	21.56534
127	1	Unknown 4	-6.01424	96.0	10829.54	10384.6	-9.6	96.0	23.71155
128	2	Unknown 4	-6.01424	105.6	11866.49	11421.6	-1046.6	105.6	25.98198
129	3	Unknown 4	-6.01424	105.8	11889.12	11444.2	-1069.2	105.8	26.03153
130	1	Unknown 4	-7.01424	98.0	11049.02	10604.1	-229.1	98.0	24.19211
131	2	Unknown 4	-7.01424	98.2	11067.31	10622.4	-247.4	98.2	24.23216
132	3	Unknown 4	-7.01424	103.6	11649.49	11204.6	-829.6	103.6	25.50685
133	1	Unknown 4	-8.01424	99.2	11182.32	10737.4	-362.4	99.2	24.48397
134	2	Unknown 4	-8.01424	107.6	12091.55	11646.6	-1271.7	107.6	26.47475
135	3	Unknown 4	-8.01424	92.2	10421.27	9976.3	398.6	92.2	22.81763
136	1	Unknown 4	-9.01424	98.3	11080.64	10635.7	-260.7	98.3	24.26134
137	2	Unknown 4	-9.01424	83.4	9466.16	9021.2	1353.7	83.4	20.7264
138	3	Unknown 4	-9.01424	89.2	10092.67	9647.7	727.2	89.2	22.09816
139	1	Unknown 4	-10.01424	110.0	12342.65	11897.7	-1522.8	110.0	27.02454
140	2	Unknown 4	-10.01424	106.6	11983.36	11538.4	-1163.5	106.6	26.23787
141	3	Unknown 4	-10.01424	110.0	12351.33	11906.4	-1531.4	110.0	27.04355
142	1	—	—	109.1	12250.89	11806.0	-1431.0	109.1	26.82363
143	2	—	—	107.3	12051.56	11606.6	-1231.7	107.3	26.3872
144	3	—	—	108.8	12219.58	11774.6	-1399.7	108.8	26.75508
145	1	-6.00	0.4	492.3	47.4	10327.6	0.4	1.077903	
146	2	-6.00	0.3	474.99	30.1	10344.9	0.3	1.040003	
147	3	-6.00	0.4	484.98	40.0	10334.9	0.4	1.061876	
148	1				45698	45253.1			
149	2				45390	44945.1			
150	3				46325	45880.1			
151	1				44935	44490.1			
152	2				46172	45727.1			
153	3				45512	45067.1			

Prism data												
standard curve				weak positive				CR42340				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	0.09866	-0.21604	-0.96826	-3	3.5529	4.4429	4.3492	-3.0	-0.2546	0.1903	-0.0770	
-6.0	0.43776	0.27778	0.37011	-4	29.1543	25.8518	30.3743	-4.0	0.1514	0.1138	0.6894	
-7.0	1.90164	1.49078	1.27790	-5	77.2130	63.9957	79.2786	-5.0	0.4009	1.3490	0.5880	
-8.0	13.81211	13.39553		-6	90.2251	79.6668	96.6827	-6.0	1.3561	0.6840	-0.1011	
-9.0	61.20904	61.57864	62.19750	-7	85.4839	102.0977	99.3389	-7.0	2.7024	1.4584	1.5452	
-10.0	89.44452	92.83106	95.58442	-8	103.1402	101.0219	97.2538	-8.0	17.9209	15.9111	18.4834	
-11.0	80.10432	104.20261	91.46728	-9	102.5940	102.4942	99.7492	-9.0	61.3494	71.3371	56.3384	
				-10	101.0968	83.0716	102.9849	-10.0	97.5957	100.7473	97.1258	

CR42350				CR42354				CR42363			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0				-3.0			
-4.0	32.3003	36.6781	31.5611	-4.0	62.3006	63.6415	61.8279	-4.0	22.1458	26.3475	24.4680
-5.0	83.0124	86.1468	81.3764	-5.0	97.3293	99.1801	102.0767	-5.0		92.6592	86.9175
-6.0	104.4863	106.1451	104.8215	-6.0	108.1708	105.5750	95.5672	-6.0	95.9769	105.5607	105.7698
-7.0	103.0394	105.3401	107.0562	-7.0	96.9568	100.5095	76.8524	-7.0	98.0054	98.1745	103.5551
-8.0	106.0506	108.1135	100.5238	-8.0	102.8360	100.3175	85.0953	-8.0	99.2374	107.6407	92.2036
-9.0	109.7351	106.5892	103.1454	-9.0	98.1114	81.8549	86.0351	-9.0	98.2977	83.3763	89.1666
-10.0	103.9247	94.1490	105.0507	-10.0	96.7992	78.8122	84.0123	-10.0	109.9614	106.6408	110.0417

Competitive Assay of a known Weak Positive
153 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
 Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:			
Run identification:	507		
Assay start date:	051905		
Tracer lot number:	3559-507		
Specific activity on day of assay:	10.39	Ci/mmole	
Cytosol vial or lot identification:	8/5/2024		
Protein (cytosol):	1000	micro gram per tube	
Standard Curve IC50:	1.64E-09	M	
Weak Positive, Max Concentration:	3.00E-02	M	
Weak Positive IC50:	3.23E-05	M	
RBA:	5.07583E-05		
Max Concentration, Unknown 1:	3.00E-02	M	5e-3)
IC50, Unknown 1:	2.00E-09	CR42340	
RBA, Unknown 1:	81.91808%		
Max Concentration, Unknown 2:	3.00E-02	M	(example 5e-3)
IC50, Unknown 2:	4.84E-05	CR42350	
RBA, Unknown 2:	0.00339%		
Max Concentration, Unknown 3:	3.00E-02	M	(example 5e-3)
IC50, Unknown 3:	1.50E-04	CR42354	
RBA, Unknown 3:	0.00109%		
Max Concentration, Unknown 4:	3.00E-02	M	(example 5e-3)
IC50, Unknown 4:	4.41E-05	CR42363	
RBA, Unknown 4:	0.00372%		
volume of ethanol counted:	2	mL	protocol calls for counting decanted EtOH supernate
multiply DPM in sample by :	3.1		reflects 100ul of reaction mixture processed
working volume	3.1E+02	uL	

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11433.3	642.60	Total Binding, solvent control, tubes
Hot	6	44490.8	496.79	Total hot R1881 added to each tube
NSB	6	417.1	42.08	Nonspecific Binding
Specific EtOH	6	11016.2	642.60	

Assay Characterization Values	
EtOH / Hot	0.26 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triangelone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3285.10	10183.81	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3740.90	11596.79	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3674.00	11389.40	TRUE	
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	145.84	437.52	TRUE		
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	152.30	456.90	TRUE		
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	115.25	345.75	TRUE		
7	1	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	212.91	660.02	TRUE		
8	2	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	183.39	568.51	TRUE		
9	3	Inert R1881	S	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	177.78	551.12	TRUE		
10	1	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	608.50	1886.35	TRUE		
11	2	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	644.65	1998.42	TRUE		
12	3	Inert R1881	S	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	652.20	2021.82	TRUE		
13	1	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2383.50	7388.85	TRUE		
14	2	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2310.50	7162.55	TRUE		
15	3	Inert R1881	S	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2350.70	7287.17	TRUE		
16	1	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3519.90	10911.69	TRUE		
17	2	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3473.50	10767.85	TRUE		
18	3	Inert R1881	S	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3429.00	10629.90	TRUE		
19	1	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3351.20	10388.72	TRUE		
20	2	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3602.40	11167.44	TRUE		
21	3	Inert R1881	S	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3636.50	11273.15	TRUE		
22	1	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	258.99	776.97	TRUE		
23	2	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	275.36	826.08	TRUE		
24	3	Weak Positive	P	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	295.75	887.25	TRUE		
25	1	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1184.60	3553.80	TRUE		
26	2	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1204.60	3613.80	TRUE		
27	3	Weak Positive	P	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1145.60	3436.80	TRUE		
28	1	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2975.30	8925.90	TRUE		
29	2	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2562.00	7686.00	TRUE		
30	3	Weak Positive	P	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2992.20	8976.60	TRUE		
31	1	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3623.00	10869.00	TRUE		
32	2	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3212.10	9636.30	TRUE		
33	3	Weak Positive	P	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3461.10	10383.30	TRUE		
34	1	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3535.20	10605.60	TRUE		
35	2	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3530.80	10592.40	TRUE		
36	3	Weak Positive	P	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3396.00	10188.00	TRUE		
37	1	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3083.80	9251.40	TRUE		
38	2	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3520.30	10560.90	TRUE		
39	3	Weak Positive	P	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3429.20	10287.60	TRUE		
40	1	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3422.00	10266.00	TRUE		
41	2	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3497.60	10492.80	TRUE		
42	3	Weak Positive	P	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3583.80	10751.40	TRUE		
43	1	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3476.70	10430.10	TRUE		
44	2	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3506.50	10519.50	TRUE		
45	3	Weak Positive	P	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3522.40	10567.20	TRUE		

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
1	1	—	88.7	10183.81	9766.7	832.4	88.7	22.88968	
2	2	—	101.5	11596.79	11179.7	-580.6	101.5	26.06557	
3	3	—	99.6	11389.4	10972.3	-373.2	99.6	25.59943	
4	1	-6.00	0.2	437.52	20.4	10578.7	0.2	0.983394	
5	2	-6.00	0.4	456.9	39.8	10559.3	0.4	1.026953	
6	3	-6.00	0.0	345.75	-71.3	10670.5	-0.6	0.777126	
7	1	cold R1881	-7.01	2.2	660.021	242.9	2.2	1.483499	
8	2	cold R1881	-7.01	1.4	568.509	151.4	1.4	1.277812	
9	3	cold R1881	-7.01	1.2	551.118	134.0	1.2	1.238723	
10	1	cold R1881	-8.01	13.3	1886.35	1469.3	13.3	4.239862	
11	2	cold R1881	-8.01	14.4	1998.415	1581.3	14.4	4.491745	
12	3	cold R1881	-8.01	14.6	2021.82	1604.7	14.6	4.544352	
13	1	cold R1881	-9.01	63.3	7388.85	6971.8	63.3	16.60758	
14	2	cold R1881	-9.01	61.2	7162.55	6745.5	61.2	16.09893	
15	3	cold R1881	-9.01	62.4	7287.17	6870.1	62.4	16.37904	
16	1	cold R1881	-10.01	95.3	10911.69	10494.6	95.3	24.5257	
17	2	cold R1881	-10.01	94.0	10767.85	10350.8	94.0	24.2024	
18	3	cold R1881	-10.01	92.7	10629.9	10212.8	92.7	23.89234	
19	1	cold R1881	-11.01	90.5	10388.72	9971.6	90.5	23.35025	
20	2	cold R1881	-11.01	97.6	11167.44	10750.4	97.6	25.10054	
21	3	cold R1881	-11.01	98.5	11273.15	10856.1	98.5	25.33814	
22	1	Weak Positive	-3	3.3	776.97	359.9	3.3	1.74636	
23	2	Weak Positive	-3	3.7	826.08	409.0	3.7	1.856742	
24	3	Weak Positive	-3	4.3	887.25	470.2	4.3	1.994231	
25	1	Weak Positive	-4	28.5	3553.8	3136.7	28.5	7.987713	
26	2	Weak Positive	-4	29.0	3613.8	3196.7	29.0	8.122572	
27	3	Weak Positive	-4	27.4	3436.8	3019.7	27.4	7.724737	
28	1	Weak Positive	-5	77.2	8925.9	8508.8	77.2	20.06233	
29	2	Weak Positive	-5	66.0	7686	7268.9	66.0	17.27547	
30	3	Weak Positive	-5	77.7	8976.6	8559.5	77.7	20.17629	
31	1	Weak Positive	-6	94.9	10869	10451.9	94.9	24.42975	
32	2	Weak Positive	-6	83.7	9636.3	9219.2	83.7	21.65907	
33	3	Weak Positive	-6	90.5	10383.3	9966.2	90.5	23.33807	
34	1	Weak Positive	-7	92.5	10605.6	10188.5	92.5	23.83772	
35	2	Weak Positive	-7	92.4	10592.4	10175.3	92.4	23.80805	
36	3	Weak Positive	-7	88.7	10188	9770.9	88.7	22.8991	
37	1	Weak Positive	-8	80.2	9251.4	8834.3	80.2	20.79395	
38	2	Weak Positive	-8	92.1	10560.9	10143.8	92.1	23.73725	
39	3	Weak Positive	-8	89.6	10287.6	9870.5	89.6	23.12297	
40	1	Weak Positive	-9	89.4	10266	9848.9	89.4	23.07442	
41	2	Weak Positive	-9	91.5	10492.8	10075.7	91.5	23.58418	
42	3	Weak Positive	-9	93.8	10751.4	10334.3	93.8	24.16543	
43	1	Weak Positive	-10	90.9	10430.1	10013.0	90.9	23.44326	
44	2	Weak Positive	-10	91.7	10519.5	10102.4	91.7	23.6442	
45	3	Weak Positive	-10	92.1	10567.2	10150.1	92.1	23.75141	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	121.11	375.44	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	114.98	356.44	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	112.31	348.16	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	122.78	380.62	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	133.65	414.32	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	119.32	369.89	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	146.22	453.28	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	153.72	476.53	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	131.28	406.97	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	137.83	427.27	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	140.00	434.00	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	138.87	430.50	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	184.09	570.68	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	207.48	643.19	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	182.33	565.22	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	663.28	2056.17	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	688.12	2133.17	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	666.52	2066.21	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2426.30	7521.53	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2564.60	7950.26	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2627.50	8145.25	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3601.40	11164.34	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3406.10	10558.91	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3557.80	11029.18	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1068.44	3312.16	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1035.21	3209.15	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1026.68	3182.71	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1437.80	4457.18	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1406.90	4361.39	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1427.20	4424.32	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3038.50	9419.35	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2992.80	9277.68	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2584.60	8012.26	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3541.80	10979.58	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3660.90	11348.79	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3758.90	11652.59	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3611.80	11196.58	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3577.70	11090.87	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3843.60	11915.16	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3753.10	11634.61	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3658.00	11339.80	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3791.30	11753.03	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3602.30	11167.13	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3630.50	11254.55	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3730.20	11563.62	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3801.20	11783.72	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3412.90	10579.99	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3663.40	11356.54	TRUE	

Check the 10% rule: **25.70%** if the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-0.4	375.441	-41.6	10640.8	-0.4	0.843861
47	2	Unknown 1	-3.01424	-0.6	356.438	-60.6	10659.8	-0.6	0.801149
48	3	Unknown 1	-3.01424	-0.6	348.161	-68.9	10668.1	-0.6	0.782545
49	1	Unknown 1	-4.01424	-0.3	380.618	-36.5	10635.6	-0.3	0.855498
50	2	Unknown 1	-4.01424	0.0	414.315	-2.8	10601.9	0.0	0.931237
51	3	Unknown 1	-4.01424	-0.4	369.892	-47.2	10646.3	-0.4	0.831389
52	1	Unknown 1	-5.01424	0.3	453.282	36.2	10563.0	0.3	1.018821
53	2	Unknown 1	-5.01424	0.5	476.532	59.5	10539.7	0.5	1.071079
54	3	Unknown 1	-5.01424	-0.1	406.968	-10.1	10609.3	-0.1	0.914723
55	1	Unknown 1	-6.01424	0.1	427.273	10.2	10589.0	0.1	0.960362
56	2	Unknown 1	-6.01424	0.2	434	16.9	10582.2	0.2	0.975482
57	3	Unknown 1	-6.01424	0.1	430.497	13.4	10585.7	0.1	0.967608
58	1	Unknown 1	-7.01424	1.4	570.679	153.6	10445.6	1.4	1.282689
59	2	Unknown 1	-7.01424	2.1	643.188	226.1	10373.0	2.1	1.445664
60	3	Unknown 1	-7.01424	1.3	565.223	148.1	10451.0	1.3	1.270426
61	1	Unknown 1	-8.01424	14.9	2056.168	1639.1	8960.1	14.9	4.621554
62	2	Unknown 1	-8.01424	15.6	2133.172	1716.1	8883.1	15.6	4.794633
63	3	Unknown 1	-8.01424	15.0	2066.212	1649.1	8950.0	15.0	4.64413
64	1	Unknown 1	-9.01424	64.5	7521.53	7104.5	3494.7	64.5	16.9058
65	2	Unknown 1	-9.01424	68.4	7950.26	7533.2	3066.0	68.4	17.86943
66	3	Unknown 1	-9.01424	70.2	8145.25	7728.2	2871.0	70.2	18.3077
67	1	Unknown 1	-10.01424	97.6	11164.34	10747.3	-148.1	97.6	25.09357
68	2	Unknown 1	-10.01424	92.1	10558.91	10141.8	457.3	92.1	23.73278
69	3	Unknown 1	-10.01424	96.3	11029.18	10612.1	-12.9	96.3	24.78978
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	36.7	4457.18	4040.1	6559.1	36.7	10.0182
74	2	Unknown 2	-4.01424	35.8	4361.39	3944.3	6654.8	35.8	9.802896
75	3	Unknown 2	-4.01424	36.4	4424.32	4007.2	6591.9	36.4	9.944341
76	1	Unknown 2	-5.01424	81.7	9419.35	9002.3	1596.9	81.7	21.17144
77	2	Unknown 2	-5.01424	80.4	9277.68	8860.6	1738.6	80.4	20.85301
78	3	Unknown 2	-5.01424	68.9	8012.26	7595.2	3004.0	68.9	18.00879
79	1	Unknown 2	-6.01424	95.9	10979.58	10562.5	36.7	95.9	24.6783
80	2	Unknown 2	-6.01424	99.2	11348.79	10931.7	-332.6	99.2	25.50815
81	3	Unknown 2	-6.01424	102.0	11652.59	11235.5	-636.4	102.0	26.19099
82	1	Unknown 2	-7.01424	97.9	11196.58	10779.5	-180.3	97.9	25.16604
83	2	Unknown 2	-7.01424	96.9	11090.87	10673.8	-74.6	96.9	24.92844
84	3	Unknown 2	-7.01424	104.4	11915.16	11498.1	-898.9	104.4	26.78116
85	1	Unknown 2	-8.01424	101.8	11634.61	11217.5	-618.4	101.8	26.15058
86	2	Unknown 2	-8.01424	99.2	11339.8	10922.7	-323.6	99.2	25.48795
87	3	Unknown 2	-8.01424	102.9	11753.03	11336.0	-736.8	102.9	26.41675
88	1	Unknown 2	-9.01424	97.6	11167.13	10750.1	-150.9	97.6	25.09984
89	2	Unknown 2	-9.01424	98.4	11254.55	10837.5	-238.3	98.4	25.29633
90	3	Unknown 2	-9.01424	101.2	11563.62	11146.5	-547.4	101.2	25.99102
91	1	Unknown 2	-10.01424	103.2	11783.72	11366.6	-767.5	103.2	26.48573
92	2	Unknown 2	-10.01424	92.3	10579.99	10162.9	436.2	92.3	23.78016
93	3	Unknown 2	-10.01424	99.3	11356.54	10939.5	-340.3	99.3	25.52557

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1+4-E supplied by Entaire to Laboratory	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacenolone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	291.32	903.09	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	258.71	802.00	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	277.17	859.23	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2215.60	6868.36	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2318.50	7187.35	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2268.70	7032.97	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3242.10	10050.51	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3198.40	9915.04	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3936.30	12202.53	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3749.40	11623.14	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3673.10	11386.61	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3847.80	11928.18	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3806.40	11799.84	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3748.10	11619.11	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3759.10	11653.21	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3543.20	10983.92	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3773.00	11696.30	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3321.80	10297.58	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3792.40	11756.44	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3456.10	10713.91	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3736.70	11583.77	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3293.90	10211.09	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3724.60	11546.26	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3823.30	11852.23	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1674.40	5190.64	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1507.80	4674.18	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1455.00	4510.50	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1115.80	3458.98	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1151.20	3568.72	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1130.20	3503.62	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2796.20	8668.22	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3398.80	10536.28	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3209.40	9949.14	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3641.40	11288.34	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3811.40	11815.34	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3752.90	11633.99	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3971.80	12312.58	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3833.20	11882.92	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3746.90	11615.39	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3791.70	11754.27	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3708.20	11495.42	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3853.60	11946.16	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3905.50	12107.05	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3913.90	12133.09	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3351.60	10389.96	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3832.20	11879.82	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3901.70	12095.27	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3774.40	11700.64	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3849.60	11933.76	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3752.80	11633.68	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3826.60	11862.46	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	147.05	441.15	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	144.67	434.01	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	129.05	387.15	TRUE	
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44995.00	44995.00	TRUE	
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	44788.00	44788.00	TRUE	
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	44148.00	44148.00	TRUE	
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44554.00	44554.00	TRUE	
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	44793.00	44793.00	TRUE	
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	43667.00	43667.00	TRUE	

Check the 10% rule: **25.70%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression							
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	58.6	6868.36	6451.3	4147.9	58.6	15.4377
98	2	Unknown 3	-4.01424	61.5	7187.35	6770.3	3828.9	61.5	16.15468
99	3	Unknown 3	-4.01424	60.1	7032.97	6615.9	3983.3	60.1	15.80768
100	1	Unknown 3	-5.01424	87.4	10050.51	9633.4	965.7	87.4	22.59007
101	2	Unknown 3	-5.01424	86.2	9915.04	9498.0	1101.2	86.2	22.28558
102	3	Unknown 3	-5.01424	107.0	12202.53	11785.5	-1186.3	107.0	27.42707
103	1	Unknown 3	-6.01424	101.7	11623.14	11206.1	-606.9	101.7	26.1248
104	2	Unknown 3	-6.01424	99.6	11386.61	10969.5	-370.4	99.6	25.59316
105	3	Unknown 3	-6.01424	104.5	11928.18	11511.1	-911.9	104.5	26.81042
106	1	Unknown 3	-7.01424	103.3	11799.84	11382.8	-783.6	103.3	26.52196
107	2	Unknown 3	-7.01424	101.7	11619.11	11202.0	-602.9	101.7	26.11574
108	3	Unknown 3	-7.01424	102.0	11653.21	11236.1	-637.0	102.0	26.19238
109	1	Unknown 3	-8.01424	95.9	10983.92	10566.8	32.3	95.9	24.68805
110	2	Unknown 3	-8.01424	102.4	11696.3	11279.2	-680.1	102.4	26.28924
111	3	Unknown 3	-8.01424	89.7	10297.58	9880.5	718.7	89.7	23.1454
112	1	Unknown 3	-9.01424	102.9	11756.44	11339.4	-740.2	102.9	26.42441
113	2	Unknown 3	-9.01424	93.5	10713.91	10296.8	302.3	93.5	24.08116
114	3	Unknown 3	-9.01424	101.4	11583.77	11166.7	-567.5	101.4	26.03631
115	1	Unknown 3	-10.01424	88.9	10211.09	9794.0	805.1	88.9	22.951
116	2	Unknown 3	-10.01424	101.0	11546.26	11129.2	-530.0	101.0	25.952
117	3	Unknown 3	-10.01424	103.8	11852.23	11435.2	-836.0	103.8	26.63971
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	27.6	3458.98	3041.9	7557.3	27.6	7.77459
122	2	Unknown 4	-4.01424	28.6	3568.72	3151.6	7447.5	28.6	8.021248
123	3	Unknown 4	-4.01424	28.0	3503.62	3086.5	7512.6	28.0	7.874926
124	1	Unknown 4	-5.01424	74.9	8668.22	8251.1	2348.0	74.9	19.48316
125	2	Unknown 4	-5.01424	91.9	10536.28	10119.2	480.0	91.9	23.68191
126	3	Unknown 4	-5.01424	86.5	9949.14	9532.1	1067.1	86.5	22.36222
127	1	Unknown 4	-6.01424	98.7	11288.34	10871.3	-272.1	98.7	25.37228
128	2	Unknown 4	-6.01424	103.5	11815.34	11398.3	-799.1	103.5	26.5568
129	3	Unknown 4	-6.01424	101.8	11633.99	11216.9	-617.8	101.8	26.14918
130	1	Unknown 4	-7.01424	108.0	12312.58	11895.5	-1296.3	108.0	27.67442
131	2	Unknown 4	-7.01424	104.1	11882.92	11465.8	-866.7	104.1	26.70869
132	3	Unknown 4	-7.01424	101.7	11615.39	11198.3	-599.2	101.7	26.10738
133	1	Unknown 4	-8.01424	102.9	11754.27	11337.2	-738.0	102.9	26.41953
134	2	Unknown 4	-8.01424	100.6	11495.42	11078.3	-479.2	100.6	25.83773
135	3	Unknown 4	-8.01424	104.7	11946.16	11529.1	-929.9	104.7	26.85083
136	1	Unknown 4	-9.01424	106.1	12107.05	11690.0	-1090.8	106.1	27.21246
137	2	Unknown 4	-9.01424	106.4	12133.09	11716.0	-1116.9	106.4	27.27099
138	3	Unknown 4	-9.01424	90.5	10389.96	9972.9	626.3	90.5	23.35304
139	1	Unknown 4	-10.01424	104.1	11879.82	11462.7	-863.6	104.1	26.70173
140	2	Unknown 4	-10.01424	106.0	12095.27	11678.2	-1079.0	106.0	27.18598
141	3	Unknown 4	-10.01424	102.4	11700.64	11283.6	-684.4	102.4	26.29899
142	1	—	—	104.5	11933.76	11516.7	-917.5	104.5	26.82296
143	2	—	—	101.8	11633.68	11216.6	-617.4	101.8	26.14849
144	3	—	—	103.9	11862.46	11445.4	-846.2	103.9	26.66271
145	1	-6.00		0.2	441.15	24.1	10575.1	0.2	0.991553
146	2	-6.00		0.2	434.01	16.9	10582.2	0.2	0.975504
147	3	-6.00		-0.3	387.15	-29.9	10629.1	-0.3	0.870179
148	1				44995	44577.9			
149	2				44788	44370.9			
150	3				44148	43730.9			
151	1				44554	44136.9			
152	2				44793	44375.9			
153	3				43667	43249.9			

Prism data												
standard curve				weak positive					CR42340			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	0.18554	0.36147	-0.64750	-3	3.2669	3.7127	4.2680	-3.0	-0.3780	-0.5505	-0.6256	
-6.0	0.21850	0.15368	-0.27169	-4	28.4736	29.0183	27.4115	-4.0	-0.3310	-0.0251	-0.4283	
-7.0	2.20530	1.37460	1.21673	-5	77.2389	65.9837	77.6991	-5.0	0.3286	0.5397	-0.0918	
-8.0	13.33731	14.35458	14.56704	-6	94.8774	83.6876	90.4685	-6.0	0.0925	0.1536	0.1218	
-9.0	63.28631	61.23207	62.36331	-7	92.4864	92.3666	88.6956	-7.0	1.3943	2.0525	1.3448	
-10.0	95.26493	93.95922	92.70698	-8	80.1936	92.0806	89.5997	-8.0	14.8788	15.5778	14.9700	
-11.0	90.51766	97.58650	98.54609	-9	89.4037	91.4625	93.8099	-9.0	64.4907	68.3825	70.1525	
				-10	90.8933	91.7048	92.1378	-10.0	97.5584	92.0626	96.3314	

CR42350				CR42354				CR42363			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0				-3.0			
-4.0	36.6740	35.8045	36.3758	-4.0	58.5616	61.4572	60.0558	-4.0	27.6129	28.6090	28.0181
-5.0	81.7182	80.4322	68.9453	-5.0	87.4476	86.2178	106.9825	-5.0	74.8998	91.8571	86.5274
-6.0	95.8812	99.2327	101.9905	-6.0	101.7231	99.5760	104.4921	-6.0	98.6840	103.4678	101.8216
-7.0	97.8510	96.8914	104.3739	-7.0	103.3271	101.6865	101.9961	-7.0	107.9815	104.0813	101.6528
-8.0	101.8272	99.1511	102.9022	-8.0	95.9206	102.3872	89.6903	-8.0	102.9135	100.5637	104.6553
-9.0	97.5837	98.3772	101.1828	-9.0	102.9332	93.4696	101.3657	-9.0	106.1158	106.3522	90.5289
-10.0	103.1808	92.2539	99.3031	-10.0	88.9052	101.0252	103.8027	-10.0	104.0531	106.0089	102.4266

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:			
Run identification:	508		
Assay start date:	9/28/2005		
Tracer lot number:	3559-507		
Specific activity on day of assay:	79.97	Ci/mmole	
Cytosol vial or lot identification:	051905		
Protein (cytosol):	1000	micro gram per tube	
Standard Curve IC50:	1.53E-09	M	
Weak Positive, Max Concentration:	3.00E-02	M	
Weak Positive IC50:	3.80E-05	M	
RBA:	4.01736E-05		
Max Concentration, Unknown 1:	3.00E-02	M	5e-3
IC50, Unknown 1:	2.19E-09	CR42340	
RBA, Unknown 1:	69.66241%		
Max Concentration, Unknown 2:	3.00E-02	M	(example 5e-3)
IC50, Unknown 2:	4.81E-05	CR42350	
RBA, Unknown 2:	0.00317%		
Max Concentration, Unknown 3:	3.00E-02	M	(example 5e-3)
IC50, Unknown 3:	1.44E-04	CR42354	
RBA, Unknown 3:	0.00106%		
Max Concentration, Unknown 4:	3.00E-02	M	(example 5e-3)
IC50, Unknown 4:	5.05E-05	CR42363	
RBA, Unknown 4:	0.00302%		
volume of ethanol counted:	2	mL	
multiply DPM in sample by :	3.1		
working volume	3.1E+02	uL	protocol calls for counting decanted EtOH supernate reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10682.0	1538.07	Total Binding, solvent control, tubes
Hot	6	44801.0	475.25	Total hot R1881 added to each tube
NSB	6	457.9	46.15	Nonspecific Binding
Specific EtOH	6	10224.1	1538.07	

Assay Characterization Values	
EtOH / Hot	0.24 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3112.90	9649.99	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2939.80	9113.38	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2961.90	9181.89	TRUE	
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	139.84	419.52	TRUE		
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	140.12	420.36	TRUE		
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	155.96	467.88	TRUE		
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	175.45	543.90	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	181.38	562.28	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	191.80	594.58	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	581.70	1803.27	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	653.17	2024.83	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	626.37	1941.75	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2344.70	7268.57	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2076.10	6435.91	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2098.30	6504.73	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2947.90	9138.49	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2947.10	9136.01	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3290.00	10199.00	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3451.10	10698.41	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3216.40	9970.84	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3035.30	9409.43	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	278.25	834.75	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	335.31	1005.93	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	282.48	847.44	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1191.90	3575.70	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	949.81	2849.43	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1039.90	3119.70	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2579.50	7738.50	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3062.80	9188.40	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3074.60	9223.80	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3502.10	10506.30	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3259.40	9778.20	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3194.60	9583.80	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3723.90	11171.70	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3517.70	10553.10	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3651.80	10955.40	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3675.90	11027.70	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3688.40	11065.20	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2978.10	8934.30	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3375.40	10126.20	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3458.80	10376.40	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3437.20	10311.60	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3705.00	11115.00	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3081.10	9243.30	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3127.20	9381.60	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot
1	1				89.9	9649.99	9192.1	89.9	21.53968
2	2				84.7	9113.38	8655.5	84.7	20.34191
3	3				85.3	9181.89	8724.0	85.3	20.49483
4	1		-6.00	-0.4	419.52	-38.4	9804.6	-0.4	0.936408
5	2		-6.00	-0.4	420.36	-37.5	9803.7	-0.4	0.938283
6	3		-6.00	0.0	467.88	10.0	9756.2	0.1	1.044352
7	1	cold R1881	-7.01	0.8	543.895	86.0	9680.2	0.8	1.214024
8	2	cold R1881	-7.01	1.0	562.278	104.4	9661.8	1.0	1.255057
9	3	cold R1881	-7.01	1.3	594.58	136.7	9629.5	1.3	1.327158
10	1	cold R1881	-8.01	13.2	1803.27	1345.4	8420.8	13.2	4.025066
11	2	cold R1881	-8.01	15.3	2024.827	1567.0	8199.3	15.3	4.519602
12	3	cold R1881	-8.01	14.5	1941.747	1483.9	8282.4	14.5	4.33416
13	1	cold R1881	-9.01	66.6	7268.57	6810.7	2955.5	66.6	16.22412
14	2	cold R1881	-9.01	58.5	6435.91	5978.0	3788.2	58.5	14.36555
15	3	cold R1881	-9.01	59.1	6504.73	6046.9	3719.4	59.1	14.51916
16	1	cold R1881	-10.01	84.9	9138.49	8680.6	1085.6	84.9	20.39796
17	2	cold R1881	-10.01	84.9	9136.01	8678.1	1088.1	84.9	20.39242
18	3	cold R1881	-10.01	95.3	10199	9741.1	25.1	95.3	22.76512
19	1	cold R1881	-11.01	100.2	10698.41	10240.5	-474.3	100.2	23.87985
20	2	cold R1881	-11.01	93.0	9970.84	9513.0	253.3	93.0	22.25584
21	3	cold R1881	-11.01	87.6	9409.43	8951.6	814.7	87.6	21.00272
22	1	Weak Positive	-3	3.7	834.75	376.9	9389.4	3.7	1.86324
23	2	Weak Positive	-3	5.4	1005.93	548.1	9218.2	5.4	2.245329
24	3	Weak Positive	-3	3.8	847.44	389.6	9376.7	3.8	1.891565
25	1	Weak Positive	-4	30.5	3575.7	3117.8	6648.4	30.5	7.981295
26	2	Weak Positive	-4	23.4	2849.43	2391.6	7374.7	23.4	6.360193
27	3	Weak Positive	-4	26.0	3119.7	2661.8	7104.4	26.0	6.963461
28	1	Weak Positive	-5	71.2	7738.5	7280.6	2485.6	71.2	17.27305
29	2	Weak Positive	-5	85.4	9188.4	8730.5	1035.7	85.4	20.50936
30	3	Weak Positive	-5	85.7	9223.8	8765.9	1000.3	85.7	20.58838
31	1	Weak Positive	-6	98.3	10506.3	10048.4	-282.2	98.3	23.45104
32	2	Weak Positive	-6	91.2	9778.2	9320.3	445.9	91.2	21.82585
33	3	Weak Positive	-6	89.3	9583.8	9125.9	640.3	89.3	21.39193
34	1	Weak Positive	-7	104.8	11171.7	10713.8	-947.6	104.8	24.93627
35	2	Weak Positive	-7	98.7	10553.1	10095.2	-329.0	98.7	23.55555
36	3	Weak Positive	-7	102.7	10955.4	10497.5	-731.3	102.7	24.45347
37	1	Weak Positive	-8	103.4	11027.7	10569.8	-803.6	103.4	24.61485
38	2	Weak Positive	-8	103.7	11065.2	10607.3	-841.1	103.7	24.69856
39	3	Weak Positive	-8	82.9	8934.3	8476.4	1289.8	82.9	19.94219
40	1	Weak Positive	-9	94.6	10126.2	9668.3	97.9	94.6	22.60262
41	2	Weak Positive	-9	97.0	10376.4	9918.5	-152.3	97.0	23.16109
42	3	Weak Positive	-9	96.4	10311.6	9853.7	-87.5	96.4	23.01645
43	1	Weak Positive	-10	104.2	11115	10657.1	-890.9	104.2	24.80971
44	2	Weak Positive	-10	85.9	9243.3	8785.4	980.8	85.9	20.63191
45	3	Weak Positive	-10	87.3	9381.6	8923.7	842.5	87.3	20.9406

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,1-E supplied by Battelle to laboratory	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	111.23	344.81	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	128.69	398.94	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	132.31	410.16	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	118.93	368.68	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	142.57	441.97	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	139.92	433.75	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	116.08	359.85	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	127.64	395.68	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	157.34	487.75	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	147.97	458.71	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	144.16	446.90	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	153.61	476.19	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	197.94	613.61	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	194.49	602.92	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	215.54	668.17	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	766.91	2377.42	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	825.62	2559.42	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	715.33	2217.52	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2263.60	7017.16	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2318.80	7188.28	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2517.90	7805.49	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3414.70	10585.57	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3456.90	10716.39	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3464.10	10738.71	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	937.87	2907.40	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1045.81	3242.01	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1016.27	3150.44	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1401.10	4343.41	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1218.30	3776.73	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1185.10	3673.81	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2539.80	7873.38	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	3199.60	9918.76	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2749.70	8524.07	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3182.60	9866.06	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3113.50	9651.85	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3280.80	10170.48	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3379.90	10477.69	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3378.20	10472.42	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3430.60	10634.86	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3568.40	11062.04	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3436.40	10652.84	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3836.60	11893.46	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3371.30	10451.03	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3857.60	11958.56	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3387.10	10500.01	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3050.20	9455.62	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3771.20	11690.72	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3247.20	10066.32	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	-1.1	344.813	-113.1	9879.3	-1.1	0.769655
47	2	Unknown 1	-3.01424	-0.6	398.939	-58.9	9825.2	-0.6	0.890469
48	3	Unknown 1	-3.01424	-0.5	410.161	-47.7	9813.9	-0.5	0.915518
49	1	Unknown 1	-4.01424	-0.9	368.683	-89.2	9855.4	-0.9	0.822935
50	2	Unknown 1	-4.01424	-0.2	441.967	-15.9	9782.1	-0.2	0.986511
51	3	Unknown 1	-4.01424	-0.2	433.752	-24.1	9790.4	-0.2	0.968175
52	1	Unknown 1	-5.01424	-1.0	359.848	-98.0	9864.3	-1.0	0.803214
53	2	Unknown 1	-5.01424	-0.6	395.684	-62.2	9828.4	-0.6	0.883203
54	3	Unknown 1	-5.01424	0.3	487.754	29.9	9736.4	0.3	1.088712
55	1	Unknown 1	-6.01424	0.0	458.707	0.8	9765.4	0.0	1.023877
56	2	Unknown 1	-6.01424	-0.1	446.896	-11.0	9777.2	-0.1	0.997513
57	3	Unknown 1	-6.01424	0.2	476.191	18.3	9747.9	0.2	1.062903
58	1	Unknown 1	-7.01424	1.5	613.614	155.7	9610.5	1.5	1.369644
59	2	Unknown 1	-7.01424	1.4	602.919	145.0	9621.2	1.4	1.345771
60	3	Unknown 1	-7.01424	2.1	668.174	210.3	9555.9	2.1	1.491427
61	1	Unknown 1	-8.01424	18.8	2377.421	1919.5	7846.7	18.8	5.306625
62	2	Unknown 1	-8.01424	20.6	2559.422	2101.5	7664.7	20.6	5.712868
63	3	Unknown 1	-8.01424	17.2	2217.523	1759.6	8006.6	17.2	4.949718
64	1	Unknown 1	-9.01424	64.2	7017.16	6559.3	3206.9	64.2	15.66295
65	2	Unknown 1	-9.01424	65.8	7188.28	6730.4	3035.8	65.8	16.04491
66	3	Unknown 1	-9.01424	71.9	7805.49	7347.6	2418.6	71.9	17.42258
67	1	Unknown 1	-10.01424	99.1	10585.57	10127.7	-361.5	99.1	23.62798
68	2	Unknown 1	-10.01424	100.3	10716.39	10258.5	-492.3	100.3	23.91998
69	3	Unknown 1	-10.01424	100.6	10738.71	10280.8	-514.6	100.6	23.9698
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	38.0	4343.41	3885.5	5880.7	38.0	9.694895
74	2	Unknown 2	-4.01424	32.5	3776.73	3318.9	6447.4	32.5	8.430013
75	3	Unknown 2	-4.01424	31.5	3673.81	3215.9	6550.3	31.5	8.200286
76	1	Unknown 2	-5.01424	72.5	7873.38	7415.5	2350.7	72.5	17.57412
77	2	Unknown 2	-5.01424	92.5	9918.76	9460.9	305.3	92.5	22.1396
78	3	Unknown 2	-5.01424	78.9	8524.07	8066.2	1700.0	78.9	19.02652
79	1	Unknown 2	-6.01424	92.0	9866.06	9408.2	358.0	92.0	22.02196
80	2	Unknown 2	-6.01424	89.9	9651.85	9194.0	572.3	89.9	21.54383
81	3	Unknown 2	-6.01424	95.0	10170.48	9712.6	53.6	95.0	22.70146
82	1	Unknown 2	-7.01424	98.0	10477.69	10019.8	-253.6	98.0	23.38718
83	2	Unknown 2	-7.01424	98.0	10472.42	10014.5	-248.3	98.0	23.37542
84	3	Unknown 2	-7.01424	99.5	10634.86	10177.0	-410.8	99.5	23.738
85	1	Unknown 2	-8.01424	103.7	11062.04	10604.2	-837.9	103.7	24.6915
86	2	Unknown 2	-8.01424	99.7	10652.84	10195.0	-428.7	99.7	23.77813
87	3	Unknown 2	-8.01424	111.8	11893.46	11435.6	-1669.4	111.8	26.54731
88	1	Unknown 2	-9.01424	97.7	10451.03	9993.2	-226.9	97.7	23.32767
89	2	Unknown 2	-9.01424	112.5	11958.56	11500.7	-1734.5	112.5	26.69262
90	3	Unknown 2	-9.01424	98.2	10500.01	10042.1	-275.9	98.2	23.437
91	1	Unknown 2	-10.01424	88.0	9455.62	8997.7	768.5	88.0	21.10582
92	2	Unknown 2	-10.01424	109.9	11690.72	11232.8	-1466.6	109.9	26.09477
93	3	Unknown 2	-10.01424	94.0	10066.32	9608.4	157.8	94.0	22.46896

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1+1-E supplied by Battelle to laboratory	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	238.21	738.45	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	243.83	755.87	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	286.04	886.72	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1884.00	5840.40	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2036.30	6312.53	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2366.30	7335.53	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3200.90	9922.79	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3401.60	10544.96	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3093.80	9590.78	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3229.00	10009.90	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3821.20	11845.72	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3012.10	9337.51	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3212.90	9959.99	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3088.80	9575.28	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3801.90	11785.89	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3797.50	11772.25	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3568.90	11063.59	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3145.10	9749.81	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3637.20	11275.32	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3533.50	10953.85	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3811.70	11816.27	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3047.90	9448.49	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3213.70	9962.47	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3451.80	10700.58	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1281.70	3973.27	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1243.10	3853.61	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	1398.00	4333.80	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1128.60	3498.66	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	984.32	3051.39	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	1082.40	3355.44	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2917.40	9043.94	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3320.10	10292.31	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3289.50	10197.45	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3086.40	9567.84	FALSE	spill
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3754.70	11639.57	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3709.30	11498.83	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	2861.50	8870.65	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3455.80	10712.98	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3703.70	11481.47	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3293.00	10208.30	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3247.90	10068.49	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3076.50	9537.15	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3854.70	11949.57	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3448.80	10691.28	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3901.20	12093.72	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3828.30	11867.73	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3706.30	11489.53	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3933.40	12193.54	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3982.40	12345.44	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3967.00	12297.70	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3710.80	11503.48	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	151.79	455.37	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	146.82	440.46	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	181.22	543.66	TRUE	
148	1	none	Hot	—	—	—	30	—	—	—	—	—	—	44935.00	44935.00	TRUE	
149	2	none	Hot	—	—	—	30	—	—	—	—	—	—	43880.00	43880.00	TRUE	
150	3	none	Hot	—	—	—	30	—	—	—	—	—	—	44953.00	44953.00	TRUE	
151	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45278.00	45278.00	TRUE	
152	2	none	Hot	—	—	—	30	—	—	—	—	—	—	44882.00	44882.00	TRUE	
153	3	none	Hot	—	—	—	30	—	—	—	—	—	—	44878.00	44878.00	TRUE	

Check the 10% rule: **23.84%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

			Values for analysis by nonlinear regression						
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICH)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.01424						
95	2	Unknown 3	-3.01424						
96	3	Unknown 3	-3.01424						
97	1	Unknown 3	-4.01424	52.6	5840.4	5382.5	4383.7	52.6	13.03632
98	2	Unknown 3	-4.01424	57.3	6312.53	5854.7	3911.6	57.3	14.09015
99	3	Unknown 3	-4.01424	67.3	7335.53	6877.7	2888.6	67.3	16.37359
100	1	Unknown 3	-5.01424	92.6	9922.79	9464.9	301.3	92.6	22.14859
101	2	Unknown 3	-5.01424	98.7	10544.96	10087.1	-320.9	98.7	23.53733
102	3	Unknown 3	-5.01424	89.3	9590.78	9132.9	633.3	89.3	21.40751
103	1	Unknown 3	-6.01424	93.4	10009.9	9552.0	214.2	93.4	22.34303
104	2	Unknown 3	-6.01424	111.4	11845.72	11387.8	-1621.6	111.4	26.44075
105	3	Unknown 3	-6.01424	86.8	9337.51	8879.6	886.6	86.8	20.84219
106	1	Unknown 3	-7.01424	92.9	9959.99	9502.1	264.1	92.9	22.23162
107	2	Unknown 3	-7.01424	89.2	9575.28	9117.4	648.8	89.2	21.37292
108	3	Unknown 3	-7.01424	110.8	11785.89	11328.0	-1561.8	110.8	26.3072
109	1	Unknown 3	-8.01424	110.7	11772.25	11314.4	-1548.1	110.7	26.27676
110	2	Unknown 3	-8.01424	103.7	11063.59	10605.7	-839.5	103.7	24.69496
111	3	Unknown 3	-8.01424	90.9	9749.81	9291.9	474.3	90.9	21.76248
112	1	Unknown 3	-9.01424	105.8	11275.32	10817.4	-1051.2	105.8	25.16756
113	2	Unknown 3	-9.01424	102.7	10953.85	10496.0	-729.7	102.7	24.45001
114	3	Unknown 3	-9.01424	111.1	11816.27	11358.4	-1592.2	111.1	26.37501
115	1	Unknown 3	-10.01424	87.9	9448.49	8990.6	775.6	87.9	21.08991
116	2	Unknown 3	-10.01424	93.0	9962.47	9504.6	261.6	93.0	22.23716
117	3	Unknown 3	-10.01424	100.2	10700.58	10242.7	-476.5	100.2	23.88469
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	29.7	3498.66	3040.8	6725.4	29.7	7.809335
122	2	Unknown 4	-4.01424	25.4	3051.392	2593.5	7172.7	25.4	6.810991
123	3	Unknown 4	-4.01424	28.3	3355.44	2897.6	6868.7	28.3	7.489654
124	1	Unknown 4	-5.01424	84.0	9043.94	8586.1	1180.2	84.0	20.18692
125	2	Unknown 4	-5.01424	96.2	10292.31	9834.4	-68.2	96.2	22.97339
126	3	Unknown 4	-5.01424	95.3	10197.45	9739.6	26.7	95.3	22.76166
127	1	Unknown 4	-6.01424						
128	2	Unknown 4	-6.01424	109.4	11639.57	11181.7	-1415.5	109.4	25.9806
129	3	Unknown 4	-6.01424	108.0	11498.83	11041.0	-1274.7	108.0	25.66646
130	1	Unknown 4	-7.01424	82.3	8870.65	8412.8	1353.5	82.3	19.80012
131	2	Unknown 4	-7.01424	100.3	10712.98	10255.1	-488.9	100.3	23.91237
132	3	Unknown 4	-7.01424	107.8	11481.47	11023.6	-1257.4	107.8	25.62771
133	1	Unknown 4	-8.01424	95.4	10208.3	9750.4	15.8	95.4	22.78588
134	2	Unknown 4	-8.01424	94.0	10068.49	9610.6	155.6	94.0	22.47381
135	3	Unknown 4	-8.01424	88.8	9537.15	9079.3	687.0	88.8	21.28781
136	1	Unknown 4	-9.01424	112.4	11949.57	11491.7	-1725.5	112.4	26.67255
137	2	Unknown 4	-9.01424	100.1	10691.28	10233.4	-467.2	100.1	23.86393
138	3	Unknown 4	-9.01424	113.8	12093.72	11635.8	-1869.6	113.8	26.99431
139	1	Unknown 4	-10.01424	111.6	11867.73	11409.9	-1643.6	111.6	26.48988
140	2	Unknown 4	-10.01424	107.9	11489.53	11031.7	-1265.4	107.9	25.6457
141	3	Unknown 4	-10.01424	114.8	12193.54	11735.7	-1969.4	114.8	27.21712
142	1	—	—	116.3	12345.44	11887.6	-2121.3	116.3	27.55617
143	2	—	—	115.8	12297.7	11839.8	-2073.6	115.8	27.44961
144	3	—	—	108.0	11503.48	11045.6	-1279.4	108.0	25.67684
145	1	-6.00	0.0	455.37	-2.5	9768.7	0.0	1.016428	
146	2	-6.00	-0.2	440.46	-17.4	9783.6	-0.2	0.983148	
147	3	-6.00	0.8	543.66	85.8	9680.4	0.8	1.2135	
148	1				44935	44477.1			
149	2				43880	43422.1			
150	3				44953	44495.1			
151	1				45278	44820.1			
152	2				44882	44424.1			
153	3				44878	44420.1			

Prism data												
standard curve				weak positive				CR42340				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	-0.37514	-0.36693	0.09786	-3	3.6861	5.3604	3.8103	-3.0	-1.1058	-0.5764	-0.4667	
-6.0	-0.02450	-0.17033	0.83905	-4	30.4948	23.3913	26.0348	-4.0	-0.8724	-0.1556	-0.2359	
-7.0	0.84135	1.02115	1.33709	-5	71.2104	85.3916	85.7378	-5.0	-0.9588	-0.6083	0.2922	
-8.0	13.15905	15.32606	14.51347	-6	98.2817	91.1603	89.2589	-6.0	0.0081	-0.1074	0.1791	
-9.0	66.61409	58.47001	59.14312	-7	104.7899	98.7394	102.6743	-7.0	1.5233	1.4186	2.0569	
-10.0	84.90342	84.87917	95.27607	-8	103.3814	103.7482	82.9063	-8.0	18.7747	20.5548	17.2108	
-11.0	100.16070	93.04448	87.55343	-9	94.5640	97.0112	96.3774	-9.0	64.1551	65.8288	71.8656	
				-10	104.2353	85.9285	87.2812	-10.0	99.0570	100.3366	100.5549	

CR42350				CR42354				CR42363			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0				-3.0			
-4.0	38.0037	32.4611	31.4544	-4.0	52.6454	57.2633	67.2690	-4.0	29.7413	25.3667	28.3405
-5.0	72.5296	92.5351	78.8939	-5.0	92.5745	98.6598	89.3272	-5.0	83.9786	96.1887	95.2609
-6.0	92.0196	89.9245	94.9971	-6.0	93.4265	111.3823	86.8500	-6.0		109.3660	107.9895
-7.0	98.0019	97.9503	99.5391	-7.0	92.9384	89.1756	110.7971	-7.0	82.2837	100.3032	107.8197
-8.0	103.7173	99.7150	111.8493	-8.0	110.6637	103.7325	90.8826	-8.0	95.3670	93.9996	88.8026
-9.0	97.7411	112.4860	98.2202	-9.0	105.8033	102.6591	111.0943	-9.0	112.3981	100.0910	113.8080
-10.0	88.0052	109.8663	93.9783	-10.0	87.9355	92.9626	100.1819	-10.0	111.5976	107.8985	114.7843

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	509	
Assay start date:	10/3/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.91	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.61E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	4.04E-05	M
RBA:	3.97919E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3
IC50, Unknown 1:	3.94E-05	CR42352
RBA, Unknown 1:	0.00407%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	4.03E-05	CR42353
RBA, Unknown 2:	0.00399%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	4.49E-03	CR42359
RBA, Unknown 3:	0.00004%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	4.16E-05	CR42360
RBA, Unknown 4:	0.00387%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11217.0	657.99	Total Binding, solvent control, tubes
Hot	6	45884.8	373.60	Total hot R1881 added to each tube
NSB	6	387.1	39.91	Nonspecific Binding
Specific EtOH	6	10829.9	657.99	

Assay Characterization Values	
EtOH / Hot	0.24 less than 0.1?
NSB / EtOH	0.03 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.45%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3302.80	10238.68	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3859.10	11963.21	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3740.70	11596.17	TRUE	
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.85	398.55	TRUE		
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	133.85	401.55	TRUE		
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	144.01	432.03	TRUE		
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	192.51	596.78	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	172.79	535.65	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	192.69	597.34	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	611.04	1894.22	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	585.47	1814.96	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	604.01	1872.43	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2275.90	7055.29	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2319.00	7188.90	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2300.50	7131.55	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3522.40	10919.44	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3364.20	10429.02	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3215.10	9966.81	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2985.00	9253.50	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3683.90	11420.09	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3412.10	10577.51	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	256.06	768.18	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	280.13	840.39	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	273.53	820.59	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1200.30	3600.90	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1221.40	3664.20	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1172.30	3516.90	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3008.60	9025.80	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2950.00	8850.00	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3061.80	9185.40	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3719.60	11158.80	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3259.20	9777.60	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2882.90	8648.70	FALSE	spill
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3864.70	11594.10	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2864.20	8592.60	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2820.00	8460.00	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3398.00	10194.00	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3690.90	11072.70	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3652.30	10956.90	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3770.90	11312.70	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3109.30	9327.90	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3517.80	10553.40	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3360.00	10080.00	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3811.70	11435.10	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3782.40	11347.20	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean MSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
1	1	—	91.0	10238.68	9851.6	591.3	91.0	22.31387	
2	2	—	106.9	11963.21	11576.2	-1133.3	106.9	26.07225	
3	3	—	103.5	11596.17	11209.1	-766.2	103.5	25.27234	
4	1	-6.00	0.1	398.55	11.5	10431.4	0.1	0.868588	
5	2	-6.00	0.1	401.55	14.5	10428.4	0.1	0.875126	
6	3	-6.00	0.0	432.03	45.0	10397.9	0.4	0.941553	
7	1	cold R1881	-7.01	1.9	596.781	209.7	1.9	1.300606	
8	2	cold R1881	-7.01	1.4	535.649	148.6	1.4	1.167377	
9	3	cold R1881	-7.01	1.9	597.339	210.3	1.9	1.301822	
10	1	cold R1881	-8.01	13.9	1894.224	1507.2	13.9	4.128214	
11	2	cold R1881	-8.01	13.2	1814.957	1427.9	13.2	3.955462	
12	3	cold R1881	-8.01	13.7	1872.431	1485.4	13.7	4.080719	
13	1	cold R1881	-9.01	61.6	7055.29	6668.2	61.6	15.37608	
14	2	cold R1881	-9.01	62.8	7188.9	6801.8	62.8	15.66727	
15	3	cold R1881	-9.01	62.3	7131.55	6744.5	62.3	15.54228	
16	1	cold R1881	-10.01	97.3	10919.44	10532.4	97.3	23.79749	
17	2	cold R1881	-10.01	92.7	10429.02	10042.0	92.7	22.72869	
18	3	cold R1881	-10.01	88.5	9966.81	9579.8	88.5	21.72136	
19	1	cold R1881	-11.01	81.9	9253.5	8866.4	81.9	20.16679	
20	2	cold R1881	-11.01	101.9	11420.09	11033.0	101.9	24.88859	
21	3	cold R1881	-11.01	94.1	10577.51	10190.5	94.1	23.0523	
22	1	Weak Positive	-3	3.5	768.18	381.1	3.5	1.674148	
23	2	Weak Positive	-3	4.2	840.39	453.3	4.2	1.83152	
24	3	Weak Positive	-3	4.0	820.59	433.5	4.0	1.788369	
25	1	Weak Positive	-4	29.7	3600.9	3213.8	29.7	7.847691	
26	2	Weak Positive	-4	30.3	3664.2	3277.1	30.3	7.985645	
27	3	Weak Positive	-4	28.9	3516.9	3129.8	28.9	7.664624	
28	1	Weak Positive	-5	79.8	9025.8	8638.7	79.8	19.67055	
29	2	Weak Positive	-5	78.1	8850	8462.9	78.1	19.28742	
30	3	Weak Positive	-5	81.2	9185.4	8798.3	81.2	20.01838	
31	1	Weak Positive	-6	99.5	11158.8	10771.7	99.5	24.31915	
32	2	Weak Positive	-6	86.7	9777.6	9390.5	86.7	21.309	
33	3	Weak Positive	-6						
34	1	Weak Positive	-7	103.5	11594.1	11207.0	103.5	25.26783	
35	2	Weak Positive	-7	75.8	8592.6	8205.5	75.8	18.72645	
36	3	Weak Positive	-7	74.5	8460	8072.9	74.5	18.43746	
37	1	Weak Positive	-8	90.6	10194	9806.9	90.6	22.21649	
38	2	Weak Positive	-8	98.7	11072.7	10685.6	98.7	24.1315	
39	3	Weak Positive	-8	97.6	10956.9	10569.8	97.6	23.87913	
40	1	Weak Positive	-9	100.9	11312.7	10925.6	100.9	24.65455	
41	2	Weak Positive	-9	82.6	9327.9	8940.8	82.6	20.32894	
42	3	Weak Positive	-9	93.9	10553.4	10166.3	93.9	22.99976	
43	1	Weak Positive	-10	89.5	10080	9692.9	89.5	21.96804	
44	2	Weak Positive	-10	102.0	11435.1	11048.0	102.0	24.92131	
45	3	Weak Positive	-10	101.2	11347.2	10960.1	101.2	24.72974	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.45%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	170.67	529.08	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	154.16	477.90	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	168.99	523.87	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1127.10	3494.01	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1141.60	3538.96	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1155.70	3582.67	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2649.50	8213.45	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3107.50	9633.25	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	3070.50	9518.55	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2949.50	9143.45	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3579.10	11095.21	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3206.70	9940.77	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3050.10	9455.31	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3482.90	10796.99	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3778.00	11711.80	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3778.00	11711.80	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3477.50	10780.25	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3746.30	11613.53	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3883.00	12037.30	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2776.60	8607.46	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3599.40	11158.14	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3877.10	12019.01	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3180.80	9860.48	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3691.80	11444.58	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	26.20	81.22	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	24.48	75.89	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	27.68	85.81	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1122.20	3478.82	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1047.70	3247.87	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1402.90	4348.99	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2571.90	7972.89	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2912.50	9028.75	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2951.80	9150.58	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3892.00	12065.20	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3655.20	11331.12	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3623.80	11233.78	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3875.90	12015.29	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3633.60	11264.16	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3816.20	11830.22	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3128.10	9697.11	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3850.80	11937.48	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3642.70	11292.37	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3853.70	11946.47	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3969.30	12304.83	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3825.30	11858.43	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3978.00	12331.80	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3957.90	12269.49	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3963.90	12288.09	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	1.3	529.077	142.0	10300.9	1.3	1.153054
47	2	Unknown 1	-3.01424	0.8	477.896	90.8	10352.0	0.8	1.041512
48	3	Unknown 1	-3.01424	1.3	523.869	136.8	10306.1	1.3	1.141704
49	1	Unknown 1	-4.01424	28.7	3494.01	3107.0	7335.9	28.7	7.614738
50	2	Unknown 1	-4.01424	29.1	3538.96	3151.9	7291.0	29.1	7.712701
51	3	Unknown 1	-4.01424	29.5	3582.67	3195.6	7247.3	29.5	7.807961
52	1	Unknown 1	-5.01424	72.3	8213.45	7826.4	2616.5	72.3	17.90014
53	2	Unknown 1	-5.01424	85.4	9633.25	9246.2	1196.7	85.4	20.99441
54	3	Unknown 1	-5.01424	84.3	9518.55	9131.5	1311.4	84.3	20.74444
55	1	Unknown 1	-6.01424	80.9	9143.45	8756.4	1686.5	80.9	19.92695
56	2	Unknown 1	-6.01424	98.9	11095.21	10708.2	-265.3	98.9	24.18056
57	3	Unknown 1	-6.01424	88.2	9940.77	9553.7	889.2	88.2	21.66461
58	1	Unknown 1	-7.01424	83.7	9455.31	9068.3	1374.6	83.7	20.60661
59	2	Unknown 1	-7.01424	96.1	10796.99	10409.9	32.9	96.1	23.53063
60	3	Unknown 1	-7.01424	104.6	11711.8	11324.7	-881.9	104.6	25.52434
61	1	Unknown 1	-8.01424	104.6	11711.8	11324.7	-881.9	104.6	25.52434
62	2	Unknown 1	-8.01424	96.0	10780.25	10393.2	49.7	96.0	23.49415
63	3	Unknown 1	-8.01424	103.7	11613.53	11226.5	-783.6	103.7	25.31017
64	1	Unknown 1	-9.01424	107.6	12037.3	11650.2	-1207.4	107.6	26.23372
65	2	Unknown 1	-9.01424	75.9	8607.46	8220.4	2222.5	75.9	18.75883
66	3	Unknown 1	-9.01424	99.5	11158.14	10771.1	-328.2	99.5	24.31771
67	1	Unknown 1	-10.01424	107.4	12019.01	11632.0	-1189.1	107.4	26.19386
68	2	Unknown 1	-10.01424	87.5	9860.48	9473.4	969.5	87.5	21.48963
69	3	Unknown 1	-10.01424	102.1	11444.58	11057.5	-614.6	102.1	24.94197
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	28.5	3478.82	3091.8	7351.1	28.5	7.581634
74	2	Unknown 2	-4.01424	26.4	3247.87	2860.8	7582.1	26.4	7.078308
75	3	Unknown 2	-4.01424	36.6	4348.99	3961.9	6480.9	36.6	9.478056
76	1	Unknown 2	-5.01424	70.0	7972.89	7585.8	2857.0	70.0	17.37587
77	2	Unknown 2	-5.01424	79.8	9028.75	8641.7	1801.2	79.8	19.67698
78	3	Unknown 2	-5.01424	80.9	9150.58	8763.5	1679.4	80.9	19.94249
79	1	Unknown 2	-6.01424	107.8	12065.2	11678.1	-1235.3	107.8	26.29453
80	2	Unknown 2	-6.01424	101.1	11331.12	10944.1	-501.2	101.1	24.6947
81	3	Unknown 2	-6.01424	100.2	11233.78	10846.7	-403.8	100.2	24.48256
82	1	Unknown 2	-7.01424	107.4	12015.29	11628.2	-1185.4	107.4	26.18575
83	2	Unknown 2	-7.01424	100.4	11264.16	10877.1	-434.2	100.4	24.54877
84	3	Unknown 2	-7.01424	105.7	11830.22	11443.2	-1000.3	105.7	25.78242
85	1	Unknown 2	-8.01424	86.0	9697.11	9310.1	1132.8	86.0	21.13358
86	2	Unknown 2	-8.01424	106.7	11937.48	11550.4	-1107.5	106.7	26.01618
87	3	Unknown 2	-8.01424	100.7	11292.37	10905.3	-462.4	100.7	24.61025
88	1	Unknown 2	-9.01424	106.7	11946.47	11559.4	-1116.5	106.7	26.03577
89	2	Unknown 2	-9.01424	110.0	12304.83	11917.8	-1474.9	110.0	26.81677
90	3	Unknown 2	-9.01424	105.9	11858.43	11471.4	-1028.5	105.9	25.8439
91	1	Unknown 2	-10.01424	110.3	12331.8	11944.7	-1501.9	110.3	26.87555
92	2	Unknown 2	-10.01424	109.7	12269.49	11882.4	-1439.6	109.7	26.73975
93	3	Unknown 2	-10.01424	109.9	12288.09	11901.0	-1458.2	109.9	26.78029

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	24.45%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	3006.20	9319.22	TRUE	
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2960.30	9176.93	TRUE	
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2967.70	9199.87	TRUE	
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3749.60	11623.76	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3090.80	9581.48	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3794.10	11761.71	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3844.20	11917.02	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	4018.90	12458.59	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3717.80	11525.18	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3913.20	12130.92	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3832.50	11880.75	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3895.80	12076.98	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3917.80	12145.18	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3924.60	12166.26	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3583.70	11109.47	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	4041.60	12528.96	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3773.10	11696.61	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	2970.80	9209.48	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3891.60	12063.96	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3586.00	11116.60	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3904.20	12103.02	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3838.40	11899.04	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3758.10	11650.11	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3756.40	11644.84	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	136.09	421.88	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	127.26	394.51	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	29.59	91.73	FALSE	spill, no sample
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	886.51	2748.18	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	911.87	2826.80	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	919.20	2849.52	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3190.00	9889.00	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3245.50	10061.05	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3249.00	10071.90	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3958.10	12270.11	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3829.90	11872.69	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3897.10	12081.01	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3946.60	12234.46	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3973.70	12318.47	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3939.30	12211.83	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3878.30	12022.73	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3978.00	12331.80	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	4026.70	12482.77	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3958.40	12271.04	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3506.80	10871.08	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3932.90	12191.99	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3951.50	12249.65	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3745.90	11612.29	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3706.90	11491.39	TRUE	
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3748.10	11619.11	TRUE	
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3630.40	11254.24	TRUE	
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3429.20	10630.52	TRUE	
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	107.47	322.41	TRUE	
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	136.79	410.37	TRUE	
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	119.14	357.42	TRUE	
148	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45990.00	45990.00	TRUE	
149	2	none	Hot	—	—	—	30	—	—	—	—	—	—	46294.00	46294.00	TRUE	
150	3	none	Hot	—	—	—	30	—	—	—	—	—	—	46282.00	46282.00	TRUE	
151	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45818.00	45818.00	TRUE	
152	2	none	Hot	—	—	—	30	—	—	—	—	—	—	45478.00	45478.00	TRUE	
153	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45447.00	45447.00	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
94	1	Unknown 3	-3.01424	82.5	9319.22	8932.2	1510.7	82.5	20.31002				
95	2	Unknown 3	-3.01424	81.2	9176.93	8789.9	1653.0	81.2	19.99992				
96	3	Unknown 3	-3.01424	81.4	9199.87	8812.8	1630.1	81.4	20.04991				
97	1	Unknown 3	-4.01424	103.8	11623.76	11236.7	-793.8	103.8	25.33247				
98	2	Unknown 3	-4.01424	84.9	9581.48	9194.4	1248.5	84.9	20.88158				
99	3	Unknown 3	-4.01424	105.0	11761.71	11374.7	-931.8	105.0	25.63311				
100	1	Unknown 3	-5.01424	106.5	11917.02	11530.0	-1087.1	106.5	25.97159				
101	2	Unknown 3	-5.01424	111.5	12458.59	12071.5	-1628.7	111.5	27.15187				
102	3	Unknown 3	-5.01424	102.8	11525.18	11138.1	-695.2	102.8	25.11762				
103	1	Unknown 3	-6.01424	108.4	12130.92	11743.9	-1301.0	108.4	26.43776				
104	2	Unknown 3	-6.01424	106.1	11880.75	11493.7	-1050.8	106.1	25.89254				
105	3	Unknown 3	-6.01424	107.9	12076.98	11689.9	-1247.0	107.9	26.3202				
106	1	Unknown 3	-7.01424	108.6	12145.18	11758.1	-1315.2	108.6	26.46883				
107	2	Unknown 3	-7.01424	108.8	12166.26	11779.2	-1336.3	108.8	26.51477				
108	3	Unknown 3	-7.01424	99.0	11109.47	10722.4	-279.5	99.0	24.21164				
109	1	Unknown 3	-8.01424	112.1	12528.96	12141.9	-1699.0	112.1	27.30523				
110	2	Unknown 3	-8.01424	104.4	11696.61	11309.6	-866.7	104.4	25.49123				
111	3	Unknown 3	-8.01424	81.5	9209.48	8822.4	1620.5	81.5	20.07086				
112	1	Unknown 3	-9.01424	107.8	12063.96	11676.9	-1234.0	107.8	26.29182				
113	2	Unknown 3	-9.01424	99.1	11116.6	10729.5	-286.7	99.1	24.22718				
114	3	Unknown 3	-9.01424	108.2	12103.02	11716.0	-1273.1	108.2	26.37695				
115	1	Unknown 3	-10.01424	106.3	11899.04	11512.0	-1069.1	106.3	25.9324				
116	2	Unknown 3	-10.01424	104.0	11650.11	11263.1	-820.2	104.0	25.38989				
117	3	Unknown 3	-10.01424	104.0	11644.84	11257.8	-814.9	104.0	25.37841				
118	1	Unknown 4	-3.01424	0.3	421.879	34.8	10408.1	0.3	0.91943				
119	2	Unknown 4	-3.01424	0.1	394.506	7.5	10435.4	0.1	0.859774				
120	3	Unknown 4	-3.01424										
121	1	Unknown 4	-4.01424	21.8	2748.181	2361.1	8081.8	21.8	5.989301				
122	2	Unknown 4	-4.01424	22.5	2826.797	2439.7	8003.1	22.5	6.160635				
123	3	Unknown 4	-4.01424	22.7	2849.52	2462.5	7980.4	22.7	6.210157				
124	1	Unknown 4	-5.01424	87.7	9889	9501.9	940.9	87.7	21.55178				
125	2	Unknown 4	-5.01424	89.3	10061.05	9674.0	768.9	89.3	21.92674				
126	3	Unknown 4	-5.01424	89.4	10071.9	9684.8	758.0	89.4	21.95039				
127	1	Unknown 4	-6.01424	109.7	12270.11	11883.1	-1440.2	109.7	26.7411				
128	2	Unknown 4	-6.01424	106.1	11872.69	11485.6	-1042.8	106.1	25.87498				
129	3	Unknown 4	-6.01424	108.0	12081.01	11694.0	-1251.1	108.0	26.32898				
130	1	Unknown 4	-7.01424	109.4	12234.46	11847.4	-1404.5	109.4	26.66341				
131	2	Unknown 4	-7.01424	110.2	12318.47	11931.4	-1488.5	110.2	26.8465				
132	3	Unknown 4	-7.01424	109.2	12211.83	11824.8	-1381.9	109.2	26.61409				
133	1	Unknown 4	-8.01424	107.4	12022.73	11635.7	-1192.8	107.4	26.20197				
134	2	Unknown 4	-8.01424	110.3	12331.8	11944.7	-1501.9	110.3	26.87555				
135	3	Unknown 4	-8.01424	111.7	12482.77	12095.7	-1652.8	111.7	27.20457				
136	1	Unknown 4	-9.01424	109.7	12271.04	11884.0	-1441.1	109.7	26.74313				
137	2	Unknown 4	-9.01424	96.8	10871.08	10484.0	-41.1	96.8	23.6921				
138	3	Unknown 4	-9.01424	109.0	12191.99	11804.9	-1362.1	109.0	26.57085				
139	1	Unknown 4	-10.01424	109.5	12249.65	11862.6	-1419.7	109.5	26.69651				
140	2	Unknown 4	-10.01424	103.7	11612.29	11225.2	-782.4	103.7	25.30747				
141	3	Unknown 4	-10.01424	102.5	11491.39	11104.3	-661.5	102.5	25.04398				
142	1	—	—	103.7	11619.11	11232.1	-789.2	103.7	25.32233				
143	2	—	—	100.3	11254.24	10867.2	-424.3	100.3	24.52715				
144	3	—	—	94.6	10630.52	10243.5	199.4	94.6	23.16783				
145	1	-6.00	-0.6	322.41	-64.6	10507.5	-0.6	0.70265					
146	2	-6.00	0.2	410.37	23.3	10419.6	0.2	0.894348					
147	3	-6.00	-0.3	357.42	-29.6	10472.5	-0.3	0.77895					
148	1			45990	45602.9								
149	2			46294	45906.9								
150	3			46282	45894.9								
151	1			45818	45430.9								
152	2			45478	45090.9								
153	3			45447	45059.9								

Prism data												
standard curve				weak positive				CR42352				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	0.10614	0.13384	0.41528	-3	3.5192	4.1859	4.0031	-3.0	1.3114	0.8388	1.2633	
-6.0	-0.59691	0.21528	-0.27364	-4	29.6756	30.2601	28.8999	-4.0	28.6886	29.1036	29.5072	
-7.0	1.93654	1.37207	1.94169	-5	79.7673	78.1440	81.2410	-5.0	72.2663	85.3763	84.3172	
-8.0	13.91670	13.18477	13.71547	-6	99.4627	86.7092		-6.0	80.8536	98.8755	88.2158	
-9.0	61.57226	62.80597	62.27642	-7	103.4821	75.7673	74.5429	-7.0	83.7332	96.1219	104.5689	
-10.0	97.25254	92.72416	88.45627	-8	90.5541	98.6677	97.5984	-8.0	104.5689	95.9673	103.6615	
-11.0	81.86980	101.87537	94.09527	-9	100.8838	82.5568	93.8726	-9.0	107.5745	75.9045	99.4566	
				-10	89.5014	102.0140	101.2023	-10.0	107.4056	87.4745	102.1015	

CR42353				CR42359				CR42360			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.0				-3.0	82.4766	81.1628	81.3746	-3.0	0.3216	0.0688	
-4.0	28.5483	26.4158	36.5832	-4.0	103.7560	84.8983	105.0298	-4.0	21.8019	22.5278	22.7376
-5.0	70.0451	79.7945	80.9195	-5.0	106.4639	111.4645	102.8457	-5.0	87.7378	89.3265	89.4266
-6.0	107.8321	101.0539	100.1550	-6.0	108.4389	106.1290	107.9409	-6.0	109.7242	106.0545	107.9781
-7.0	107.3713	100.4356	105.6624	-7.0	108.5706	108.7653	99.0072	-7.0	109.3950	110.1707	109.1860
-8.0	85.9659	106.6528	100.6960	-8.0	112.1143	104.4287	81.4633	-8.0	107.4400	110.2938	111.6878
-9.0	106.7358	110.0448	105.9229	-9.0	107.8207	99.0730	108.1813	-9.0	109.7328	96.8060	109.0028
-10.0	110.2938	109.7185	109.8902	-10.0	106.2978	103.9993	103.9506	-10.0	109.5353	103.6501	102.5337

Competitive Assay of a known Weak Positive**153 Assay Tubes**

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
by nonlinear regression softwareProvide information in all blue cells in
this column

Laboratory Code:		
Run identification:	510	
Assay start date:	10/4/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.90	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.35E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	1.86E-05	M
RBA:	7.26491E-05	
Max Concentration, Unknown 1:	3.00E-02	M (example 5e-3)
IC50, Unknown 1:	2.36E-05	CR42352
RBA, Unknown 1:	0.00573%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	3.01E-05	CR42353
RBA, Unknown 2:	0.00449%	
Max Concentration, Unknown 3:	3.00E-02	M (example 5e-3)
IC50, Unknown 3:	2.46E-03	CR42359
RBA, Unknown 3:	0.00005%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	3.19E-05	CR42360
RBA, Unknown 4:	0.00423%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11607.4	427.69	Total Binding, solvent control, tubes
Hot	6	45051.0	436.89	Total hot R1881 added to each tube
NSB	6	405.0	43.58	Nonspecific Binding
Specific EtOH	6	11202.4	427.69	

Assay Characterization Values	
EtOH / Hot	0.26 less than 0.1?
NSB / EtOH	0.03 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)															Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	transcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3582.10	11104.51	TRUE		
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3632.10	11259.51	TRUE		
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3677.70	11400.87	TRUE		
4	1	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	119.08	357.24	TRUE			
5	2	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	124.68	374.04	TRUE			
6	3	Inert R1881	NSB	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	123.89	371.67	TRUE			
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	170.47	528.46	TRUE		
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	167.01	517.73	TRUE		
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	158.89	492.56	TRUE		
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	551.82	1710.64	TRUE		
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	595.12	1844.87	TRUE		
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	598.95	1856.75	TRUE		
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2197.50	6812.25	TRUE		
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2246.60	6964.46	TRUE		
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2288.10	7093.11	TRUE		
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3415.80	10588.98	TRUE		
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3284.60	10182.26	TRUE		
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3344.10	10366.71	TRUE		
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3558.30	11030.73	TRUE		
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3532.90	10951.99	TRUE		
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3447.20	10686.32	TRUE		
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	240.28	720.84	TRUE		
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	234.87	704.61	TRUE		
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	246.92	740.76	TRUE		
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1029.39	3088.17	TRUE		
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1108.60	3325.80	TRUE		
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1070.31	3210.93	TRUE		
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2431.50	7294.50	TRUE		
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2484.40	7453.20	TRUE		
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2562.20	7686.60	TRUE		
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3073.30	9219.90	TRUE		
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3010.00	9030.00	TRUE		
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3385.80	10157.40	TRUE		
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3185.30	9555.90	TRUE		
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2785.20	8355.60	TRUE		
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2829.30	8487.90	TRUE		
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3658.00	10974.00	TRUE		
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2937.00	8811.00	TRUE		
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2891.00	8673.00	TRUE		
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3049.10	9147.30	TRUE		
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	2943.90	8831.70	TRUE		
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3509.40	10528.20	TRUE		
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3653.60	10960.80	TRUE		
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	2745.50	8236.50	FALSE	spill	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3603.20	10809.60	TRUE		

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean MSE)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot
1	1				95.5	11104.51	10699.5	97.9	95.5
2	2				96.9	11259.51	10854.5	-57.1	96.9
3	3				98.2	11400.87	10995.8	-198.5	98.2
4	1		-6.00	-0.4	357.24	-47.8	10845.2	-0.4	0.792968
5	2		-6.00	-0.3	374.04	-31.0	10828.4	-0.3	0.830259
6	3		-6.00	0.0	371.67	-33.4	10830.7	-0.3	0.824998
7	1	cold R1881	-7.01	1.1	528.457	123.4	10673.9	1.1	1.173019
8	2	cold R1881	-7.01	1.0	517.731	112.7	10684.7	1.0	1.149211
9	3	cold R1881	-7.01	0.8	492.559	87.5	10709.8	0.8	1.093336
10	1	cold R1881	-8.01	11.7	1710.642	1305.6	9491.8	11.7	3.797123
11	2	cold R1881	-8.01	12.9	1844.872	1439.8	9357.5	12.9	4.095074
12	3	cold R1881	-8.01	13.0	1856.745	1451.7	9345.7	13.0	4.121429
13	1	cold R1881	-9.01	57.2	6812.25	6407.2	4390.2	57.2	15.1212
14	2	cold R1881	-9.01	58.6	6964.46	6559.4	4237.9	58.6	15.45906
15	3	cold R1881	-9.01	59.7	7093.11	6688.1	4109.3	59.7	15.74462
16	1	cold R1881	-10.01	90.9	10588.98	10184.0	613.4	90.9	23.50443
17	2	cold R1881	-10.01	87.3	10182.26	9777.2	1020.1	87.3	22.60163
18	3	cold R1881	-10.01	88.9	10366.71	9961.7	835.7	88.9	23.01105
19	1	cold R1881	-11.01	94.9	11030.73	10625.7	171.7	94.9	24.48498
20	2	cold R1881	-11.01	94.1	10951.99	10547.0	250.4	94.1	24.3102
21	3	cold R1881	-11.01	91.8	10686.32	10281.3	516.1	91.8	23.72049
22	1	Weak Positive	-3	2.8	720.84	315.8	10481.6	2.8	1.600053
23	2	Weak Positive	-3	2.7	704.61	299.6	10497.8	2.7	1.564027
24	3	Weak Positive	-3	3.0	740.76	335.7	10461.6	3.0	1.64427
25	1	Weak Positive	-4	24.0	3088.17	2683.1	8114.2	24.0	6.854831
26	2	Weak Positive	-4	26.1	3325.8	2920.8	7876.6	26.1	7.3823
27	3	Weak Positive	-4	25.0	3210.93	2805.9	7991.5	25.0	7.127322
28	1	Weak Positive	-5	61.5	7294.5	6889.5	3907.9	61.5	16.19165
29	2	Weak Positive	-5	62.9	7453.2	7048.2	3749.2	62.9	16.54392
30	3	Weak Positive	-5	65.0	7686.6	7281.6	3515.8	65.0	17.062
31	1	Weak Positive	-6	78.7	9219.9	8814.9	1982.5	78.7	20.46547
32	2	Weak Positive	-6	77.0	9030	8625.0	2172.4	77.0	20.04395
33	3	Weak Positive	-6	87.1	10157.4	9752.4	1045.0	87.1	22.54645
34	1	Weak Positive	-7	81.7	9555.9	9150.9	1646.5	81.7	21.21129
35	2	Weak Positive	-7	71.0	8355.6	7950.6	2846.8	71.0	18.54698
36	3	Weak Positive	-7	72.2	8487.9	8082.9	2714.5	72.2	18.84065
37	1	Weak Positive	-8	94.3	10974	10569.0	228.4	94.3	24.35906
38	2	Weak Positive	-8	75.0	8811	8406.0	2391.4	75.0	19.55783
39	3	Weak Positive	-8	73.8	8673	8268.0	2529.4	73.8	19.25151
40	1	Weak Positive	-9	78.0	9147.3	8742.3	2055.1	78.0	20.30432
41	2	Weak Positive	-9	75.2	8831.7	8426.7	2370.7	75.2	19.60378
42	3	Weak Positive	-9	90.4	10528.2	10123.2	674.2	90.4	23.36951
43	1	Weak Positive	-10	94.2	10960.8	10555.8	241.6	94.2	24.32976
44	2	Weak Positive	-10						
45	3	Weak Positive	-10	92.9	10809.6	10404.6	392.8	92.9	23.99414

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)															Check the 10% rule:	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1,3-E supplied by Bartelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	160.63	497.95	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	167.21	518.35	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	168.50	522.35	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	894.23	2772.11	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1049.63	3253.85	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	1074.04	3329.52	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2731.80	8468.58	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2323.40	7202.54	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	2757.20	8547.32	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	2936.60	9103.46	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3323.10	10301.61	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	3502.30	10857.13	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3834.60	11887.26	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3759.60	11654.76	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3193.10	9898.61	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3382.30	10485.13	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3278.90	10164.59	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3713.80	11512.78	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3634.80	11267.88	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3334.20	10336.02	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3149.90	9764.69	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3369.30	10444.83	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3390.00	10509.00	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3607.50	11183.25	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1203.90	3732.09	FALSE	precipitate in tube
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1148.30	3559.73	FALSE	precipitate in tube
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	1201.80	3725.58	FALSE	precipitate in tube
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1071.12	3320.47	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1231.70	3818.27	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	1228.60	3808.66	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2282.20	7074.82	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2921.10	9055.41	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	2865.60	8883.36	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3638.60	11279.66	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	3625.20	11238.12	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2856.20	8854.22	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3236.00	10031.60	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3708.80	11497.28	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3773.80	11698.78	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3844.00	11916.40	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3746.30	11613.53	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3573.20	11076.92	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3867.10	11988.01	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3803.60	11791.16	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3687.20	11430.32	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3825.10	11857.81	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3673.10	11386.61	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3781.30	11722.03	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ETOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424	0.8	497.953	92.9	10704.5	0.8	1.10531
47	2	Unknown 1	-3.01424	1.0	518.351	113.3	10684.1	1.0	1.150587
48	3	Unknown 1	-3.01424	1.0	522.35	117.3	10680.1	1.0	1.159464
49	1	Unknown 1	-4.01424	21.1	2772.113	2367.1	8430.3	21.1	6.153277
50	2	Unknown 1	-4.01424	25.4	3253.853	2848.8	7948.6	25.4	7.222599
51	3	Unknown 1	-4.01424	26.1	3329.524	2924.5	7872.9	26.1	7.390566
52	1	Unknown 1	-5.01424	72.0	8468.58	8063.6	2733.8	72.0	18.79776
53	2	Unknown 1	-5.01424	60.7	7202.54	6797.5	3999.9	60.7	15.98753
54	3	Unknown 1	-5.01424	72.7	8547.32	8142.3	2655.1	72.7	18.97254
55	1	Unknown 1	-6.01424	77.6	9103.46	8698.4	2098.9	77.6	20.20701
56	2	Unknown 1	-6.01424	88.3	10301.61	9896.6	900.8	88.3	22.86655
57	3	Unknown 1	-6.01424	93.3	10857.13	10452.1	345.3	93.3	24.09964
58	1	Unknown 1	-7.01424	102.5	11887.26	11482.2	-684.9	102.5	26.38623
59	2	Unknown 1	-7.01424	100.4	11654.76	11249.7	-452.4	100.4	25.87015
60	3	Unknown 1	-7.01424	84.7	9898.61	9493.6	1303.8	84.7	21.97201
61	1	Unknown 1	-8.01424	90.0	10485.13	10080.1	717.3	90.0	23.27391
62	2	Unknown 1	-8.01424	87.1	10164.59	9759.6	1037.8	87.1	22.56241
63	3	Unknown 1	-8.01424	99.2	11512.78	11107.8	-310.4	99.2	25.55499
64	1	Unknown 1	-9.01424	97.0	11267.88	10862.9	-65.5	97.0	25.01139
65	2	Unknown 1	-9.01424	88.7	10336.02	9931.0	866.4	88.7	22.94293
66	3	Unknown 1	-9.01424	83.6	9764.69	9359.7	1437.7	83.6	21.67475
67	1	Unknown 1	-10.01424	89.6	10444.83	10039.8	757.6	89.6	23.18446
68	2	Unknown 1	-10.01424	90.2	10509	10104.0	693.4	90.2	23.3269
69	3	Unknown 1	-10.01424	96.2	11183.25	10778.2	19.2	96.2	24.82353
70	1	Unknown 2	-3.01424						
71	2	Unknown 2	-3.01424						
72	3	Unknown 2	-3.01424						
73	1	Unknown 2	-4.01424	26.0	3320.472	2915.4	7881.9	26.0	7.370473
74	2	Unknown 2	-4.01424	30.5	3818.27	3413.2	7384.1	30.5	8.475439
75	3	Unknown 2	-4.01424	30.4	3808.66	3403.6	7393.7	30.4	8.454108
76	1	Unknown 2	-5.01424	59.5	7074.82	6669.8	4127.6	59.5	15.70402
77	2	Unknown 2	-5.01424	77.2	9055.41	8650.4	2147.0	77.2	20.10035
78	3	Unknown 2	-5.01424	75.7	8883.36	8478.3	2319.0	75.7	19.71845
79	1	Unknown 2	-6.01424	97.1	11279.66	10874.6	-77.3	97.1	25.03754
80	2	Unknown 2	-6.01424	96.7	11238.12	10833.1	-35.7	96.7	24.94533
81	3	Unknown 2	-6.01424	75.4	8854.22	8449.2	2348.2	75.4	19.65377
82	1	Unknown 2	-7.01424	85.9	10031.6	9626.6	1170.8	85.9	22.26721
83	2	Unknown 2	-7.01424	99.0	11497.28	11092.3	-294.9	99.0	25.52059
84	3	Unknown 2	-7.01424	100.8	11698.78	11293.8	-496.4	100.8	25.96786
85	1	Unknown 2	-8.01424	102.8	11916.4	11511.4	-714.0	102.8	26.45091
86	2	Unknown 2	-8.01424	100.1	11613.53	11208.5	-411.1	100.1	25.77863
87	3	Unknown 2	-8.01424	95.3	11076.92	10671.9	125.5	95.3	24.58751
88	1	Unknown 2	-9.01424	103.4	11988.01	11583.0	-785.6	103.4	26.60986
89	2	Unknown 2	-9.01424	101.6	11791.16	11386.1	-588.8	101.6	26.17292
90	3	Unknown 2	-9.01424	98.4	11430.32	11025.3	-227.9	98.4	25.37196
91	1	Unknown 2	-10.01424	102.2	11857.81	11452.8	-655.4	102.2	26.32086
92	2	Unknown 2	-10.01424	98.0	11386.61	10981.6	-184.2	98.0	25.27493
93	3	Unknown 2	-10.01424	101.0	11722.03	11317.0	-519.6	101.0	26.01947

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)															Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triacelone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"	
94	1	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2993.40	9279.54	TRUE		
95	2	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2966.60	9196.46	TRUE		
96	3	Unknown 3	U3	1	E-1-U3	3.00E-02	300	30	10	50	310	9.7E-04	100	2314.60	7175.26	TRUE		
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3696.60	11459.46	TRUE		
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3109.80	9640.38	TRUE		
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	3031.80	9398.58	TRUE		
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3924.00	12164.40	TRUE		
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3869.60	11995.76	TRUE		
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3866.80	11987.08	TRUE		
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2860.70	8868.17	TRUE		
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3291.30	10203.03	TRUE		
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3561.10	11039.41	TRUE		
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3898.50	12085.35	TRUE		
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3722.60	11540.06	TRUE		
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3621.60	11226.96	TRUE		
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3625.80	11239.98	TRUE		
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3642.50	11291.75	TRUE		
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3713.10	11510.61	TRUE		
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3713.60	11512.16	TRUE		
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3671.60	11381.96	TRUE		
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2817.70	8734.87	TRUE		
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3784.90	11733.19	TRUE		
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3527.40	10934.94	TRUE		
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3753.80	11636.78	TRUE		
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	137.05	424.86	TRUE		
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	145.97	452.51	TRUE		
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	117.82	365.24	TRUE		
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	859.06	2663.09	TRUE		
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	795.39	2465.71	TRUE		
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	825.74	2559.79	TRUE		
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3187.90	9882.49	TRUE		
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2990.70	9271.17	TRUE		
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3094.60	9593.26	TRUE		
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3434.40	10646.64	TRUE		
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3721.40	11536.34	TRUE		
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3589.60	11127.76	TRUE		
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3408.40	10566.04	TRUE		
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3802.10	11786.51	TRUE		
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3827.80	11866.18	TRUE		
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3739.00	11590.90	TRUE		
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3284.90	10183.19	TRUE		
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3749.20	11622.52	TRUE		
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3795.60	11766.36	TRUE		
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3581.70	11103.27	TRUE		
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3812.50	11818.75	TRUE		
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3797.10	11771.01	TRUE		
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	4010.90	12433.79	TRUE		
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3951.90	12250.89	TRUE		
142	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3792.50	11756.75	TRUE		
143	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3833.40	11883.54	TRUE		
144	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3948.20	12239.42	TRUE		
145	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	155.20	465.60	TRUE		
146	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	140.82	422.46	TRUE		
147	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	146.39	439.17	TRUE		
148	1	none	Hot	—	—	—	—	30	—	—	—	—	—	44823.00	44823.00	TRUE		
149	2	none	Hot	—	—	—	—	30	—	—	—	—	—	44402.00	44402.00	TRUE		
150	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45025.00	45025.00	TRUE		
151	1	none	Hot	—	—	—	—	30	—	—	—	—	—	45103.00	45103.00	TRUE		
152	2	none	Hot	—	—	—	—	30	—	—	—	—	—	45717.00	45717.00	TRUE		
153	3	none	Hot	—	—	—	—	30	—	—	—	—	—	45236.00	45236.00	TRUE		

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
94	1	Unknown 3	-3.01424	79.2	9279.54	8874.5	1922.9	79.2	20.59786				
95	2	Unknown 3	-3.01424	78.5	9196.46	8791.4	2005.9	78.5	20.41344				
96	3	Unknown 3	-3.01424	60.4	7175.26	6770.2	4027.1	60.4	15.92697				
97	1	Unknown 3	-4.01424	98.7	11459.46	11054.4	-257.1	98.7	25.43664				
98	2	Unknown 3	-4.01424	82.4	9640.38	9235.4	1562.0	82.4	21.39881				
99	3	Unknown 3	-4.01424	80.3	9398.58	8993.6	1803.8	80.3	20.86209				
100	1	Unknown 3	-5.01424	105.0	12164.4	11759.4	-962.0	105.0	27.0014				
101	2	Unknown 3	-5.01424	103.5	11995.76	11590.7	-793.4	103.5	26.62707				
102	3	Unknown 3	-5.01424	103.4	11987.08	11582.1	-784.7	103.4	26.6078				
103	1	Unknown 3	-6.01424	75.5	8868.17	8463.1	2334.2	75.5	19.68474				
104	2	Unknown 3	-6.01424	87.5	10203.03	9798.0	999.4	87.5	22.64773				
105	3	Unknown 3	-6.01424	94.9	11039.41	10634.4	163.0	94.9	24.50425				
106	1	Unknown 3	-7.01424	104.3	12085.35	11680.3	-882.9	104.3	26.82593				
107	2	Unknown 3	-7.01424	99.4	11540.06	11135.0	-337.7	99.4	25.61555				
108	3	Unknown 3	-7.01424	96.6	11226.96	10821.9	-24.6	96.6	24.92056				
109	1	Unknown 3	-8.01424	96.7	11239.98	10835.0	-37.6	96.7	24.94946				
110	2	Unknown 3	-8.01424	97.2	11291.75	10886.7	-89.3	97.2	25.06437				
111	3	Unknown 3	-8.01424	99.1	11510.61	11105.6	-308.2	99.1	25.55018				
112	1	Unknown 3	-9.01424	99.1	11512.16	11107.1	-309.8	99.1	25.55362				
113	2	Unknown 3	-9.01424	98.0	11381.96	10976.9	-179.6	98.0	25.26461				
114	3	Unknown 3	-9.01424	74.4	8734.87	8329.8	2467.5	74.4	19.38885				
115	1	Unknown 3	-10.01424	101.1	11733.19	11328.2	-530.8	101.1	26.04424				
116	2	Unknown 3	-10.01424	94.0	10934.94	10529.9	267.5	94.0	24.27236				
117	3	Unknown 3	-10.01424	100.3	11636.78	11231.8	-434.4	100.3	25.83024				
118	1	Unknown 4	-3.01424	0.2	424.855	19.8	10777.5	0.2	0.943053				
119	2	Unknown 4	-3.01424	0.4	452.507	47.5	10749.9	0.4	1.004433				
120	3	Unknown 4	-3.01424	-0.4	365.242	-39.8	10837.2	-0.4	0.81073				
121	1	Unknown 4	-4.01424	20.2	2663.086	2258.1	8539.3	20.2	5.911269				
122	2	Unknown 4	-4.01424	18.4	2465.709	2060.7	8736.7	18.4	5.47315				
123	3	Unknown 4	-4.01424	19.2	2559.794	2154.8	8642.6	19.2	5.681992				
124	1	Unknown 4	-5.01424	84.6	9882.49	9477.5	1319.9	84.6	21.93623				
125	2	Unknown 4	-5.01424	79.1	9271.17	8866.1	1931.2	79.1	20.57928				
126	3	Unknown 4	-5.01424	82.0	9593.26	9188.2	1609.1	82.0	21.29422				
127	1	Unknown 4	-6.01424	91.4	10646.64	10241.6	555.8	91.4	23.63242				
128	2	Unknown 4	-6.01424	99.4	11536.34	11131.3	-333.9	99.4	25.60729				
129	3	Unknown 4	-6.01424	95.7	11127.76	10722.7	74.6	95.7	24.70036				
130	1	Unknown 4	-7.01424	90.7	10566.04	10161.0	636.4	90.7	23.45351				
131	2	Unknown 4	-7.01424	101.6	11786.51	11381.5	-584.1	101.6	26.16259				
132	3	Unknown 4	-7.01424	102.3	11866.18	11461.2	-663.8	102.3	26.33944				
133	1	Unknown 4	-8.01424	99.9	11590.9	11185.9	-388.5	99.9	25.7284				
134	2	Unknown 4	-8.01424	87.3	10183.19	9778.2	1019.2	87.3	22.60369				
135	3	Unknown 4	-8.01424	100.1	11622.52	11217.5	-420.1	100.1	25.79858				
136	1	Unknown 4	-9.01424	101.4	11766.36	11361.3	-564.0	101.4	26.11787				
137	2	Unknown 4	-9.01424	95.5	11103.27	10698.2	99.1	95.5	24.646				
138	3	Unknown 4	-9.01424	101.9	11818.75	11413.7	-616.3	101.9	26.23416				
139	1	Unknown 4	-10.01424	101.5	11771.01	11366.0	-568.6	101.5	26.12819				
140	2	Unknown 4	-10.01424	107.4	12433.79	12028.8	-1231.4	107.4	27.59937				
141	3	Unknown 4	-10.01424	105.7	12250.89	11845.9	-1048.5	105.7	27.19338				
142	1	—	—	101.3	11756.75	11351.7	-554.3	101.3	26.09654				
143	2	—	—	102.5	11883.54	11478.5	-681.1	102.5	26.37797				
144	3	—	—	105.6	12239.42	11834.4	-1037.0	105.6	27.16792				
145	1	-6.00	0.5	465.6	60.6	10736.8	0.5	1.033495					
146	2	-6.00	0.2	422.46	17.4	10779.9	0.2	0.937737					
147	3	-6.00	0.3	439.17	34.1	10763.2	0.3	0.974829					
148	1			44823	44418.0								
149	2			44402	43997.0								
150	3			45025	44620.0								
151	1			45103	44698.0								
152	2			45717	45312.0								
153	3			45236	44831.0								

Prism data												
standard curve				weak positive				CR42352				
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-6.0	-0.42660	-0.27664	-0.29779	-3	2.8191	2.6742	2.9969	-3.0	0.8295	1.0116	1.0473	
-6.0	0.54069	0.15559	0.30476	-4	23.9515	26.0727	25.0473	-4.0	21.1301	25.4305	26.1060	
-7.0	1.10179	1.00604	0.78134	-5	61.4999	62.9166	65.0001	-5.0	71.9805	60.6790	72.6834	
-8.0	11.65475	12.85297	12.95896	-6	78.6873	76.9921	87.0561	-6.0	77.6479	88.3434	93.3023	
-9.0	57.19505	58.55377	59.70219	-7	81.6867	70.9720	72.1530	-7.0	102.4979	100.4225	84.7459	
-10.0	90.90862	87.27797	88.92449	-8	94.3456	75.0372	73.8053	-8.0	89.9816	87.1202	99.1551	
-11.0	94.85197	94.14908	91.77754	-9	78.0392	75.2220	90.3661	-9.0	96.9689	88.6505	83.5505	
				-10	94.2277		92.8780	-10.0	89.6218	90.1947	96.2135	

CR42353					CR42359					CR42360				
conce ntratio n (log)					conce ntratio n (log)					conce ntratio n (log)				
	y1-U1	y2-U1	y3-U1			y1-U1	y2-U1	y3-U1			y1-U1	y2-U1	y3-U1	
-3.0					-3.0	79.2197	78.4781	60.4355		-3.0	0.1770	0.4238	-0.3552	
-4.0	26.0251	30.4688	30.3830		-4.0	98.6791	82.4408	80.2823		-4.0	20.1569	18.3950	19.2348	
-5.0	59.5389	77.2190	75.6831		-5.0	104.9718	103.4665	103.3890		-5.0	84.6020	79.1450	82.0202	
-6.0	97.0741	96.7033	75.4230		-6.0	75.5475	87.4634	94.9295		-6.0	91.4233	99.3654	95.7181	
-7.0	85.9331	99.0167	100.8154		-7.0	104.2662	99.3986	96.6036		-7.0	90.7038	101.5986	102.3097	
-8.0	102.7580	100.0544	95.2643		-8.0	96.7199	97.1820	99.1357		-8.0	99.8524	87.2863	100.1347	
-9.0	103.3973	101.6401	98.4190		-9.0	99.1495	97.9873	74.3576		-9.0	101.4187	95.4995	101.8864	
-10.0	102.2350	98.0288	101.0230		-10.0	101.1226	93.9969	100.2620		-10.0	101.4602	107.3766	105.7439	

Competitive Assay of a known Weak Positive
177 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:		
Run identification:	511	
Assay start date:	10/6/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.87	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.67E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.47E-05	M
RBA:	4.81002E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	4.84E-08	CR42342
RBA, Unknown 1:	3.45248%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	2.01E-06	CR42345
RBA, Unknown 2:	0.08309%	
Max Concentration, Unknown 3:	7.50E-03	M (example 5e-3) non standard dilutions
IC50, Unknown 3:	9.08E-05	CR42351
RBA, Unknown 3:	0.00184%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	1.72E-03	CR42358
RBA, Unknown 4:	0.00010%	
Max Concentration, Unknown 5:	7.50E-03	M (example 5e-3) non standard dilutions
IC50, Unknown 5:	3.89E-04	CR43261
RBA, Unknown 5:	0.00043%	
volume of ethanol counted:	2	mL
multitply DPM in sample by :	3.1	

protocol calls for counting decanted EtOH supernate
 reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

working volume

3.1E+02 uL

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	9980.1	1105.28	Total Binding, solvent control, tubes
Hot	6	45599.2	680.09	Total hot R1881 added to each tube
NSB	6	445.6	106.16	Nonspecific Binding
Specific EtOH	6	9534.5	1105.28	

Assay Characterization Values	
EtOH / Hot	0.22 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-3-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2855.10	8850.81	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2974.10	9219.71	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	2894.70	8973.57	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.34	397.02	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	131.76	395.28	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	118.92	356.76	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	168.32	521.79	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	125.28	388.37	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	151.75	470.43	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	557.06	1726.89	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	477.13	1479.10	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	562.93	1745.08	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2105.80	6527.98	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2134.90	6618.19	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2055.90	6373.29	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2846.60	8824.46	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3075.70	9534.67	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3147.40	9756.94	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3495.40	10835.74	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3404.00	10552.40	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2783.70	8629.47	FALSE	spill
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	254.52	763.56	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	272.13	816.39	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	317.17	951.51	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1112.00	3336.00	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	938.00	2814.00	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1125.10	3375.30	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2510.90	7532.70	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2541.30	7623.90	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2510.10	7530.30	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3339.90	10019.70	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3327.20	9981.60	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2870.00	8610.00	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	2756.00	8268.00	FALSE	pipetting error
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3389.60	10168.80	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3336.30	10008.90	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3426.80	10280.40	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2927.70	8783.10	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	2598.60	7795.80	FALSE	pipetting error
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3275.70	9827.10	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3067.10	9201.30	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3410.10	10230.30	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3462.90	10388.70	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3466.40	10399.20	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3021.90	9065.70	FALSE	spill

Check the 10% rule: 21.89% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICP)	Ratio Total binding/ Hot					
1	1	—	88.2	8850.81	8405.3	683.7	88.2	19.41003					
2	2	—	92.0	9219.71	8774.2	314.8	92.0	20.21903					
3	3	—	89.4	8973.57	8528.0	561.0	89.4	19.67924					
4	1	-6.00	-0.5	397.02	-48.5	9137.5	-0.5	0.870674					
5	2	-6.00	-0.5	395.28	-50.3	9139.3	-0.5	0.866858					
6	3	-6.00	0.0	356.76	-88.8	9177.8	-0.9	0.782383					
7	1	cold R1881	-7.01	0.8	521.792	76.2	0.8	1.144302					
8	2	cold R1881	-7.01	-0.6	388.368	-57.2	-0.6	0.8517					
9	3	cold R1881	-7.01	0.3	470.425	24.9	0.3	1.031653					
10	1	cold R1881	-8.01	13.4	1726.886	1281.3	13.4	3.7871					
11	2	cold R1881	-8.01	10.8	1479.103	1033.5	10.8	3.243706					
12	3	cold R1881	-8.01	13.6	1745.083	1299.5	13.6	3.827006					
13	1	cold R1881	-9.01	63.8	6527.98	6082.4	63.8	14.31601					
14	2	cold R1881	-9.01	64.7	6618.19	6172.6	64.7	14.51384					
15	3	cold R1881	-9.01	62.2	6373.29	5927.7	62.2	13.97677					
16	1	cold R1881	-10.01	87.9	8824.46	8378.9	87.9	19.35224					
17	2	cold R1881	-10.01	95.3	9534.67	9089.1	95.3	20.90975					
18	3	cold R1881	-10.01	97.7	9756.94	9311.4	97.7	21.39719					
19	1	cold R1881	-11.01	109.0	10835.74	10390.2	109.0	23.76302					
20	2	cold R1881	-11.01	106.0	10552.4	10106.8	106.0	23.14165					
21	3	cold R1881	-11.01										
22	1	Weak Positive	-3	3.3	763.56	318.0	3.3	1.674504					
23	2	Weak Positive	-3	3.9	816.39	370.8	3.9	1.790362					
24	3	Weak Positive	-3	5.3	951.51	506.0	5.3	2.086683					
25	1	Weak Positive	-4	30.3	3336	2890.4	30.3	7.315923					
26	2	Weak Positive	-4	24.8	2814	2368.4	24.8	6.171165					
27	3	Weak Positive	-4	30.7	3375.3	2929.7	30.7	7.402109					
28	1	Weak Positive	-5	74.3	7532.7	7087.1	74.3	16.51938					
29	2	Weak Positive	-5	75.3	7623.9	7178.3	75.3	16.71938					
30	3	Weak Positive	-5	74.3	7530.3	7084.7	74.3	16.51412					
31	1	Weak Positive	-6	100.4	10019.7	9574.1	100.4	21.97343					
32	2	Weak Positive	-6	100.0	9981.6	9536.0	100.0	21.88987					
33	3	Weak Positive	-6	85.6	8610	8164.4	85.6	18.88192					
34	1	Weak Positive	-7										
35	2	Weak Positive	-7	102.0	10168.8	9723.2	102.0	22.30041					
36	3	Weak Positive	-7	100.3	10008.9	9563.3	100.3	21.94974					
37	1	Weak Positive	-8	103.1	10280.4	9834.8	103.1	22.54515					
38	2	Weak Positive	-8	87.4	8783.1	8337.5	87.4	19.26154					
39	3	Weak Positive	-8										
40	1	Weak Positive	-9	98.4	9827.1	9381.5	98.4	21.55105					
41	2	Weak Positive	-9	91.8	9201.3	8755.7	91.8	20.17866					
42	3	Weak Positive	-9	102.6	10230.3	9784.7	102.6	22.43528					
43	1	Weak Positive	-10	104.3	10388.7	9943.1	104.3	22.78265					
44	2	Weak Positive	-10	104.4	10399.2	9953.6	104.4	22.80568					
45	3	Weak Positive	-10										

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	21.89%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	131.86	408.77	FALSE	precipitate in tube
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	133.30	413.23	FALSE	precipitate in tube
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	181.57	562.87	FALSE	precipitate in tube
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	126.90	393.39	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	131.91	408.92	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	114.54	355.07	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	148.16	459.30	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	161.08	499.35	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	164.80	510.88	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	196.25	608.38	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	171.11	530.44	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	189.94	588.81	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	879.90	2727.69	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	847.62	2627.62	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	1065.10	3301.81	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	2903.60	9001.16	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3158.20	9790.42	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3041.80	9429.58	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3375.50	10464.05	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3464.20	10739.02	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2767.30	8578.63	FALSE	spill
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3091.10	9582.41	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3334.40	10336.64	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3059.20	9483.52	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	126.58	392.40	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	123.97	384.31	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	113.02	350.36	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	195.79	606.95	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	158.13	490.20	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	190.48	590.49	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	754.77	2339.79	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	708.22	2195.48	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	737.67	2286.78	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2012.70	6239.37	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2111.10	6544.41	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2231.90	6918.89	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3268.90	10133.59	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3267.40	10128.94	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3146.50	9754.15	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3618.10	11216.11	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3048.30	9449.73	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3359.50	10414.45	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3515.00	10896.50	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3295.90	10217.29	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	2811.30	8715.03	FALSE	spill
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	2967.10	9198.01	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	2965.90	9194.29	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	2899.20	8987.52	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICR)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424						
47	2	Unknown 1	-3.01424						
48	3	Unknown 1	-3.01424						
49	1	Unknown 1	-4.01424	-0.5	393.39	-52.2	9141.1	-0.5	0.862713
50	2	Unknown 1	-4.01424	-0.4	408.921	-36.6	9125.6	-0.4	0.896773
51	3	Unknown 1	-4.01424	-0.9	355.074	-90.5	9179.5	-0.9	0.778685
52	1	Unknown 1	-5.01424	0.1	459.296	13.7	9075.2	0.1	1.007246
53	2	Unknown 1	-5.01424	0.6	499.348	53.8	9035.2	0.6	1.095081
54	3	Unknown 1	-5.01424	0.7	510.88	65.3	9023.7	0.7	1.120371
55	1	Unknown 1	-6.01424	1.7	608.375	162.8	8926.2	1.7	1.33418
56	2	Unknown 1	-6.01424	0.9	530.441	84.9	9004.1	0.9	1.163269
57	3	Unknown 1	-6.01424	1.5	588.814	143.3	8945.7	1.5	1.291282
58	1	Unknown 1	-7.01424	23.9	2727.69	2282.1	6806.8	23.9	5.981886
59	2	Unknown 1	-7.01424	22.9	2627.622	2182.1	6906.9	22.9	5.762434
60	3	Unknown 1	-7.01424	30.0	3301.81	2856.3	6232.7	30.0	7.240944
61	1	Unknown 1	-8.01424	89.7	9001.16	8555.6	533.4	89.7	19.73975
62	2	Unknown 1	-8.01424	98.0	9790.42	9344.9	-255.9	98.0	21.47061
63	3	Unknown 1	-8.01424	94.2	9429.58	8984.0	105.0	94.2	20.67928
64	1	Unknown 1	-9.01424	105.1	10464.05	10018.5	-929.5	105.1	22.9479
65	2	Unknown 1	-9.01424	108.0	10739.02	10293.5	-1204.5	108.0	23.55091
66	3	Unknown 1	-9.01424						
67	1	Unknown 1	-10.01424	95.8	9582.41	9136.9	-47.9	95.8	21.01444
68	2	Unknown 1	-10.01424	103.7	10336.64	9891.1	-802.1	103.7	22.66848
69	3	Unknown 1	-10.01424	94.8	9483.52	9038.0	51.0	94.8	20.79757
70	1	Unknown 2	-3.01424	-0.6	392.398	-53.2	9142.1	-0.6	0.860538
71	2	Unknown 2	-3.01424	-0.6	384.307	-61.2	9150.2	-0.6	0.842794
72	3	Unknown 2	-3.01424	-1.0	350.362	-95.2	9184.2	-1.0	0.768352
73	1	Unknown 2	-4.01424	1.7	606.949	161.4	8927.6	1.7	1.331053
74	2	Unknown 2	-4.01424	0.5	490.203	44.6	9044.3	0.5	1.075026
75	3	Unknown 2	-4.01424	1.5	590.488	144.9	8944.0	1.5	1.294953
76	1	Unknown 2	-5.01424	19.9	2339.787	1894.2	7194.7	19.9	5.131206
77	2	Unknown 2	-5.01424	18.4	2195.482	1749.9	7339.1	18.4	4.814741
78	3	Unknown 2	-5.01424	19.3	2286.777	1841.2	7247.8	19.3	5.014953
79	1	Unknown 2	-6.01424	60.8	6239.37	5793.8	3295.2	60.8	13.68308
80	2	Unknown 2	-6.01424	64.0	6544.41	6098.9	2990.1	64.0	14.35204
81	3	Unknown 2	-6.01424	67.9	6918.89	6473.3	2615.6	67.9	15.17328
82	1	Unknown 2	-7.01424	101.6	10133.59	9688.0	-599.1	101.6	22.22319
83	2	Unknown 2	-7.01424	101.6	10128.94	9683.4	-594.4	101.6	22.21299
84	3	Unknown 2	-7.01424	97.6	9754.15	9308.6	-219.6	97.6	21.39107
85	1	Unknown 2	-8.01424	113.0	11216.11	10770.6	-1681.6	113.0	24.59718
86	2	Unknown 2	-8.01424	94.4	9449.73	9004.2	84.8	94.4	20.72347
87	3	Unknown 2	-8.01424	104.6	10414.45	9968.9	-879.9	104.6	22.83912
88	1	Unknown 2	-9.01424	109.6	10896.5	10450.9	-1362.0	109.6	23.89627
89	2	Unknown 2	-9.01424	102.5	10217.29	9771.7	-682.8	102.5	22.40675
90	3	Unknown 2	-9.01424						
91	1	Unknown 2	-10.01424	91.8	9198.01	8752.5	336.5	91.8	20.17144
92	2	Unknown 2	-10.01424	91.8	9194.29	8748.7	340.2	91.8	20.16329
93	3	Unknown 2	-10.01424	89.6	8987.52	8542.0	547.0	89.6	19.70983

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:	21.89%	If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	446.72	1384.83		
95	2	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	379.48	1176.39	TRUE	
96	3	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	411.17	1274.63	TRUE	
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1854.80	5749.88	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1894.20	5872.02	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1777.40	5509.94	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3443.00	10673.30	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3449.60	10693.76	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3469.20	10754.52	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3513.10	10890.61	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2881.40	8932.34	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3098.90	9606.59	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3497.40	10841.94	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3454.90	10710.19	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3578.40	11093.04	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3446.60	10684.46	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3480.50	10789.55	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3550.30	11005.93	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3042.50	9431.75	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2928.40	9078.04	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3311.60	10265.96	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3556.80	11026.08	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3551.80	11010.58	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3455.90	10713.29	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	2872.10	8903.51	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	2843.90	8816.09	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	2901.30	8994.03	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2993.00	9278.30	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3174.50	9840.95	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	2983.30	9248.23	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3398.90	10536.59	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	2922.40	9059.44	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3274.10	10149.71	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3011.40	9335.34	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3778.00	11711.80	FALSE	pipetting error
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3536.90	10964.39	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3163.80	9807.78	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3610.90	11193.79	FALSE	pipetting error
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3319.40	10290.14	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3687.20	11430.32	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3679.10	11405.21	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3724.80	11546.88	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3676.70	11397.77	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3741.50	11598.65	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3739.20	11591.52	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3657.00	11336.70	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3678.00	11401.80	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3730.60	11564.86	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific E(Ch)	Ratio Total binding/ Hot					
94	1	Unknown 3	-3.6163	9.9	1384.832	939.3	8149.7	9.9	3.036968				
95	2	Unknown 3	-3.6163	7.7	1176.388	730.8	8358.1	7.7	2.579845				
96	3	Unknown 3	-3.6163	8.7	1274.627	829.1	8259.9	8.7	2.795286				
97	1	Unknown 3	-4.01424	55.6	5749.88	5304.3	3784.7	55.6	12.60962				
98	2	Unknown 3	-4.01424	56.9	5872.02	5426.5	3662.5	56.9	12.87747				
99	3	Unknown 3	-4.01424	53.1	5509.94	5064.4	4024.6	53.1	12.08342				
100	1	Unknown 3	-5.01424	107.3	10673.3	10227.7	-1138.8	107.3	23.40679				
101	2	Unknown 3	-5.01424	107.5	10693.76	10248.2	-1159.2	107.5	23.45166				
102	3	Unknown 3	-5.01424	108.1	10754.52	10309.0	-1220.0	108.1	23.5849				
103	1	Unknown 3	-6.01424	109.5	10890.61	10445.1	-1356.1	109.5	23.88335				
104	2	Unknown 3	-6.01424	89.0	8932.34	8486.8	602.2	89.0	19.58882				
105	3	Unknown 3	-6.01424	96.1	9606.59	9161.0	-72.1	96.1	21.06747				
106	1	Unknown 3	-7.01424	109.0	10841.94	10396.4	-1307.4	109.0	23.77662				
107	2	Unknown 3	-7.01424	107.7	10710.19	10264.6	-1175.7	107.7	23.48769				
108	3	Unknown 3	-7.01424	111.7	11093.04	10647.5	-1558.5	111.7	24.32729				
109	1	Unknown 3	-8.01424	107.4	10684.46	10238.9	-1149.9	107.4	23.43126				
110	2	Unknown 3	-8.01424	108.5	10789.55	10344.0	-1255.0	108.5	23.66173				
111	3	Unknown 3	-8.01424	110.8	11005.93	10560.4	-1471.4	110.8	24.13625				
112	1	Unknown 3	-9.01424	94.2	9431.75	8986.2	102.8	94.2	20.68404				
113	2	Unknown 3	-9.01424	90.5	9078.04	8632.5	456.5	90.5	19.90835				
114	3	Unknown 3	-9.01424	103.0	10265.96	9820.4	-731.4	103.0	22.51348				
115	1	Unknown 3	-10.01424	111.0	11026.08	10580.5	-1491.5	111.0	24.18044				
116	2	Unknown 3	-10.01424	110.8	11010.58	10565.0	-1476.0	110.8	24.14645				
117	3	Unknown 3	-10.01424	107.7	10713.29	10267.7	-1178.8	107.7	23.49449				
118	1	Unknown 4	-3.01424										
119	2	Unknown 4	-3.01424										
120	3	Unknown 4	-3.01424										
121	1	Unknown 4	-4.01424	92.6	9278.3	8832.7	256.2	92.6	20.34752				
122	2	Unknown 4	-4.01424	98.5	9840.95	9395.4	-306.4	98.5	21.58143				
123	3	Unknown 4	-4.01424	92.3	9248.23	8802.7	286.3	92.3	20.28158				
124	1	Unknown 4	-5.01424	105.8	10536.59	10091.0	-1002.1	105.8	23.10698				
125	2	Unknown 4	-5.01424	90.3	9059.44	8613.9	475.1	90.3	19.86756				
126	3	Unknown 4	-5.01424	101.8	10149.71	9704.2	-615.2	101.8	22.25854				
127	1	Unknown 4	-6.01424	93.2	9335.34	8889.8	199.2	93.2	20.47261				
128	2	Unknown 4	-6.01424										
129	3	Unknown 4	-6.01424	110.3	10964.39	10518.8	-1429.9	110.3	24.04515				
130	1	Unknown 4	-7.01424	98.2	9807.78	9362.2	-273.2	98.2	21.50868				
131	2	Unknown 4	-7.01424										
132	3	Unknown 4	-7.01424	103.3	10290.14	9844.6	-755.6	103.3	22.56651				
133	1	Unknown 4	-8.01424	115.2	11430.32	10984.8	-1895.8	115.2	25.06695				
134	2	Unknown 4	-8.01424	114.9	11405.21	10959.7	-1870.7	114.9	25.01188				
135	3	Unknown 4	-8.01424	116.4	11546.88	11101.3	-2012.3	116.4	25.32257				
136	1	Unknown 4	-9.01424	114.9	11397.77	10952.2	-1863.2	114.9	24.99557				
137	2	Unknown 4	-9.01424	117.0	11598.65	11153.1	-2064.1	117.0	25.4361				
138	3	Unknown 4	-9.01424	116.9	11591.52	11146.0	-2057.0	116.9	25.42046				
139	1	Unknown 4	-10.01424	114.2	11336.7	10891.1	-1802.2	114.2	24.86164				
140	2	Unknown 4	-10.01424	114.9	11401.8	10956.2	-1867.3	114.9	25.0044				
141	3	Unknown 4	-10.01424	116.6	11564.86	11119.3	-2030.3	116.6	25.362				

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1881.10	5831.41	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1901.60	5894.96	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1860.70	5768.17	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2725.40	8448.74	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2851.80	8840.58	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2459.20	7623.52	FALSE	spill
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3384.10	10490.71	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3616.30	11210.53	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3451.90	10700.89	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3738.90	11590.59	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3805.50	11797.05	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3787.80	11742.18	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3486.70	10808.77	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3725.90	11550.29	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3765.20	11672.12	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3202.80	9928.68	FALSE	spill
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3744.10	11606.71	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3781.40	11722.34	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3169.90	9826.69	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3151.80	9770.58	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3805.10	11795.81	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3288.10	10193.11	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3783.10	11727.61	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3804.00	11792.40	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3651.20	11318.72	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3581.60	11102.96	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3359.60	10414.76	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.40	397.20	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	160.56	481.68	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	215.13	645.39	TRUE	
172	1	none	Hot	—	—	—	30	—	—	—	—	—	—	44889.00	44889.00	TRUE	
173	2	none	Hot	—	—	—	30	—	—	—	—	—	—	45636.00	45636.00	TRUE	
174	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45486.00	45486.00	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45897.00	45897.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	—	44953.00	44953.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	—	46734.00	46734.00	TRUE	

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
142	1	Unknown 5	-3.6163	56.5	5831.41	5385.9	3703.1	56.5	12.78841
143	2	Unknown 5	-3.6163	57.2	5894.96	5449.4	3639.6	57.2	12.92778
144	3	Unknown 5	-3.6163	55.8	5768.17	5322.6	3766.4	55.8	12.64973
145	1	Unknown 5	-4.01424	83.9	8448.74	8003.2	1085.8	83.9	18.52828
146	2	Unknown 5	-4.01424	88.0	8840.58	8395.0	694.0	88.0	19.38759
147	3	Unknown 5	-4.01424						
148	1	Unknown 5	-5.01424	105.4	10490.71	10045.2	-956.2	105.4	23.00636
149	2	Unknown 5	-5.01424	112.9	11210.53	10765.0	-1676.0	112.9	24.58494
150	3	Unknown 5	-5.01424	107.6	10700.89	10255.3	-1166.4	107.6	23.46729
151	1	Unknown 5	-6.01424	116.9	11590.59	11145.0	-2056.1	116.9	25.41843
152	2	Unknown 5	-6.01424	119.1	11797.05	11351.5	-2262.5	119.1	25.8712
153	3	Unknown 5	-6.01424	118.5	11742.18	11296.6	-2207.6	118.5	25.75087
154	1	Unknown 5	-7.01424	108.7	10808.77	10363.2	-1274.2	108.7	23.70388
155	2	Unknown 5	-7.01424	116.5	11550.29	11104.7	-2015.8	116.5	25.33005
156	3	Unknown 5	-7.01424	117.7	11672.12	11226.6	-2137.6	117.7	25.59722
157	1	Unknown 5	-8.01424						
158	2	Unknown 5	-8.01424	117.1	11606.71	11161.2	-2072.2	117.1	25.45378
159	3	Unknown 5	-8.01424	118.3	11722.34	11276.8	-2187.8	118.3	25.70736
160	1	Unknown 5	-9.01424	98.4	9826.69	9381.1	-292.2	98.4	21.55015
161	2	Unknown 5	-9.01424	97.8	9770.58	9325.0	-236.0	97.8	21.4271
162	3	Unknown 5	-9.01424	119.0	11795.81	11350.3	-2261.3	119.0	25.86848
163	1	Unknown 5	-10.01424	102.2	10193.11	9747.6	-658.6	102.2	22.35372
164	2	Unknown 5	-10.01424	118.3	11727.61	11282.1	-2193.1	118.3	25.71891
165	3	Unknown 5	-10.01424	119.0	11792.4	11346.8	-2257.9	119.0	25.861
166	1	—	—	114.0	11318.72	10873.2	-1784.2	114.0	24.82221
167	2	—	—	111.8	11102.96	10657.4	-1568.4	111.8	24.34904
168	3	—	—	104.6	10414.76	9969.2	-880.2	104.6	22.8398
169	1	-6.00	-0.5	397.2	-48.4	9137.3	-0.5	0.871069	
170	2	-6.00	0.4	481.68	36.1	9052.9	0.4	1.056335	
171	3	-6.00	2.1	645.39	199.8	8889.1	2.1	1.415355	
172	1				44889	44443.4			
173	2				45636	45190.4			
174	3				45486	45040.4			
175	1				45897	45451.4			
176	2				44953	44507.4			
177	3				46734	46288.4			

Prism data															
standard curve				weak positive				CR42342				CR42345			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-6.0	-0.50904	-0.52729	-0.93130	-3	3.3353	3.8894	5.3066	-3.0				-3.0	-0.5575	-0.6424	-0.9984
-6.0	-0.50716	0.37889	2.09591	-4	30.3155	24.8407	30.7277	-4.0	-0.5471	-0.3842	-0.9490	-4.0	1.6927	0.4683	1.5201
-7.0	0.79959	-0.59979	0.26084	-5	74.3313	75.2878	74.3062	-5.0	0.1441	0.5642	0.6851	-5.0	19.8671	18.3536	19.3111
-8.0	13.43884	10.84005	13.62970	-6	100.4155	100.0159	85.6303	-6.0	1.7077	0.8903	1.5025	-6.0	60.7666	63.9660	67.8936
-9.0	63.79363	64.73977	62.17121	-7		101.9792	100.3022	-7.0	23.9355	22.8859	29.9569	-7.0	101.6100	101.5612	97.6303
-10.0	87.87955	95.32837	97.65958	-8	103.1497	87.4458		-8.0	89.7328	98.0107	94.2262	-8.0	112.9636	94.4375	104.5557
-11.0	108.97424	106.00251		-9	98.3954	91.8319	102.6243	-9.0	105.0759	107.9598		-9.0	109.6115	102.4878	
				-10	104.2856	104.3957		-10.0	95.8291	103.7396	94.7919	-10.0	91.7974	91.7584	89.5898

CR42351					CR42358					CR43261				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.6	9.8513	7.6651	8.6955		-3.0					-3.6	56.4879	57.1544	55.8246	
-4.0	55.6328	56.9138	53.1162		-4.0	92.6395	98.5407	92.3241		-4.0	83.9389	88.0486		
-5.0	107.2705	107.4851	108.1224		-5.0	105.8367	90.3441	101.7790		-5.0	105.3555	112.9051	107.5599	
-6.0	109.5497	89.0110	96.0827		-6.0	93.2378		110.3235		-6.0	116.8912	119.0566	118.4812	
-7.0	109.0393	107.6574	111.6728		-7.0	98.1928		103.2519		-7.0	108.6914	116.4686	117.7464	
-8.0	107.3876	108.4898	110.7592		-8.0	115.2103	114.9469	116.4328		-8.0		117.0603	118.2731	
-9.0	94.2489	90.5391	102.9983		-9.0	114.8689	116.9758	116.9010		-9.0	98.3911	97.8026	119.0436	
-10.0	110.9706	110.8080	107.6900		-10.0	114.2284	114.9112	116.6214		-10.0	102.2342	118.3283	119.0079	

Competitive Assay of a known Weak Positive
177 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:		
Run identification:	512	
Assay start date:	10/10/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.82	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.41E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.53E-05	M
RBA:	3.99094E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	5.56E-08	CR42342
RBA, Unknown 1:	2.53415%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	1.82E-06	CR42345
RBA, Unknown 2:	0.07769%	
Max Concentration, Unknown 3:	7.50E-03	M (example 5e-3)
IC50, Unknown 3:	9.70E-05	CR42351
RBA, Unknown 3:	0.00145%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	6.86E-04	CR42358
RBA, Unknown 4:	0.00021%	
Max Concentration, Unknown 5:	7.50E-03	M (example 5e-3)
IC50, Unknown 5:	3.04E-04	CR43261
RBA, Unknown 5:	0.00046%	
volume of ethanol counted:	2	mL
multitply DPM in sample by :	3.1	
working volume	3.1E+02	uL

protocol calls for counting decanted EtOH supernate
 reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10857.5	718.50	Total Binding, solvent control, tubes
Hot	6	45304.2	1267.27	Total hot R1881 added to each tube
NSB	6	430.7	60.15	Nonspecific Binding
Specific EtOH	6	10426.9	718.50	

Assay Characterization Values	
EtOH / Hot	0.24 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3199.90	9919.69	TRUE	
2	2	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3451.40	10699.34	TRUE	
3	3	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3272.60	10145.06	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	130.81	392.43	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	123.83	371.49	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	122.18	366.54	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	160.40	497.24	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	158.95	492.75	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	161.43	500.43	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	627.09	1943.98	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	568.68	1762.91	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	592.14	1835.63	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2181.20	6761.72	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2035.90	6311.29	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2149.10	6662.21	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3183.90	9870.09	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3229.30	10010.83	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3065.60	9503.36	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3420.00	10602.00	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3475.60	10774.36	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3359.90	10415.69	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	253.59	760.77	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	264.19	792.57	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	299.04	897.12	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1165.60	3496.80	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1142.40	3427.20	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1120.50	3361.50	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2914.10	8742.30	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2754.10	8262.30	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2588.40	7765.20	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3635.30	10905.90	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3410.10	10230.30	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3463.80	10391.40	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3475.80	10427.40	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3608.00	10824.00	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3553.90	10661.70	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3382.10	10146.30	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3169.10	9507.30	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3472.80	10418.40	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3547.10	10641.30	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3550.20	10650.60	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3551.90	10655.70	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3488.40	10465.20	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3192.50	9577.70	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3595.70	10787.10	TRUE	

Check the 10% rule: 23.97% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
9919.69	TRUE	
10699.34	TRUE	
10145.06	TRUE	
392.43	TRUE	
371.49	TRUE	
366.54	TRUE	
497.24	TRUE	
492.75	TRUE	
500.43	TRUE	
1943.98	TRUE	
1762.91	TRUE	
1835.63	TRUE	
6761.72	TRUE	
6311.29	TRUE	
6662.21	TRUE	
9870.09	TRUE	
10010.83	TRUE	
9503.36	TRUE	
10602.00	TRUE	
10774.36	TRUE	
10415.69	TRUE	
760.77	TRUE	
792.57	TRUE	
897.12	TRUE	
3496.80	TRUE	
3427.20	TRUE	
3361.50	TRUE	
8742.30	TRUE	
8262.30	TRUE	
7765.20	TRUE	
10905.90	TRUE	
10230.30	TRUE	
10391.40	TRUE	
10427.40	TRUE	
10824.00	TRUE	
10661.70	TRUE	
10146.30	TRUE	
9507.30	TRUE	
10418.40	TRUE	
10641.30	TRUE	
10650.60	TRUE	
10655.70	TRUE	
10465.20	TRUE	
9577.70	TRUE	
10787.10	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
1	1	—	91.0	9919.69	9489.0	507.2	91.0	21.89576					
2	2	—	98.5	10699.34	10268.7	-272.5	98.5	23.61668					
3	3	—	93.2	10145.06	9714.4	281.8	93.2	22.39322					
4	1	-6.00	-0.4	392.43	-38.2	10034.4	-0.4	0.866212					
5	2	-6.00	-0.6	371.49	-59.2	10055.4	-0.6	0.819991					
6	3	-6.00	0.0	366.54	-64.1	10060.3	-0.6	0.809065					
7	1	cold R1881	-7.01	0.6	497.24	66.6	0.6	1.097559					
8	2	cold R1881	-7.01	0.6	492.745	62.1	0.6	1.087637					
9	3	cold R1881	-7.01	0.7	500.433	69.8	0.7	1.104607					
10	1	cold R1881	-8.01	14.5	1943.979	1513.3	14.5	4.29095					
11	2	cold R1881	-8.01	12.8	1762.908	1332.2	12.8	3.891271					
12	3	cold R1881	-8.01	13.5	1835.634	1405.0	13.5	4.0518					
13	1	cold R1881	-9.01	60.7	6761.72	6331.1	60.7	14.92516					
14	2	cold R1881	-9.01	56.4	6311.29	5880.6	56.4	13.93093					
15	3	cold R1881	-9.01	59.8	6662.21	6231.5	59.8	14.70551					
16	1	cold R1881	-10.01	90.5	9870.09	9439.4	90.5	21.78627					
17	2	cold R1881	-10.01	91.9	10010.83	9580.2	91.9	22.09693					
18	3	cold R1881	-10.01	87.0	9503.36	9072.7	87.0	20.97679					
19	1	cold R1881	-11.01	97.5	10602	10171.3	97.5	23.40182					
20	2	cold R1881	-11.01	99.2	10774.36	10343.7	99.2	23.78227					
21	3	cold R1881	-11.01	95.8	10415.69	9985.0	95.8	22.99058					
22	1	Weak Positive	-3	3.2	760.77	330.1	3.2	1.67925					
23	2	Weak Positive	-3	3.5	792.57	361.9	3.5	1.749442					
24	3	Weak Positive	-3	4.5	897.12	466.5	4.5	1.980215					
25	1	Weak Positive	-4	29.4	3496.8	3066.1	29.4	7.718495					
26	2	Weak Positive	-4	28.7	3427.2	2996.5	28.7	7.564867					
27	3	Weak Positive	-4	28.1	3361.5	2930.8	28.1	7.419847					
28	1	Weak Positive	-5	79.7	8742.3	8311.6	79.7	19.2969					
29	2	Weak Positive	-5	75.1	8262.3	7831.6	75.1	18.2374					
30	3	Weak Positive	-5	70.3	7765.2	7334.5	70.3	17.14015					
31	1	Weak Positive	-6	100.5	10905.9	10475.2	100.5	24.07262					
32	2	Weak Positive	-6	94.0	10230.3	9799.6	94.0	22.58137					
33	3	Weak Positive	-6	95.5	10391.4	9960.7	95.5	22.93696					
34	1	Weak Positive	-7	95.9	10427.4	9996.7	95.9	23.01643					
35	2	Weak Positive	-7	99.7	10824	10393.3	99.7	23.89184					
36	3	Weak Positive	-7	98.1	10661.7	10231.0	98.1	23.5336					
37	1	Weak Positive	-8	93.2	10146.3	9715.6	93.2	22.39595					
38	2	Weak Positive	-8	87.1	9507.3	9076.6	87.1	20.98549					
39	3	Weak Positive	-8	95.8	10418.4	9987.7	95.8	22.99656					
40	1	Weak Positive	-9	97.9	10641.3	10210.6	97.9	23.48857					
41	2	Weak Positive	-9	98.0	10650.6	10219.9	98.0	23.5091					
42	3	Weak Positive	-9	98.1	10655.7	10225.0	98.1	23.52035					
43	1	Weak Positive	-10	96.2	10465.2	10034.5	96.2	23.09986					
44	2	Weak Positive	-10	87.7	9577.5	9146.8	87.7	21.14044					
45	3	Weak Positive	-10	99.3	10787.1	10356.4	99.3	23.81039					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: **23.97%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	164.04	508.52	FALSE	precipitate in tube
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	139.94	433.81	FALSE	precipitate in tube
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	110.05	341.16	FALSE	precipitate in tube
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	107.36	332.82	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	119.14	369.33	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	113.18	350.86	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	130.20	403.62	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	176.51	547.18	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	146.48	454.09	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	259.07	803.12	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	211.93	656.98	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	218.32	676.79	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	1149.60	3563.76	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	1160.00	3596.00	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	1428.80	4429.28	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3226.40	10001.84	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3124.00	9684.40	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3164.00	9808.40	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3462.70	10734.37	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3650.40	11316.24	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3650.10	11315.31	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3721.70	11537.27	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3621.00	11225.10	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3654.20	11328.02	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	114.86	356.07	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	139.14	431.33	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	136.33	422.62	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	208.18	645.36	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	202.98	629.24	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	219.94	681.81	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	821.68	2547.21	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	785.45	2434.90	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	726.49	2252.12	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2042.70	6332.37	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2429.10	7530.21	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2187.40	6780.94	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3467.00	10747.70	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3461.50	10730.65	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3275.90	10155.29	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3589.30	11126.83	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3592.80	11137.68	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3442.70	10672.37	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3633.80	11264.78	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3496.30	10838.53	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3324.80	10306.88	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3331.60	10327.96	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3530.10	10943.31	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3629.40	11251.14	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424						
47	2	Unknown 1	-3.01424						
48	3	Unknown 1	-3.01424						
49	1	Unknown 1	-4.01424	-0.9	332.816	-97.9	10094.1	-0.9	0.734626
50	2	Unknown 1	-4.01424	-0.6	369.334	-61.3	10057.5	-0.6	0.815232
51	3	Unknown 1	-4.01424	-0.8	350.858	-79.8	10076.0	-0.8	0.77445
52	1	Unknown 1	-5.01424	-0.3	403.62	-27.1	10023.3	-0.3	0.890911
53	2	Unknown 1	-5.01424	1.1	547.181	116.5	9879.7	1.1	1.207794
54	3	Unknown 1	-5.01424	0.2	454.088	23.4	9972.8	0.2	1.00231
55	1	Unknown 1	-6.01424	3.6	803.117	372.4	9623.8	3.6	1.772722
56	2	Unknown 1	-6.01424	2.2	656.983	226.3	9769.9	2.2	1.45016
57	3	Unknown 1	-6.01424	2.4	676.792	246.1	9750.1	2.4	1.493885
58	1	Unknown 1	-7.01424	30.0	3563.76	3133.1	6863.1	30.0	7.866296
59	2	Unknown 1	-7.01424	30.4	3596	3165.3	6830.9	30.4	7.93746
60	3	Unknown 1	-7.01424	38.3	4429.28	3998.6	5997.6	38.3	9.776761
61	1	Unknown 1	-8.01424	91.8	10001.84	9571.2	425.0	91.8	22.07709
62	2	Unknown 1	-8.01424	88.7	9684.4	9253.7	742.5	88.7	21.3764
63	3	Unknown 1	-8.01424	89.9	9808.4	9377.7	618.5	89.9	21.65011
64	1	Unknown 1	-9.01424	98.8	10734.37	10303.7	-307.5	98.8	23.694
65	2	Unknown 1	-9.01424	104.4	11316.24	10885.6	-889.4	104.4	24.97836
66	3	Unknown 1	-9.01424	104.4	11315.31	10884.6	-888.4	104.4	24.97631
67	1	Unknown 1	-10.01424	106.5	11537.27	11106.6	-1110.4	106.5	25.46624
68	2	Unknown 1	-10.01424	103.5	11225.1	10794.4	-798.2	103.5	24.77719
69	3	Unknown 1	-10.01424	104.5	11328.02	10897.4	-901.1	104.5	25.00437
70	1	Unknown 2	-3.01424	-0.7	356.066	-74.6	10070.8	-0.7	0.785945
71	2	Unknown 2	-3.01424	0.0	431.334	0.7	9995.5	0.0	0.952085
72	3	Unknown 2	-3.01424	-0.1	422.623	-8.0	10004.3	-0.1	0.932857
73	1	Unknown 2	-4.01424	2.1	645.358	214.7	9781.5	2.1	1.4245
74	2	Unknown 2	-4.01424	1.9	629.238	198.6	9797.6	1.9	1.388919
75	3	Unknown 2	-4.01424	2.4	681.814	251.1	9745.1	2.4	1.50497
76	1	Unknown 2	-5.01424	20.3	2547.208	2116.5	7879.7	20.3	5.622459
77	2	Unknown 2	-5.01424	19.2	2434.895	2004.2	7992.0	19.2	5.37455
78	3	Unknown 2	-5.01424	17.5	2252.119	1821.4	8174.8	17.5	4.971108
79	1	Unknown 2	-6.01424	56.6	6332.37	5901.7	4094.5	56.6	13.97746
80	2	Unknown 2	-6.01424	68.1	7530.21	7099.5	2896.7	68.1	16.62145
81	3	Unknown 2	-6.01424	60.9	6780.94	6350.3	3645.9	60.9	14.96759
82	1	Unknown 2	-7.01424	98.9	10747.7	10317.0	-320.8	98.9	23.72342
83	2	Unknown 2	-7.01424	98.8	10730.65	10300.0	-303.8	98.8	23.68579
84	3	Unknown 2	-7.01424	93.3	10155.29	9724.6	271.6	93.3	22.4158
85	1	Unknown 2	-8.01424	102.6	11126.83	10696.2	-700.0	102.6	24.56028
86	2	Unknown 2	-8.01424	102.7	11137.68	10707.0	-710.8	102.7	24.58423
87	3	Unknown 2	-8.01424	98.2	10672.37	10241.7	-245.5	98.2	23.55715
88	1	Unknown 2	-9.01424	103.9	11264.78	10834.1	-837.9	103.9	24.86478
89	2	Unknown 2	-9.01424	99.8	10838.53	10407.9	-411.7	99.8	23.92391
90	3	Unknown 2	-9.01424	94.7	10306.88	9876.2	120.0	94.7	22.7504
91	1	Unknown 2	-10.01424	94.9	10327.96	9897.3	98.9	94.9	22.79693
92	2	Unknown 2	-10.01424	100.8	10943.31	10512.6	-516.4	100.8	24.1552
93	3	Unknown 2	-10.01424	103.8	11251.14	10820.5	-824.3	103.8	24.83467

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: **23.97%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	444.41	1377.67	TRUE	
95	2	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	450.83	1397.57	TRUE	
96	3	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	560.85	1738.64	TRUE	
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2164.40	6709.64	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2085.80	6465.98	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2261.30	7010.03	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3531.60	10947.96	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3459.30	10723.83	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3386.40	10497.84	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3670.90	11379.79	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3680.80	11410.48	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3505.30	10866.43	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3644.40	11297.64	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3648.50	11310.35	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3733.60	11574.16	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3705.80	11487.98	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3628.40	11248.04	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3571.90	11072.89	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3668.30	11371.73	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3581.70	11103.27	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3544.10	10986.71	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3068.60	9512.66	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3641.30	11288.03	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3807.30	11802.63	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	3057.90	9479.49	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	2976.10	9225.91	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	3048.80	9451.28	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3060.20	9486.62	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3163.20	9805.92	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3030.50	9394.55	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3310.90	10263.79	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3315.90	10279.29	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3515.00	10896.50	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3277.50	10160.25	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3673.70	11388.47	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3435.00	10648.50	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3463.50	10736.85	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3156.40	9784.84	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3589.60	11127.76	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3538.40	10969.04	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3642.60	11292.06	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3654.20	11328.02	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3581.90	11103.89	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3627.10	11244.01	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3756.70	11645.77	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3509.60	10879.76	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3573.50	11077.85	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3647.50	11307.25	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EIOH)	Ratio Total binding/ Hot					
94	1	Unknown 3	-3.6163	9.1	1377.671	947.0	9049.2	9.1 3.040937					
95	2	Unknown 3	-3.6163	9.3	1397.573	966.9	9029.3	9.3 3.084866					
96	3	Unknown 3	-3.6163	12.5	1738.635	1308.0	8688.2	12.5 3.837693					
97	1	Unknown 3	-4.01424	60.2	6709.64	6279.0	3717.2	60.2 14.81021					
98	2	Unknown 3	-4.01424	57.9	6465.98	6035.3	3960.9	57.9 14.27237					
99	3	Unknown 3	-4.01424	63.1	7010.03	6579.4	3416.8	63.1 15.47326					
100	1	Unknown 3	-5.01424	100.9	10947.96	10517.3	-521.1	100.9 24.16546					
101	2	Unknown 3	-5.01424	98.7	10723.83	10293.2	-297.0	98.7 23.67074					
102	3	Unknown 3	-5.01424	96.6	10497.84	10067.2	-71.0	96.6 23.17191					
103	1	Unknown 3	-6.01424	105.0	11379.79	10949.1	-952.9	105.0 25.11864					
104	2	Unknown 3	-6.01424	105.3	11410.48	10979.8	-983.6	105.3 25.18638					
105	3	Unknown 3	-6.01424	100.1	10866.43	10435.8	-439.6	100.1 23.9855					
106	1	Unknown 3	-7.01424	104.2	11297.64	10867.0	-870.8	104.2 24.93731					
107	2	Unknown 3	-7.01424	104.3	11310.35	10879.7	-883.5	104.3 24.96536					
108	3	Unknown 3	-7.01424	106.9	11574.16	11143.5	-1147.3	106.9 25.54767					
109	1	Unknown 3	-8.01424	106.0	11487.98	11057.3	-1061.1	106.0 25.35745					
110	2	Unknown 3	-8.01424	103.7	11248.04	10817.4	-821.2	103.7 24.82783					
111	3	Unknown 3	-8.01424	102.1	11072.89	10642.2	-646.0	102.1 24.44122					
112	1	Unknown 3	-9.01424	104.9	11371.73	10941.1	-944.9	104.9 25.10085					
113	2	Unknown 3	-9.01424	102.4	11103.27	10672.6	-676.4	102.4 24.50828					
114	3	Unknown 3	-9.01424	101.2	10986.71	10556.0	-559.8	101.2 24.25099					
115	1	Unknown 3	-10.01424	87.1	9512.66	9082.0	914.2	87.1 20.99732					
116	2	Unknown 3	-10.01424	104.1	11288.03	10857.4	-861.2	104.1 24.9161					
117	3	Unknown 3	-10.01424	109.1	11802.63	11372.0	-1375.8	109.1 26.05197					
118	1	Unknown 4	-3.01424										
119	2	Unknown 4	-3.01424										
120	3	Unknown 4	-3.01424										
121	1	Unknown 4	-4.01424	86.9	9486.62	9056.0	940.3	86.9 20.93984					
122	2	Unknown 4	-4.01424	89.9	9805.92	9375.3	621.0	89.9 21.64463					
123	3	Unknown 4	-4.01424	86.0	9394.55	8963.9	1032.3	86.0 20.73661					
124	1	Unknown 4	-5.01424	94.3	10263.79	9833.1	163.1	94.3 22.65529					
125	2	Unknown 4	-5.01424	94.5	10279.29	9848.6	147.6	94.5 22.6895					
126	3	Unknown 4	-5.01424	100.4	10896.5	10465.8	-469.6	100.4 24.05187					
127	1	Unknown 4	-6.01424	93.3	10160.25	9729.6	266.6	93.3 22.42675					
128	2	Unknown 4	-6.01424	105.1	11388.47	10957.8	-961.6	105.1 25.1378					
129	3	Unknown 4	-6.01424	98.0	10648.5	10217.8	-221.6	98.0 23.50446					
130	1	Unknown 4	-7.01424	98.8	10736.85	10306.2	-310.0	98.8 23.69948					
131	2	Unknown 4	-7.01424	89.7	9784.84	9354.2	642.0	89.7 21.5981					
132	3	Unknown 4	-7.01424	102.6	11127.76	10697.1	-700.9	102.6 24.56233					
133	1	Unknown 4	-8.01424	101.1	10969.04	10538.4	-542.2	101.1 24.21199					
134	2	Unknown 4	-8.01424	104.2	11292.06	10861.4	-865.2	104.2 24.92499					
135	3	Unknown 4	-8.01424	104.5	11328.02	10897.4	-901.1	104.5 25.00437					
136	1	Unknown 4	-9.01424	102.4	11103.89	10673.2	-677.0	102.4 24.50964					
137	2	Unknown 4	-9.01424	103.7	11244.01	10813.3	-817.1	103.7 24.81893					
138	3	Unknown 4	-9.01424	107.6	11645.77	11215.1	-1218.9	107.6 25.70574					
139	1	Unknown 4	-10.01424	100.2	10879.76	10449.1	-452.9	100.2 24.01492					
140	2	Unknown 4	-10.01424	102.1	11077.85	10647.2	-651.0	102.1 24.45217					
141	3	Unknown 4	-10.01424	104.3	11307.25	10876.6	-880.4	104.3 24.95852					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-4-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1888.10	5853.11	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1916.50	5941.15	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	2001.10	6203.41	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2468.00	7650.80	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2717.80	8425.18	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2803.00	8689.30	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3813.00	11820.30	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3745.90	11612.29	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3738.40	11589.04	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3671.80	11382.58	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3678.80	11404.28	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3602.20	11166.82	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3510.80	10883.48	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3625.70	11239.67	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3723.90	11544.09	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3657.70	11338.87	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3601.10	11163.41	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3671.90	11382.89	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3667.60	11369.56	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3589.30	11126.83	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3659.50	11344.45	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3576.50	11087.15	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3638.00	11277.80	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3739.70	11593.07	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3641.80	11289.58	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3681.80	11413.58	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3767.10	11678.01	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	162.19	486.57	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	165.29	495.87	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	157.04	471.12	TRUE	
172	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45174.00	45174.00	TRUE	
173	2	none	Hot	—	—	—	30	—	—	—	—	—	—	46200.00	46200.00	TRUE	
174	3	none	Hot	—	—	—	30	—	—	—	—	—	—	46603.00	46603.00	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45073.00	45073.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	—	45764.00	45764.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	—	43011.00	43011.00	TRUE	

Check the 10% rule: 23.97% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
142	1	Unknown 5	-3.6163	52.0	5853.11	5422.4	4573.8	52.0	12.91958
143	2	Unknown 5	-3.6163	52.8	5941.15	5510.5	4485.7	52.8	13.11392
144	3	Unknown 5	-3.6163	55.4	6203.41	5772.7	4223.5	55.4	13.6928
145	1	Unknown 5	-4.01424	69.2	7650.8	7220.1	2776.1	69.2	16.88763
146	2	Unknown 5	-4.01424	76.7	8425.18	7994.5	2001.7	76.7	18.59692
147	3	Unknown 5	-4.01424	79.2	8689.3	8258.6	1737.6	79.2	19.17991
148	1	Unknown 5	-5.01424	109.2	11820.3	11389.6	-1393.4	109.2	26.09098
149	2	Unknown 5	-5.01424	107.2	11612.29	11181.6	-1185.4	107.2	25.63184
150	3	Unknown 5	-5.01424	107.0	11589.04	11158.4	-1162.2	107.0	25.58052
151	1	Unknown 5	-6.01424	105.0	11382.58	10951.9	-955.7	105.0	25.1248
152	2	Unknown 5	-6.01424	105.2	11404.28	10973.6	-977.4	105.2	25.1727
153	3	Unknown 5	-6.01424	103.0	11166.82	10736.2	-739.9	103.0	24.64855
154	1	Unknown 5	-7.01424	100.2	10883.48	10452.8	-456.6	100.2	24.02313
155	2	Unknown 5	-7.01424	103.7	11239.67	10809.0	-812.8	103.7	24.80935
156	3	Unknown 5	-7.01424	106.6	11544.09	11113.4	-1117.2	106.6	25.4813
157	1	Unknown 5	-8.01424	104.6	11338.87	10908.2	-912.0	104.6	25.02832
158	2	Unknown 5	-8.01424	102.9	11163.41	10732.7	-736.5	102.9	24.64102
159	3	Unknown 5	-8.01424	105.0	11382.89	10952.2	-956.0	105.0	25.12548
160	1	Unknown 5	-9.01424	104.9	11369.56	10938.9	-942.7	104.9	25.09606
161	2	Unknown 5	-9.01424	102.6	11126.83	10696.2	-700.0	102.6	24.56028
162	3	Unknown 5	-9.01424	104.7	11344.45	10913.8	-917.6	104.7	25.04063
163	1	Unknown 5	-10.01424	102.2	11087.15	10656.5	-660.3	102.2	24.47269
164	2	Unknown 5	-10.01424	104.0	11277.8	10847.1	-850.9	104.0	24.89352
165	3	Unknown 5	-10.01424	107.1	11593.07	11162.4	-1166.2	107.1	25.58941
166	1	—	—	104.1	11289.58	10858.9	-862.7	104.1	24.91952
167	2	—	—	105.3	11413.58	10982.9	-986.7	105.3	25.19322
168	3	—	—	107.9	11678.01	11247.3	-1251.1	107.9	25.7769
169	1	-6.00	0.5	486.57	55.9	9940.3	0.5	1.074007	
170	2	-6.00	0.6	495.87	65.2	9931.0	0.6	1.094535	
171	3	-6.00	0.4	471.12	40.5	9955.8	0.4	1.039904	
172	1			45174	44743.3				
173	2			46200	45769.3				
174	3			46603	46172.3				
175	1			45073	44642.3				
176	2			45764	45333.3				
177	3			43011	42580.3				

Prism data

<i>standard curve</i>				<i>weak positive</i>				<i>CR42342</i>				<i>CR42345</i>			
<i>conce</i> <i>ntratio</i> <i>n (log)</i>	Y1-SC	Y2-SC	Y3-SC	<i>conce</i> <i>ntratio</i> <i>n (log)</i>	y1-PC	y2-PC	y3-PC	<i>conce</i> <i>ntratio</i> <i>n (log)</i>	y1-U1	y2-U1	y3-U1	<i>conce</i> <i>ntratio</i> <i>n (log)</i>	y1-U1	y2-U1	y3-U1
-6.0	-0.36674	-0.56757	-0.61505	-3	3.1659	3.4708	4.4735	-3.0				-3.0	-0.7155	0.0064	-0.0772
-6.0	0.53611	0.62531	0.38794	-4	29.4060	28.7385	28.1084	-4.0	-0.9385	-0.5882	-0.7654	-4.0	2.0590	1.9044	2.4086
-7.0	0.63845	0.59534	0.66907	-5	79.7135	75.1101	70.3426	-5.0	-0.2594	1.1174	0.2246	-5.0	20.2989	19.2217	17.4688
-8.0	14.51355	12.77697	13.47445	-6	100.4638	93.9844	95.5294	-6.0	3.5720	2.1705	2.3605	-6.0	56.6009	68.0889	60.9029
-9.0	60.71859	56.39869	59.76422	-7	95.8747	99.6783	98.1217	-7.0	30.0482	30.3574	38.3491	-7.0	98.9465	98.7830	93.2650
-10.0	90.52973	91.87951	87.01257	-8	93.1787	87.0504	95.7884	-8.0	91.7933	88.7488	89.9381	-8.0	102.5826	102.6867	98.2241
-11.0	97.54919	99.20222	95.76236	-9	97.9261	98.0153	98.0642	-9.0	98.8187	104.3992	104.3903	-9.0	103.9056	99.8177	94.7188
				-10	96.2372	87.7236	99.3244	-10.0	106.5190	103.5251	104.5122	-10.0	94.9210	100.8226	103.7748

CR42351					CR42358					CR43261				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.6	9.0823	9.2732	12.5442		-3.0					-3.6	52.0045	52.8488	55.3641	
-4.0	60.2191	57.8823	63.1000		-4.0	86.8520	89.9143	85.9690		-4.0	69.2454	76.6722	79.2052	
-5.0	100.8672	98.7176	96.5502		-5.0	94.3055	94.4542	100.3736		-5.0	109.2334	107.2385	107.0155	
-6.0	105.0087	105.3030	100.0852		-6.0	93.3125	105.0919	97.9951		-6.0	105.0354	105.2435	102.9661	
-7.0	104.2208	104.3427	106.8728		-7.0	98.8425	89.7121	102.5915		-7.0	100.2487	103.6648	106.5844	
-8.0	106.0463	103.7451	102.0653		-8.0	101.0693	104.1673	104.5122		-8.0	104.6162	102.9334	105.0384	
-9.0	104.9314	102.3567	101.2388		-9.0	102.3626	103.7064	107.5596		-9.0	104.9105	102.5826	104.6697	
-10.0	87.1018	104.1286	109.0640		-10.0	100.2131	102.1129	104.3130		-10.0	102.2021	104.0305	107.0541	

Competitive Assay of a known Weak Positive
177 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
 Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:		
Run identification:	513	
Assay start date:	10/13/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.79	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.58E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.92E-05	M
RBA:	4.01836E-05	
Max Concentration, Unknown 1:	3.00E-02	M 5e-3)
IC50, Unknown 1:	3.05E-08	CR42342
RBA, Unknown 1:	5.16383%	
Max Concentration, Unknown 2:	3.00E-02	M (example 5e-3)
IC50, Unknown 2:	1.92E-06	CR42345
RBA, Unknown 2:	0.08200%	
Max Concentration, Unknown 3:	7.50E-03	M (example 5e-3)
IC50, Unknown 3:	8.86E-05	CR42351
RBA, Unknown 3:	0.00178%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	5.94E-04	CR42358
RBA, Unknown 4:	0.00027%	
Max Concentration, Unknown 5:	7.50E-03	M (example 5e-3)
IC50, Unknown 5:	3.07E-04	CR43261
RBA, Unknown 5:	0.00051%	
volume of ethanol counted:	2	mL
multitply DPM in sample by :	3.1	
working volume	3.1E+02	uL

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

protocol calls for counting decanted EtOH supernate
 reflects 100ul of reaction mixture processed

Summary values				
	n	Mean	SD	
EtOH	6	11147.2	214.24	Total Binding, solvent control, tubes
Hot	6	45166.0	477.75	Total hot R1881 added to each tube
NSB	6	501.0	138.77	Nonspecific Binding
Specific EtOH	6	10646.1	214.24	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3560.80	11038.48	TRUE	
2	2	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3490.00	10819.00	TRUE	
3	3	ethanol	EIOH	0	—	—	300	30	10	50	310	—	100	3680.60	11409.86	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	152.66	457.98	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	250.99	752.97	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	190.33	570.99	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	184.73	572.66	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	266.48	826.09	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	198.84	616.40	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	667.46	2069.13	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	602.69	1868.34	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	657.28	2037.57	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2253.30	6985.23	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2268.40	7032.04	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2265.00	7021.50	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3349.00	10381.90	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3266.30	10125.53	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3469.20	10754.52	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3618.90	11218.59	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3612.00	11197.20	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3547.40	10996.94	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	317.03	951.09	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	293.58	880.74	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	299.45	898.35	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1172.50	3517.50	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1145.20	3435.60	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1212.10	3636.30	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2995.30	8985.90	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	3060.60	9181.80	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2889.20	8667.60	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3744.50	11233.50	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3589.20	10767.60	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3600.60	10801.80	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3288.70	9866.10	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3818.90	11456.70	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3553.40	10660.20	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3555.60	10666.80	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3766.90	11300.70	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3472.80	10418.40	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3815.40	11446.20	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3592.70	10778.10	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3457.90	10373.70	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3812.20	11436.60	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3757.70	11273.10	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3826.90	11480.70	TRUE	

Check the 10% rule: 24.68% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot					
1	1	—	99.0	11038.48	10537.4	-392.3	99.0	24.4398					
2	2	—	96.9	10819	10318.0	-172.9	96.9	23.95386					
3	3	—	102.5	11409.86	10908.8	-763.7	102.5	25.26206					
4	1	-6.00	-0.4	457.98	-43.1	10188.2	-0.4	1.013993					
5	2	-6.00	2.4	752.97	251.9	9893.2	2.4	1.667117					
6	3	-6.00	0.0	570.99	70.0	10075.2	0.7	1.264203					
7	1	cold R1881	-7.01	0.7	572.663	71.6	10073.5	0.7	1.267907				
8	2	cold R1881	-7.01	3.1	826.088	325.0	9820.1	3.1	1.829004				
9	3	cold R1881	-7.01	1.1	616.404	115.4	10029.7	1.1	1.364752				
10	1	cold R1881	-8.01	14.7	2069.126	1568.1	8577.0	14.7	4.581158				
11	2	cold R1881	-8.01	12.8	1868.339	1367.3	8777.8	12.8	4.136605				
12	3	cold R1881	-8.01	14.4	2037.568	1536.5	8608.6	14.4	4.511287				
13	1	cold R1881	-9.01	60.9	6985.23	6484.2	3660.9	60.9	15.46568				
14	2	cold R1881	-9.01	61.3	7032.04	6531.0	3614.1	61.3	15.56932				
15	3	cold R1881	-9.01	61.2	7021.5	6520.5	3624.6	61.2	15.54599				
16	1	cold R1881	-10.01	92.8	10381.9	9880.9	264.2	92.8	22.9861				
17	2	cold R1881	-10.01	90.4	10125.53	9624.5	520.6	90.4	22.41848				
18	3	cold R1881	-10.01	96.3	10754.52	10253.5	-108.4	96.3	23.8111				
19	1	cold R1881	-11.01	100.7	11218.59	10717.6	-572.4	100.7	24.83857				
20	2	cold R1881	-11.01	100.5	11197.2	10696.2	-551.1	100.5	24.79121				
21	3	cold R1881	-11.01	98.6	10996.94	10495.9	-350.8	98.6	24.34783				
22	1	Weak Positive	-3	4.2	951.09	450.1	9695.1	4.2	2.105765				
23	2	Weak Positive	-3	3.6	880.74	379.7	9765.4	3.6	1.950007				
24	3	Weak Positive	-3	3.7	898.35	397.3	9747.8	3.7	1.988996				
25	1	Weak Positive	-4	28.3	3517.5	3016.5	7128.6	28.3	7.787938				
26	2	Weak Positive	-4	27.6	3435.6	2934.6	7210.5	27.6	7.606607				
27	3	Weak Positive	-4	29.4	3636.3	3135.3	7009.8	29.4	8.050968				
28	1	Weak Positive	-5	79.7	8985.9	8484.9	1660.2	79.7	19.89528				
29	2	Weak Positive	-5	81.5	9181.8	8680.8	1464.3	81.5	20.32901				
30	3	Weak Positive	-5	76.7	8667.6	8166.6	1978.5	76.7	19.19054				
31	1	Weak Positive	-6	100.8	11233.5	10732.5	-587.4	100.8	24.87158				
32	2	Weak Positive	-6	96.4	10767.6	10266.6	-121.5	96.4	23.84006				
33	3	Weak Positive	-6	96.8	10801.8	10300.8	-155.7	96.8	23.91578				
34	1	Weak Positive	-7	88.0	9866.1	9365.1	780.0	88.0	21.84409				
35	2	Weak Positive	-7	102.9	11456.7	10955.7	-810.6	102.9	25.36576				
36	3	Weak Positive	-7	95.4	10660.2	10159.2	-14.1	95.4	23.60227				
37	1	Weak Positive	-8	95.5	10666.8	10165.8	-20.7	95.5	23.61688				
38	2	Weak Positive	-8	101.4	11300.7	10799.7	-654.6	101.4	25.02037				
39	3	Weak Positive	-8	93.2	10418.4	9917.4	227.7	93.2	23.06691				
40	1	Weak Positive	-9	102.8	11446.2	10945.2	-800.1	102.8	25.34251				
41	2	Weak Positive	-9	96.5	10778.1	10277.1	-132.0	96.5	23.8633				
42	3	Weak Positive	-9	92.7	10373.7	9872.7	272.4	92.7	22.96794				
43	1	Weak Positive	-10	102.7	11436.6	10935.6	-790.5	102.7	25.32126				
44	2	Weak Positive	-10	101.2	11273.1	10772.1	-627.0	101.2	24.95926				
45	3	Weak Positive	-10	103.1	11480.7	10979.7	-834.6	103.1	25.4189				

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: **24.68%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	272.80	845.68	FALSE	precipitate in tube
47	2	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	331.99	1029.17	FALSE	precipitate in tube
48	3	Unknown 1	U1	1	E-1-U1	3.00E-02	300	30	10	50	310	9.7E-04	100	258.53	801.44	FALSE	precipitate in tube
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	170.13	527.40	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	155.33	481.52	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	170.78	529.42	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	202.68	628.31	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	199.34	617.95	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	207.29	642.60	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	244.22	757.08	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	312.56	968.94	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	279.38	866.08	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	755.14	2340.93	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	785.86	2436.17	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	822.37	2549.35	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3200.60	9921.86	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	2531.40	7847.34	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	2891.70	8964.27	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3672.50	11384.75	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3796.90	11770.39	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3682.70	11416.37	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3806.90	11801.39	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3749.90	11624.69	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3751.40	11629.34	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	146.65	454.62	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	149.42	463.20	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	3.00E-02	300	30	10	50	310	9.7E-04	100	141.94	440.01	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	246.98	765.64	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	226.86	703.27	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	207.90	644.49	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	744.21	2307.05	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	787.49	2441.22	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	798.53	2475.44	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2359.40	7314.14	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2365.60	7333.36	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	2285.80	7085.98	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3581.30	11102.03	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3633.90	11265.09	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	3641.80	11289.58	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3858.50	11961.35	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3944.20	12227.02	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3748.40	11620.04	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3690.40	11440.24	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3750.00	11625.00	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3847.40	11926.94	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3691.50	11443.65	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3757.40	11647.94	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3773.10	11696.61	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
46	1	Unknown 1	-3.01424						
47	2	Unknown 1	-3.01424						
48	3	Unknown 1	-3.01424						
49	1	Unknown 1	-4.01424	0.2	527.403	26.4	10118.7	0.2	1.167699
50	2	Unknown 1	-4.01424	-0.2	481.523	-19.5	10164.6	-0.2	1.066118
51	3	Unknown 1	-4.01424	0.3	529.418	28.4	10116.7	0.3	1.17216
52	1	Unknown 1	-5.01424	1.2	628.308	127.3	10017.8	1.2	1.391108
53	2	Unknown 1	-5.01424	1.1	617.954	116.9	10028.2	1.1	1.368184
54	3	Unknown 1	-5.01424	1.3	642.599	141.6	10003.5	1.3	1.422749
55	1	Unknown 1	-6.01424	2.4	757.082	256.0	9889.1	2.4	1.676221
56	2	Unknown 1	-6.01424	4.4	968.936	467.9	9677.2	4.4	2.145277
57	3	Unknown 1	-6.01424	3.4	866.078	365.0	9780.1	3.4	1.917544
58	1	Unknown 1	-7.01424	17.3	2340.934	1839.9	8305.2	17.3	5.182956
59	2	Unknown 1	-7.01424	18.2	2436.166	1935.1	8210.0	18.2	5.393805
60	3	Unknown 1	-7.01424	19.2	2549.347	2048.3	8096.8	19.2	5.644394
61	1	Unknown 1	-8.01424	88.5	9921.86	9420.8	724.3	88.5	21.96754
62	2	Unknown 1	-8.01424	69.0	7847.34	7346.3	2798.8	69.0	17.37444
63	3	Unknown 1	-8.01424	79.5	8964.27	8463.2	1681.9	79.5	19.84739
64	1	Unknown 1	-9.01424	102.2	11384.75	10883.7	-738.6	102.2	25.20646
65	2	Unknown 1	-9.01424	105.9	11770.39	11269.4	-1124.2	105.9	26.06029
66	3	Unknown 1	-9.01424	102.5	11416.37	10915.3	-770.2	102.5	25.27647
67	1	Unknown 1	-10.01424	106.1	11801.39	11300.4	-1155.2	106.1	26.12892
68	2	Unknown 1	-10.01424	104.5	11624.69	11123.7	-978.5	104.5	25.7377
69	3	Unknown 1	-10.01424	104.5	11629.34	11128.3	-983.2	104.5	25.748
70	1	Unknown 2	-3.01424	-0.4	454.615	-46.4	10191.5	-0.4	1.006543
71	2	Unknown 2	-3.01424	-0.4	463.202	-37.8	10182.9	-0.4	1.025555
72	3	Unknown 2	-3.01424	-0.6	440.014	-61.0	10206.1	-0.6	0.974215
73	1	Unknown 2	-4.01424	2.5	765.638	264.6	9880.5	2.5	1.695165
74	2	Unknown 2	-4.01424	1.9	703.266	202.2	9942.9	1.9	1.557069
75	3	Unknown 2	-4.01424	1.3	644.49	143.5	10001.7	1.3	1.426936
76	1	Unknown 2	-5.01424	17.0	2307.051	1806.0	8339.1	17.0	5.107937
77	2	Unknown 2	-5.01424	18.2	2441.219	1940.2	8204.9	18.2	5.404993
78	3	Unknown 2	-5.01424	18.5	2475.443	1974.4	8170.7	18.5	5.480767
79	1	Unknown 2	-6.01424	64.0	7314.14	6813.1	3332.0	64.0	16.19391
80	2	Unknown 2	-6.01424	64.2	7333.36	6832.3	3312.8	64.2	16.23646
81	3	Unknown 2	-6.01424	61.9	7085.98	6584.9	3560.2	61.9	15.68875
82	1	Unknown 2	-7.01424	99.6	11102.03	10601.0	-455.9	99.6	24.5805
83	2	Unknown 2	-7.01424	101.1	11265.09	10764.1	-618.9	101.1	24.94153
84	3	Unknown 2	-7.01424	101.3	11289.58	10788.5	-643.4	101.3	24.99575
85	1	Unknown 2	-8.01424	107.6	11961.35	11460.3	-1315.2	107.6	26.48308
86	2	Unknown 2	-8.01424	110.1	12227.02	11726.0	-1580.9	110.1	27.07129
87	3	Unknown 2	-8.01424	104.4	11620.04	11119.0	-973.9	104.4	25.72741
88	1	Unknown 2	-9.01424	102.8	11440.24	10939.2	-794.1	102.8	25.32932
89	2	Unknown 2	-9.01424	104.5	11625	11124.0	-978.9	104.5	25.73839
90	3	Unknown 2	-9.01424	107.3	11926.94	11425.9	-1280.8	107.3	26.4069
91	1	Unknown 2	-10.01424	102.8	11443.65	10942.6	-797.5	102.8	25.33687
92	2	Unknown 2	-10.01424	104.7	11647.94	11146.9	-1001.8	104.7	25.78918
93	3	Unknown 2	-10.01424	105.2	11696.61	11195.6	-1050.5	105.2	25.89694

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: **24.68%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	413.05	1280.46	TRUE	
95	2	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	394.50	1222.95	TRUE	
96	3	Unknown 3	U3	1	E-1-U3	7.50E-03	300	30	10	50	310	2.4E-04	100	385.53	1195.14	TRUE	
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2149.20	6662.52	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2192.30	6796.13	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2150.40	6666.24	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3291.80	10204.58	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3685.10	11423.81	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	3661.30	11350.03	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3748.70	11620.97	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3802.90	11788.99	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3845.80	11921.98	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3770.40	11688.24	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3768.90	11683.59	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3387.30	10500.63	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3773.20	11696.92	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3813.80	11822.78	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3850.80	11937.48	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3737.20	11585.32	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3679.90	11407.69	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3694.90	11454.19	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3712.20	11507.82	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3685.50	11425.05	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3692.50	11446.75	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	3005.30	9316.43	FALSE	precipitate in tube
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	2783.00	8627.30	FALSE	precipitate in tube
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	3021.60	9366.96	FALSE	precipitate in tube
121	1	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3093.00	9588.30	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3061.00	9489.10	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	3.00E-03	300	30	10	50	310	9.7E-05	100	3204.10	9932.71	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3345.00	10369.50	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3441.80	10669.58	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	3.00E-04	300	30	10	50	310	9.7E-06	100	3425.80	10619.98	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3495.70	10836.67	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3583.00	11107.30	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	3.00E-05	300	30	10	50	310	9.7E-07	100	3620.60	11223.86	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3675.40	11393.74	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3561.60	11040.96	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	3.00E-06	300	30	10	50	310	9.7E-08	100	3366.40	10435.84	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3710.90	11503.79	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3501.80	10855.58	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	3.00E-07	300	30	10	50	310	9.7E-09	100	3340.60	10355.86	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3724.00	11544.40	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3744.90	11609.19	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	3.00E-08	300	30	10	50	310	9.7E-10	100	3785.00	11733.50	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3664.00	11358.40	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3707.30	11492.63	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	3.00E-09	300	30	10	50	310	9.7E-11	100	3849.00	11931.90	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
94	1	Unknown 3	-3.6163	7.3	1280.455	779.4	9365.7	7.3	2.834998
95	2	Unknown 3	-3.6163	6.8	1222.95	721.9	9423.2	6.8	2.707678
96	3	Unknown 3	-3.6163	6.5	1195.143	694.1	9451.0	6.5	2.646112
97	1	Unknown 3	-4.01424	57.9	6662.52	6161.5	3983.6	57.9	14.75118
98	2	Unknown 3	-4.01424	59.1	6796.13	6295.1	3850.0	59.1	15.047
99	3	Unknown 3	-4.01424	57.9	6666.24	6165.2	3979.9	57.9	14.75942
100	1	Unknown 3	-5.01424	91.1	10204.58	9703.5	441.6	91.1	22.5935
101	2	Unknown 3	-5.01424	102.6	11423.81	10922.8	-777.7	102.6	25.29294
102	3	Unknown 3	-5.01424	101.9	11350.03	10849.0	-703.9	101.9	25.12959
103	1	Unknown 3	-6.01424	104.5	11620.97	11119.9	-974.8	104.5	25.72946
104	2	Unknown 3	-6.01424	106.0	11788.99	11288.0	-1142.8	106.0	26.10147
105	3	Unknown 3	-6.01424	107.3	11921.98	11420.9	-1275.8	107.3	26.39592
106	1	Unknown 3	-7.01424	105.1	11688.24	11187.2	-1042.1	105.1	25.8784
107	2	Unknown 3	-7.01424	105.0	11683.59	11182.6	-1037.4	105.0	25.86811
108	3	Unknown 3	-7.01424	93.9	10500.63	9999.6	145.5	93.9	23.24897
109	1	Unknown 3	-8.01424	105.2	11696.92	11195.9	-1050.8	105.2	25.89762
110	2	Unknown 3	-8.01424	106.3	11822.78	11321.7	-1176.6	106.3	26.17628
111	3	Unknown 3	-8.01424	107.4	11937.48	11436.4	-1291.3	107.4	26.43024
112	1	Unknown 3	-9.01424	104.1	11585.32	11084.3	-939.2	104.1	25.65053
113	2	Unknown 3	-9.01424	102.4	11407.69	10906.7	-761.5	102.4	25.25725
114	3	Unknown 3	-9.01424	102.9	11454.19	10953.2	-808.0	102.9	25.3602
115	1	Unknown 3	-10.01424	103.4	11507.82	11006.8	-861.7	103.4	25.47894
116	2	Unknown 3	-10.01424	102.6	11425.05	10924.0	-778.9	102.6	25.29569
117	3	Unknown 3	-10.01424	102.8	11446.75	10945.7	-800.6	102.8	25.34373
118	1	Unknown 4	-3.01424						
119	2	Unknown 4	-3.01424						
120	3	Unknown 4	-3.01424						
121	1	Unknown 4	-4.01424	85.4	9588.3	9087.3	1057.8	85.4	21.22902
122	2	Unknown 4	-4.01424	84.4	9489.1	8988.1	1157.0	84.4	21.00939
123	3	Unknown 4	-4.01424	88.6	9932.71	9431.7	713.4	88.6	21.99156
124	1	Unknown 4	-5.01424	92.7	10369.5	9868.5	276.6	92.7	22.95864
125	2	Unknown 4	-5.01424	95.5	10669.58	10168.5	-23.4	95.5	23.62304
126	3	Unknown 4	-5.01424	95.0	10619.98	10118.9	26.2	95.0	23.51322
127	1	Unknown 4	-6.01424	97.1	10836.67	10335.6	-190.5	97.1	23.99298
128	2	Unknown 4	-6.01424	99.6	11107.3	10606.3	-461.2	99.6	24.59217
129	3	Unknown 4	-6.01424	100.7	11223.86	10722.8	-577.7	100.7	24.85024
130	1	Unknown 4	-7.01424	102.3	11393.74	10892.7	-747.6	102.3	25.22636
131	2	Unknown 4	-7.01424	99.0	11040.96	10539.9	-394.8	99.0	24.44529
132	3	Unknown 4	-7.01424	93.3	10435.84	9934.8	210.3	93.3	23.10552
133	1	Unknown 4	-8.01424	103.3	11503.79	11002.8	-857.6	103.3	25.47002
134	2	Unknown 4	-8.01424	97.3	10855.58	10354.5	-209.4	97.3	24.03485
135	3	Unknown 4	-8.01424	92.6	10355.86	9854.8	290.3	92.6	22.92844
136	1	Unknown 4	-9.01424	103.7	11544.4	11043.4	-898.3	103.7	25.55993
137	2	Unknown 4	-9.01424	104.3	11609.19	11108.2	-963.0	104.3	25.70338
138	3	Unknown 4	-9.01424	105.5	11733.5	11232.5	-1087.4	105.5	25.97861
139	1	Unknown 4	-10.01424	102.0	11358.4	10857.4	-712.3	102.0	25.14812
140	2	Unknown 4	-10.01424	103.2	11492.63	10991.6	-846.5	103.2	25.44531
141	3	Unknown 4	-10.01424	107.4	11931.9	11430.9	-1285.8	107.4	26.41788

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-4-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1995.30	6185.43	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1899.30	5887.83	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	7.50E-03	300	30	10	50	310	2.4E-04	100	1904.60	5904.26	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2846.80	8825.08	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2922.50	9059.75	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	2832.60	8781.06	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3839.10	11901.21	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3721.90	11537.89	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3671.00	11380.10	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3809.30	11808.83	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3563.10	11045.61	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3066.40	9505.84	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3448.40	10690.04	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3572.30	11074.13	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3482.90	10796.99	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3322.10	10298.51	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3665.30	11362.43	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3090.30	9579.93	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3605.50	11177.05	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3478.60	10783.66	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3418.90	10598.59	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3533.10	10952.61	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3598.80	11156.28	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3520.00	10912.00	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3643.20	11293.92	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3568.80	11063.28	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3631.80	11258.58	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	136.26	408.78	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	138.90	416.70	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	132.94	398.82	TRUE	
172	1	none	Hot	—	—	—	30	—	—	—	—	—	—	44631.00	44631.00	TRUE	
173	2	none	Hot	—	—	—	30	—	—	—	—	—	—	45079.00	45079.00	TRUE	
174	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45980.00	45980.00	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45184.00	45184.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	—	44776.00	44776.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45346.00	45346.00	TRUE	

Check the 10% rule: **24.68%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Values for analysis by nonlinear regression										
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
142	1	Unknown 5	-3.6163	53.4	6185.43	5684.4	4460.7	53.4	13.69488	
143	2	Unknown 5	-3.6163	50.6	5887.83	5386.8	4758.3	50.6	13.03598	
144	3	Unknown 5	-3.6163	50.8	5904.26	5403.2	4741.9	50.8	13.07236	
145	1	Unknown 5	-4.01424	78.2	8825.08	8324.0	1821.1	78.2	19.53921	
146	2	Unknown 5	-4.01424	80.4	9059.75	8558.7	1586.4	80.4	20.05878	
147	3	Unknown 5	-4.01424	77.8	8781.06	8280.0	1865.1	77.8	19.44175	
148	1	Unknown 5	-5.01424	107.1	11901.21	11400.2	-1255.1	107.1	26.34993	
149	2	Unknown 5	-5.01424	103.7	11537.89	11036.9	-891.7	103.7	25.54552	
150	3	Unknown 5	-5.01424	102.2	11380.1	10879.1	-734.0	102.2	25.19617	
151	1	Unknown 5	-6.01424	106.2	11808.83	11307.8	-1162.7	106.2	26.1454	
152	2	Unknown 5	-6.01424	99.0	11045.61	10544.6	-399.5	99.0	24.45559	
153	3	Unknown 5	-6.01424	84.6	9505.84	9004.8	1140.3	84.6	21.04645	
154	1	Unknown 5	-7.01424	95.7	10690.04	10189.0	-43.9	95.7	23.66833	
155	2	Unknown 5	-7.01424	99.3	11074.13	10573.1	-428.0	99.3	24.51873	
156	3	Unknown 5	-7.01424	96.7	10796.99	10296.0	-150.8	96.7	23.90513	
157	1	Unknown 5	-8.01424	92.0	10298.51	9797.5	347.6	92.0	22.80147	
158	2	Unknown 5	-8.01424	102.0	11362.43	10861.4	-716.3	102.0	25.15704	
159	3	Unknown 5	-8.01424	85.3	9579.93	9078.9	1066.2	85.3	21.21049	
160	1	Unknown 5	-9.01424	100.3	11177.05	10676.0	-530.9	100.3	24.7466	
161	2	Unknown 5	-9.01424	96.6	10783.66	10282.6	-137.5	96.6	23.87561	
162	3	Unknown 5	-9.01424	94.8	10598.59	10097.6	47.6	94.8	23.46586	
163	1	Unknown 5	-10.01424	98.2	10952.61	10451.6	-306.5	98.2	24.24968	
164	2	Unknown 5	-10.01424	100.1	11156.28	10655.2	-510.1	100.1	24.70062	
165	3	Unknown 5	-10.01424	97.8	10912	10411.0	-265.9	97.8	24.15977	
166	1	—	—	101.4	11293.92	10792.9	-647.8	101.4	25.00536	
167	2	—	—	99.2	11063.28	10562.2	-417.1	99.2	24.49471	
168	3	—	—	101.0	11258.58	10757.5	-612.4	101.0	24.92711	
169	1		-6.00	-0.9	408.78	-92.3	10237.4	-0.9	0.905061	
170	2		-6.00	-0.8	416.7	-84.3	10229.4	-0.8	0.922597	
171	3		-6.00	-1.0	398.82	-102.2	10247.3	-1.0	0.883009	
172	1				44631	44130.0				
173	2				45079	44578.0				
174	3				45980	45479.0				
175	1				45184	44683.0				
176	2				44776	44275.0				
177	3				45346	44845.0				

Prism data															
standard curve				weak positive				CR42342				CR42345			
concentration (log)	Y1-SC	Y2-SC	Y3-SC	concentration (log)	y1-PC	y2-PC	y3-PC	concentration (log)	y1-U1	y2-U1	y3-U1	concentration (log)	y1-U1	y2-U1	y3-U1
-6.0	-0.40447	2.36640	0.65705	-3	4.2274	3.5665	3.7320	-3.0				-3.0	-0.4361	-0.3554	-0.5732
-6.0	-0.86660	-0.79221	-0.96016	-4	28.3338	27.5645	29.4497	-4.0	0.2476	-0.1833	0.2666	-4.0	2.4854	1.8995	1.3474
-7.0	0.67276	3.05320	1.08362	-5	79.6989	81.5390	76.7091	-5.0	1.1954	1.0982	1.3297	-5.0	16.9640	18.2242	18.5457
-8.0	14.72914	12.84314	14.43271	-6	100.8107	96.4345	96.7558	-6.0	2.4050	4.3950	3.4288	-6.0	63.9959	64.1765	61.8528
-9.0	60.90645	61.34614	61.24714	-7	87.9667	102.9073	95.4257	-7.0	17.2823	18.1768	19.2399	-7.0	99.5758	101.1075	101.3375
-10.0	92.81161	90.40351	96.31165	-8	95.4877	101.4420	93.1545	-8.0	88.4904	69.0043	79.4957	-8.0	107.6475	110.1430	104.4415
-11.0	100.67070	100.46978	98.58872	-9	102.8087	96.5331	92.7346	-9.0	102.2314	105.8538	102.5285	-9.0	102.7527	104.4881	107.3243
				-10	102.7185	101.1827	103.1327	-10.0	106.1450	104.4852	104.5289	-10.0	102.7847	104.7036	105.1608

CR42351					CR42358					CR43261				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.6	7.3211	6.7810	6.5198		-3.0					-3.6	53.3939	50.5985	50.7528	
-4.0	57.8752	59.1302	57.9102		-4.0	85.3573	84.4255	88.5923		-4.0	78.1883	80.3926	77.7748	
-5.0	91.1460	102.5983	101.9053		-5.0	92.6951	95.5138	95.0479		-5.0	107.0826	103.6699	102.1878	
-6.0	104.4503	106.0285	107.2777		-6.0	97.0833	99.6253	100.7202		-6.0	106.2149	99.0459	84.5827	
-7.0	105.0822	105.0385	93.9268		-7.0	102.3159	99.0022	93.3183		-7.0	95.7060	99.3138	96.7106	
-8.0	105.1637	106.3459	107.4233		-8.0	103.3496	97.2609	92.5670		-8.0	92.0283	102.0218	85.2786	
-9.0	104.1154	102.4469	102.8837		-9.0	103.7311	104.3396	105.5073		-9.0	100.2805	96.5854	94.8470	
-10.0	103.3875	102.6100	102.8138		-10.0	101.9839	103.2448	107.3709		-10.0	98.1723	100.0854	97.7909	

Competitive Assay of a known Weak Positive
177 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
 Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:			
Run identification:	514		
Assay start date:	10/18/2005		
Tracer lot number:	3559-507		
Specific activity on day of assay:	79.73	Ci/mmole	
Cytosol vial or lot identification:	051905		
Protein (cytosol):	1000	micro gram per tube	
Standard Curve IC50:	1.39E-09	M	
Weak Positive, Max Concentration:	3.00E-02	M	
Weak Positive IC50:	3.43E-05	M	
RBA:	4.05831E-05		
Max Concentration, Unknown 1:	3.75E-03	M	5e-3)
IC50, Unknown 1:	5.13E-07	CR42341	
RBA, Unknown 1:	0.27135%		
Max Concentration, Unknown 2:	1.50E-02	M	(example 5e-3)
IC50, Unknown 2:	9.22E-08	CR42346	
RBA, Unknown 2:	1.51042%		
Max Concentration, Unknown 3:	1.50E-02	M	(example 5e-3)
IC50, Unknown 3:	5.20E-05	CR42347	non standard dilutions
RBA, Unknown 3:	0.00268%		
Max Concentration, Unknown 4:	3.00E-02	M	(example 5e-3)
IC50, Unknown 4:	5.09E-05	CR42355	
RBA, Unknown 4:	0.00274%		
Max Concentration, Unknown 5:	1.50E-02	M	(example 5e-3)
IC50, Unknown 5:	2.96E-05	CR42369	non standard dilutions
RBA, Unknown 5:	0.00471%		
volume of ethanol counted:	2	mL	
multitply DPM in sample by :	3.1		
working volume	3.1E+02	uL	protocol calls for counting decanted EtOH supernate reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11262.8	377.89	Total Binding, solvent control, tubes
Hot	6	45957.7	490.19	Total hot R1881 added to each tube
NSB	6	421.5	23.99	Nonspecific Binding
Specific EtOH	6	10841.3	377.89	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	Corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3584.90	11113.19	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3438.60	10659.66	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3665.20	11362.12	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	145.49	436.47	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	128.54	385.62	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	143.44	430.32	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	171.96	533.08	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	169.00	523.90	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	167.42	519.00	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	547.29	1696.60	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	568.18	1761.36	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	467.76	1450.06	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2208.60	6846.66	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2235.40	6929.74	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2249.60	6973.76	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3220.70	9984.17	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3217.60	9974.56	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3306.60	10250.46	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3514.40	10894.64	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3425.00	10617.50	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3404.70	10554.57	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	296.48	889.44	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	304.91	914.73	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	278.20	834.60	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1166.70	3500.10	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1114.00	3342.00	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1087.79	3263.37	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2892.30	8676.90	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2859.20	8577.60	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2983.50	8950.50	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3380.20	10140.60	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3644.20	10932.60	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3205.90	9617.70	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3478.60	10435.80	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3327.30	9981.90	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3497.10	10491.30	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3470.30	10410.90	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3495.70	10487.10	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3511.70	10535.10	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3662.80	10988.40	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3554.90	10664.70	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3536.40	10609.20	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3373.60	10120.80	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3433.30	10299.90	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3615.70	10847.10	TRUE	

Check the 10% rule: 24.51% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
11113.19	TRUE	
10659.66	TRUE	
11362.12	TRUE	
436.47	TRUE	
385.62	TRUE	
430.32	TRUE	
533.08	TRUE	
523.90	TRUE	
519.00	TRUE	
1696.60	TRUE	
1761.36	TRUE	
1450.06	TRUE	
6846.66	TRUE	
6929.74	TRUE	
6973.76	TRUE	
9984.17	TRUE	
9974.56	TRUE	
10250.46	TRUE	
10894.64	TRUE	
10617.50	TRUE	
10554.57	TRUE	
889.44	TRUE	
914.73	TRUE	
834.60	TRUE	
3500.10	TRUE	
3342.00	TRUE	
3263.37	TRUE	
8676.90	TRUE	
8577.60	TRUE	
8950.50	TRUE	
10140.60	TRUE	
10932.60	TRUE	
9617.70	TRUE	
10435.80	TRUE	
9981.90	TRUE	
10491.30	TRUE	
10410.90	TRUE	
10487.10	TRUE	
10535.10	TRUE	
10988.40	TRUE	
10664.70	TRUE	
10609.20	TRUE	
10120.80	TRUE	
10299.90	TRUE	
10847.10	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICN)	Ratio Total binding/ Hot					
1	1	—	98.6	11113.19	10691.7	-271.9	98.6	24.18136					
2	2	—	94.4	10659.66	10238.2	181.6	94.4	23.19452					
3	3	—	100.9	11362.12	10940.6	-520.8	100.9	24.72301					
4	1	-6.00	0.1	436.47	15.0	10404.8	0.1	0.949722					
5	2	-6.00	-0.3	385.62	-35.9	10455.7	-0.3	0.839077					
6	3	-6.00	0.0	430.32	8.8	10411.0	0.1	0.93634					
7	1	cold R1881	-7.01	1.0	533.076	111.6	1.0	1.159928					
8	2	cold R1881	-7.01	0.9	523.9	102.4	0.9	1.139962					
9	3	cold R1881	-7.01	0.9	519.002	97.5	0.9	1.129305					
10	1	cold R1881	-8.01	11.8	1696.599	1275.1	11.8	3.691656					
11	2	cold R1881	-8.01	12.4	1761.358	1339.8	12.4	3.832566					
12	3	cold R1881	-8.01	9.5	1450.056	1028.5	9.5	3.155199					
13	1	cold R1881	-9.01	59.3	6846.66	6425.2	59.3	14.89775					
14	2	cold R1881	-9.01	60.0	6929.74	6508.2	60.0	15.07853					
15	3	cold R1881	-9.01	60.4	6973.76	6552.3	60.4	15.17431					
16	1	cold R1881	-10.01	88.2	9984.17	9562.7	88.2	21.72471					
17	2	cold R1881	-10.01	88.1	9974.56	9553.1	88.1	21.7038					
18	3	cold R1881	-10.01	90.7	10250.46	9829.0	90.7	22.30413					
19	1	cold R1881	-11.01	96.6	10894.64	10473.1	96.6	23.70582					
20	2	cold R1881	-11.01	94.0	10617.5	10196.0	94.0	23.10278					
21	3	cold R1881	-11.01	93.5	10554.57	10133.1	93.5	22.96585					
22	1	Weak Positive	-3	4.3	889.44	467.9	4.3	1.935346					
23	2	Weak Positive	-3	4.5	914.73	493.2	4.5	1.990375					
24	3	Weak Positive	-3	3.8	834.6	413.1	3.8	1.816019					
25	1	Weak Positive	-4	28.4	3500.1	3078.6	28.4	7.615922					
26	2	Weak Positive	-4	26.9	3342	2920.5	26.9	7.27191					
27	3	Weak Positive	-4	26.2	3263.37	2841.9	26.2	7.100817					
28	1	Weak Positive	-5	76.1	8676.9	8255.4	76.1	18.8802					
29	2	Weak Positive	-5	75.2	8577.6	8156.1	75.2	18.66413					
30	3	Weak Positive	-5	78.7	8950.5	8529.0	78.7	19.47553					
31	1	Weak Positive	-6	89.6	10140.6	9719.1	89.6	22.06509					
32	2	Weak Positive	-6	97.0	10932.6	10511.1	97.0	23.78841					
33	3	Weak Positive	-6	84.8	9617.7	9196.2	84.8	20.9273					
34	1	Weak Positive	-7	92.4	10435.8	10014.3	92.4	22.70742					
35	2	Weak Positive	-7	88.2	9981.9	9560.4	88.2	21.71977					
36	3	Weak Positive	-7	92.9	10491.3	10069.8	92.9	22.82818					
37	1	Weak Positive	-8	92.1	10410.9	9989.4	92.1	22.65324					
38	2	Weak Positive	-8	92.8	10487.1	10065.6	92.8	22.81904					
39	3	Weak Positive	-8	93.3	10535.1	10113.6	93.3	22.92349					
40	1	Weak Positive	-9	97.5	10988.4	10566.9	97.5	23.90983					
41	2	Weak Positive	-9	94.5	10664.7	10243.2	94.5	23.20549					
42	3	Weak Positive	-9	94.0	10609.2	10187.7	94.0	23.08472					
43	1	Weak Positive	-10	89.5	10120.8	9699.3	89.5	22.02201					
44	2	Weak Positive	-10	91.1	10299.9	9878.4	91.1	22.41171					
45	3	Weak Positive	-10	96.2	10847.1	10425.6	96.2	23.60237					

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: **24.51%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	116.97	362.61	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	120.32	372.99	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	119.01	368.93	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	148.28	459.67	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	143.18	443.86	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	108.01	334.83	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	262.82	814.74	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	325.25	1008.28	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	349.96	1084.88	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1221.00	3785.10	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1510.40	4682.24	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1411.20	4374.72	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3090.80	9581.48	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	2973.40	9217.54	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	2822.70	8750.37	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3565.10	11051.81	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3555.90	11023.29	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3630.00	11253.00	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3615.90	11209.29	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3634.80	11267.88	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3779.80	11717.38	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3701.90	11475.89	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3202.90	9928.99	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3651.10	11318.41	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	140.70	436.17	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	108.91	337.62	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	114.33	354.42	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	132.56	410.94	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	138.09	428.08	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	136.55	423.31	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	214.82	665.94	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	195.90	607.29	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	189.92	588.75	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	454.22	1408.08	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	440.23	1364.71	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	460.99	1429.07	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1836.80	5694.08	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1842.80	5712.68	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1785.90	5536.29	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3371.90	10452.89	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3290.10	10199.31	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3093.00	9588.30	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3607.10	11182.01	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3441.80	10669.58	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3035.30	9409.43	FALSE	spill
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3649.10	11312.21	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3508.70	10876.97	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3522.70	10920.37	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific E(Ch)	Ratio Total binding/ Hot					
46	1	Unknown 1	-3.91733	-0.5	362.607	-58.9	10478.7	-0.5	0.789002				
47	2	Unknown 1	-3.91733	-0.4	372.992	-48.5	10468.3	-0.4	0.811599				
48	3	Unknown 1	-3.91733	-0.5	368.931	-52.6	10472.4	-0.5	0.802763				
49	1	Unknown 1	-4.01424	0.4	459.668	38.2	10381.6	0.4	1.000199				
50	2	Unknown 1	-4.01424	0.2	443.858	22.3	10397.4	0.2	0.965798				
51	3	Unknown 1	-4.01424	-0.8	334.831	-86.7	10506.5	-0.8	0.728564				
52	1	Unknown 1	-5.01424	3.6	814.742	393.2	10026.6	3.6	1.77281				
53	2	Unknown 1	-5.01424	5.4	1008.275	586.8	9833.0	5.4	2.193921				
54	3	Unknown 1	-5.01424	6.1	1084.876	663.4	9756.4	6.1	2.360599				
55	1	Unknown 1	-6.01424	31.0	3785.1	3363.6	7056.2	31.0	8.236058				
56	2	Unknown 1	-6.01424	39.3	4682.24	4260.7	6159.1	39.3	10.18816				
57	3	Unknown 1	-6.01424	36.5	4374.72	3953.2	6466.6	36.5	9.519021				
58	1	Unknown 1	-7.01424	84.5	9581.48	9160.0	1259.8	84.5	20.84849				
59	2	Unknown 1	-7.01424	81.1	9217.54	8796.0	1623.8	81.1	20.05659				
60	3	Unknown 1	-7.01424	76.8	8750.37	8328.9	2090.9	76.8	19.04007				
61	1	Unknown 1	-8.01424	98.1	11051.81	10630.3	-210.5	98.1	24.0478				
62	2	Unknown 1	-8.01424	97.8	11023.29	10601.8	-182.0	97.8	23.98575				
63	3	Unknown 1	-8.01424	99.9	11253	10831.5	-411.7	99.9	24.48558				
64	1	Unknown 1	-9.01424	99.5	11209.29	10787.8	-368.0	99.5	24.39047				
65	2	Unknown 1	-9.01424	100.0	11267.88	10846.4	-426.6	100.0	24.51795				
66	3	Unknown 1	-9.01424	104.2	11717.38	11295.9	-876.1	104.2	25.49603				
67	1	Unknown 1	-10.01424	102.0	11475.89	11054.4	-634.6	102.0	24.97057				
68	2	Unknown 1	-10.01424	87.7	9928.99	9507.5	912.3	87.7	21.60464				
69	3	Unknown 1	-10.01424	100.5	11318.41	10896.9	-477.1	100.5	24.6279				
70	1	Unknown 2	-3.31527	0.1	436.17	14.7	10405.1	0.1	0.949069				
71	2	Unknown 2	-3.31527	-0.8	337.621	-83.9	10503.7	-0.8	0.734635				
72	3	Unknown 2	-3.31527	-0.6	354.423	-67.1	10486.9	-0.6	0.771195				
73	1	Unknown 2	-4.01424	-0.1	410.936	-10.6	10430.4	-0.1	0.894162				
74	2	Unknown 2	-4.01424	0.1	428.079	6.6	10413.2	0.1	0.931464				
75	3	Unknown 2	-4.01424	0.0	423.305	1.8	10418.0	0.0	0.921076				
76	1	Unknown 2	-5.01424	2.3	665.942	244.4	10175.4	2.3	1.449034				
77	2	Unknown 2	-5.01424	1.7	607.29	185.8	10234.0	1.7	1.321412				
78	3	Unknown 2	-5.01424	1.5	588.752	167.2	10252.6	1.5	1.281075				
79	1	Unknown 2	-6.01424	9.1	1408.082	986.6	9433.2	9.1	3.063867				
80	2	Unknown 2	-6.01424	8.7	1364.713	943.2	9476.6	8.7	2.9695				
81	3	Unknown 2	-6.01424	9.3	1429.069	1007.6	9412.2	9.3	3.109533				
82	1	Unknown 2	-7.01424	48.6	5694.08	5272.6	5147.2	48.6	12.38984				
83	2	Unknown 2	-7.01424	48.8	5712.68	5291.2	5128.6	48.8	12.43031				
84	3	Unknown 2	-7.01424	47.2	5536.29	5114.8	5305.0	47.2	12.0465				
85	1	Unknown 2	-8.01424	92.5	10452.89	10031.4	388.4	92.5	22.74461				
86	2	Unknown 2	-8.01424	90.2	10199.31	9777.8	642.0	90.2	22.19284				
87	3	Unknown 2	-8.01424	84.6	9588.3	9166.8	1253.0	84.6	20.86333				
88	1	Unknown 2	-9.01424	99.3	11182.01	10760.5	-340.7	99.3	24.33111				
89	2	Unknown 2	-9.01424	94.5	10669.58	10248.1	171.7	94.5	23.2161				
90	3	Unknown 2	-9.01424										
91	1	Unknown 2	-10.01424	100.5	11312.21	10890.7	-470.9	100.5	24.61441				
92	2	Unknown 2	-10.01424	96.4	10876.97	10455.5	-35.7	96.4	23.66737				
93	3	Unknown 2	-10.01424	96.8	10920.37	10498.9	-79.1	96.8	23.7618				

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2473.60	7668.16	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	1914.40	5934.64	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2030.40	6294.24	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1476.80	4578.08	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1785.70	5535.67	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2101.00	6513.10	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2627.00	8143.70	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2356.10	7303.91	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2168.80	6723.28	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2792.40	8656.44	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3430.10	10633.31	FALSE	pipette error
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2762.40	8563.44	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3573.60	11078.16	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3531.90	10948.89	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3547.80	10998.18	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3270.60	10138.86	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3045.90	9442.29	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3619.70	11221.07	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3648.30	11309.73	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	2933.50	9093.85	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3655.90	11333.29	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3186.60	9878.46	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3655.60	11332.36	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3492.80	10827.68	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	113.40	351.54	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	159.47	494.36	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	114.36	354.52	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	709.37	2199.05	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	712.00	2207.20	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	591.01	1832.13	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	2962.30	9183.13	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	2959.30	9173.83	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	2694.20	8352.02	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3402.10	10546.51	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3264.80	10120.88	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3144.60	9748.26	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3512.30	10888.13	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3586.30	11117.53	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3590.20	11129.62	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3378.30	10472.73	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3286.60	10188.46	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	2919.50	9050.45	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3181.50	9862.65	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3706.20	11489.22	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3681.80	11413.58	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3707.60	11493.56	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3618.30	11216.73	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3605.00	11175.50	TRUE	

Check the 10% rule: 24.51% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific ELOH)	Ratio Total binding/ Hot	
94	1	Unknown 3	-3.31527						
95	2	Unknown 3	-3.31527						
96	3	Unknown 3	-3.31527						
97	1	Unknown 3	-4.01424	38.3	4578.08	4156.6	6263.2	38.3	9.961515
98	2	Unknown 3	-4.01424	47.2	5535.67	5114.2	5305.6	47.2	12.04515
99	3	Unknown 3	-4.01424	56.2	6513.1	6091.6	4328.2	56.2	14.17196
100	1	Unknown 3	-5.01424	71.2	8143.7	7722.2	2697.6	71.2	17.72
101	2	Unknown 3	-5.01424	63.5	7303.91	6882.4	3537.4	63.5	15.89269
102	3	Unknown 3	-5.01424	58.1	6723.28	6301.8	4118.0	58.1	14.62929
103	1	Unknown 3	-6.01424	76.0	8656.44	8234.9	2184.9	76.0	18.83568
104	2	Unknown 3	-6.01424						
105	3	Unknown 3	-6.01424	75.1	8563.44	8141.9	2277.9	75.1	18.63332
106	1	Unknown 3	-7.01424	98.3	11078.16	10656.7	-236.9	98.3	24.10514
107	2	Unknown 3	-7.01424	97.1	10948.89	10527.4	-107.6	97.1	23.82386
108	3	Unknown 3	-7.01424	97.6	10998.18	10576.7	-156.9	97.6	23.93111
109	1	Unknown 3	-8.01424	89.6	10138.86	9717.4	702.4	89.6	22.0613
110	2	Unknown 3	-8.01424	83.2	9442.29	9020.8	1399.0	83.2	20.54563
111	3	Unknown 3	-8.01424	99.6	11221.07	10799.6	-379.8	99.6	24.4161
112	1	Unknown 3	-9.01424	100.4	11309.73	10888.2	-468.4	100.4	24.60902
113	2	Unknown 3	-9.01424	80.0	9093.85	8672.3	1747.5	80.0	19.78745
114	3	Unknown 3	-9.01424	100.7	11333.29	10911.8	-492.0	100.7	24.66028
115	1	Unknown 3	-10.01424	87.2	9878.46	9457.0	962.8	87.2	21.49469
116	2	Unknown 3	-10.01424	100.6	11332.36	10910.9	-491.1	100.6	24.65826
117	3	Unknown 3	-10.01424	96.0	10827.68	10406.2	13.6	96.0	23.56012
118	1	Unknown 4	-3.01424	-0.6	351.54	-70.0	10489.8	-0.6	0.764921
119	2	Unknown 4	-3.01424	0.7	494.357	72.8	10346.9	0.7	1.075679
120	3	Unknown 4	-3.01424	-0.6	354.516	-67.0	10486.8	-0.6	0.771397
121	1	Unknown 4	-3.71321	16.4	2199.047	1777.5	8642.3	16.4	4.78494
122	2	Unknown 4	-3.71321	16.5	2207.2	1785.7	8634.1	16.5	4.802681
123	3	Unknown 4	-3.71321	13.0	1832.131	1410.6	9009.2	13.0	3.986562
124	1	Unknown 4	-4.71321	80.8	9183.13	8761.6	1658.2	80.8	19.98172
125	2	Unknown 4	-4.71321	80.7	9173.83	8752.3	1667.5	80.7	19.96148
126	3	Unknown 4	-4.71321	73.2	8352.02	7930.5	2489.3	73.2	18.17329
127	1	Unknown 4	-5.71321	93.4	10546.51	10125.0	294.8	93.4	22.94831
128	2	Unknown 4	-5.71321	89.5	10120.88	9699.4	720.4	89.5	22.02218
129	3	Unknown 4	-5.71321	86.0	9748.26	9326.8	1093.0	86.0	21.21139
130	1	Unknown 4	-6.71321	96.5	10888.13	10466.6	-46.8	96.5	23.69165
131	2	Unknown 4	-6.71321	98.7	11117.53	10696.0	-276.2	98.7	24.19081
132	3	Unknown 4	-6.71321	98.8	11129.62	10708.1	-288.3	98.8	24.21711
133	1	Unknown 4	-7.71321	92.7	10472.73	10051.2	368.6	92.7	22.78778
134	2	Unknown 4	-7.71321	90.1	10188.46	9767.0	652.8	90.1	22.16923
135	3	Unknown 4	-7.71321	79.6	9050.45	8628.9	1790.9	79.6	19.69301
136	1	Unknown 4	-8.71321	87.1	9862.65	9441.1	978.7	87.1	21.46029
137	2	Unknown 4	-8.71321	102.1	11489.22	11067.7	-647.9	102.1	24.99957
138	3	Unknown 4	-8.71321	101.4	11413.58	10992.1	-572.3	101.4	24.83499
139	1	Unknown 4	-9.71321	102.1	11493.56	11072.1	-652.3	102.1	25.00902
140	2	Unknown 4	-9.71321	99.6	11216.73	10795.2	-375.4	99.6	24.40666
141	3	Unknown 4	-9.71321	99.2	11175.5	10754.0	-334.2	99.2	24.31694

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	258.71	802.00	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	276.26	856.41	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	266.01	824.63	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	673.61	2088.19	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	730.60	2264.86	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	733.92	2275.15	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3018.70	9357.97	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2992.30	9276.13	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2996.70	9289.77	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3567.30	11058.63	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3167.70	9819.87	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3483.10	10797.61	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	2976.70	9227.77	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3027.30	9384.63	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3284.20	10181.02	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	2936.60	9103.46	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3227.50	10005.25	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3512.20	10887.82	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3365.30	10432.43	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3623.00	11231.30	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3674.30	11390.33	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3613.30	11201.23	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3802.30	11787.13	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3694.80	11453.88	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3765.90	11674.29	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3593.40	11139.54	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3751.00	11628.10	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	137.45	412.35	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	151.42	454.26	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	136.68	410.04	TRUE	
172	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45792.00	45792.00	TRUE	
173	2	none	Hot	—	—	—	30	—	—	—	—	—	—	46774.00	46774.00	TRUE	
174	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45885.00	45885.00	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	—	46180.00	46180.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	—	45815.00	45815.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	—	45300.00	45300.00	TRUE	

Check the 10% rule: **24.51%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Values for analysis by nonlinear regression									
Position	Replicate		concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
142	1	Unknown 5	-3.31527	3.5	802.001	380.5	10039.3	3.5	1.745086
143	2	Unknown 5	-3.31527	4.0	856.406	434.9	9984.9	4.0	1.863467
144	3	Unknown 5	-3.31527	3.7	824.631	403.1	10016.7	3.7	1.794327
145	1	Unknown 5	-4.01424	15.4	2088.191	1666.7	8753.1	15.4	4.543727
146	2	Unknown 5	-4.01424	17.0	2264.86	1843.4	8576.4	17.0	4.928144
147	3	Unknown 5	-4.01424	17.1	2275.152	1853.6	8566.2	17.1	4.950539
148	1	Unknown 5	-5.01424	82.4	9357.97	8936.5	1483.3	82.4	20.36215
149	2	Unknown 5	-5.01424	81.7	9276.13	8854.6	1565.2	81.7	20.18408
150	3	Unknown 5	-5.01424	81.8	9289.77	8868.3	1551.5	81.8	20.21375
151	1	Unknown 5	-6.01424	98.1	11058.63	10637.1	-217.3	98.1	24.06264
152	2	Unknown 5	-6.01424	86.7	9819.87	9398.4	1021.4	86.7	21.36721
153	3	Unknown 5	-6.01424	95.7	10797.61	10376.1	43.7	95.7	23.49469
154	1	Unknown 5	-7.01424	81.2	9227.77	8806.3	1613.5	81.2	20.07885
155	2	Unknown 5	-7.01424	82.7	9384.63	8963.1	1456.7	82.7	20.42016
156	3	Unknown 5	-7.01424	90.0	10181.02	9759.5	660.3	90.0	22.15304
157	1	Unknown 5	-8.01424	80.1	9103.46	8682.0	1737.8	80.1	19.80836
158	2	Unknown 5	-8.01424	88.4	10005.25	9583.7	836.1	88.4	21.77058
159	3	Unknown 5	-8.01424	96.5	10887.82	10466.3	-46.5	96.5	23.69098
160	1	Unknown 5	-9.01424	92.3	10432.43	10010.9	408.9	92.3	22.70009
161	2	Unknown 5	-9.01424	99.7	11231.3	10809.8	-390.0	99.7	24.43836
162	3	Unknown 5	-9.01424	101.2	11390.33	10968.8	-549.0	101.2	24.7844
163	1	Unknown 5	-10.01424	99.4	11201.23	10779.7	-359.9	99.4	24.37293
164	2	Unknown 5	-10.01424	104.8	11787.13	11365.6	-945.8	104.8	25.6478
165	3	Unknown 5	-10.01424	101.8	11453.88	11032.4	-612.6	101.8	24.92268
166	1	—	—	103.8	11674.29	11252.8	-833.0	103.8	25.40227
167	2	—	—	98.9	11139.54	10718.0	-298.2	98.9	24.2387
168	3	—	—	103.4	11628.1	11206.6	-786.8	103.4	25.30176
169	1	-6.00	-0.1	412.35	-9.2	10429.0	-0.1	0.897239	
170	2	-6.00	0.3	454.26	32.8	10387.0	0.3	0.988431	
171	3	-6.00	-0.1	410.04	-11.5	10431.3	-0.1	0.892212	
172	1				45792	45370.5			
173	2				46774	46352.5			
174	3				45885	45463.5			
175	1				46180	45758.5			
176	2				45815	45393.5			
177	3				45300	44878.5			

Prism data															
standard curve				weak positive				CR42341				CR42346			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-6.0	0.13799	-0.33105	0.08126	-3	4.3162	4.5495	3.8103	-3.9	-0.5433	-0.4475	-0.4850	-3.3	0.1352	-0.7738	-0.6188
-6.0	-0.08449	0.30209	-0.10580	-4	28.3969	26.9385	26.2133	-4.0	0.3520	0.2061	-0.7995	-4.0	-0.0975	0.0606	0.0166
-7.0	1.02908	0.94444	0.89926	-5	76.1476	75.2316	78.6712	-5.0	3.6272	5.4123	6.1189	-5.0	2.2546	1.7136	1.5426
-8.0	11.76140	12.35873	9.48729	-6	89.6487	96.9541	84.8255	-6.0	31.0257	39.3009	36.4643	-6.0	9.1001	8.7001	9.2937
-9.0	59.26546	60.03179	60.43783	-7	92.3716	88.1848	92.8835	-7.0	84.4914	81.1344	76.8252	-7.0	48.6341	48.8056	47.1786
-10.0	88.20579	88.11715	90.66204	-8	92.1419	92.8448	93.2876	-8.0	98.0537	97.7906	99.9095	-8.0	92.5293	90.1902	84.5543
-11.0	96.60395	94.04761	93.46715	-9	97.4688	94.4830	93.9711	-9.0	99.5063	100.0467	104.1929	-9.0	99.2546	94.5280	
				-10	89.4661	91.1181	96.1654	-10.0	101.9654	87.6968	100.5128	-10.0	100.4556	96.4410	96.8413

CR42347					CR42355					CR42369				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.3					-3.0	-0.6454	0.6719	-0.6180		-3.3	3.5096	4.0115	3.7184	
-4.0	38.3401	47.1729	56.1887		-3.7	16.3960	16.4712	13.0115		-4.0	15.3734	17.0030	17.0980	
-5.0	71.2293	63.4831	58.1274		-4.7	80.8170	80.7312	73.1509		-5.0	82.4297	81.6748	81.8007	
-6.0	75.9588		75.1010		-5.7	93.3928	89.4668	86.0298		-6.0	98.1166	86.6903	95.7089	
-7.0	98.2967	97.1043	97.5590		-6.7	96.5439	98.6599	98.7714		-7.0	81.2288	82.6756	90.0215	
-8.0	89.6326	83.2075	99.6149		-7.7	92.7123	90.0902	79.5932		-8.0	80.0821	88.4002	96.5410	
-9.0	100.4327	79.9935	100.6500		-8.7	87.0849	102.0883	101.3906		-9.0	92.3405	99.7093	101.1762	
-10.0	87.2307	100.6415	95.9863		-9.7	102.1284	99.5749	99.1946		-10.0	99.4319	104.8363	101.7624	

Competitive Assay of a known Weak Positive
177 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,
 Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:			
Run identification:	515		
Assay start date:	10/19/2005		
Tracer lot number:	3559-507		
Specific activity on day of assay:	79.71	Ci/mmole	
Cytosol vial or lot identification:	051905		
Protein (cytosol):	1000	micro gram per tube	
Standard Curve IC50:	1.21E-09	M	
Weak Positive, Max Concentration:	3.00E-02	M	
Weak Positive IC50:	2.98E-05	M	
RBA:	4.0605E-05		
Max Concentration, Unknown 1:	3.75E-03	M	5e-3)
IC50, Unknown 1:	7.42E-07	CR42341	
RBA, Unknown 1:	0.16291%		
Max Concentration, Unknown 2:	1.50E-02	M	(example 5e-3)
IC50, Unknown 2:	1.06E-07	CR42346	
RBA, Unknown 2:	1.14502%		
Max Concentration, Unknown 3:	1.50E-02	M	(example 5e-3)
IC50, Unknown 3:	1.18E-04	CR42347	non standard dilutions
RBA, Unknown 3:	0.00102%		
Max Concentration, Unknown 4:	3.00E-02	M	(example 5e-3)
IC50, Unknown 4:	6.72E-05	CR42355	
RBA, Unknown 4:	0.00180%		
Max Concentration, Unknown 5:	1.50E-02	M	(example 5e-3)
IC50, Unknown 5:	3.18E-05	CR42369	non standard dilutions
RBA, Unknown 5:	0.00380%		
volume of ethanol counted:	2	mL	
multitply DPM in sample by :	3.1		
working volume	3.1E+02	uL	protocol calls for counting decanted EtOH supernate reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	10785.9	712.45	Total Binding, solvent control, tubes
Hot	6	45528.7	1111.09	Total hot R1881 added to each tube
NSB	6	474.9	42.32	Nonspecific Binding
Specific EtOH	6	10311.0	712.45	

Assay Characterization Values	
EtOH / Hot	0.24 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3545.60	10991.36	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3296.80	10220.08	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3104.50	9623.95	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	164.76	494.28	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	142.68	428.04	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	159.31	477.93	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	176.49	547.12	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	190.10	589.31	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	141.13	437.50	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	607.52	1883.31	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	536.54	1663.27	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	560.13	1736.40	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	1914.80	5935.88	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2248.20	6969.42	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2042.90	6332.99	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3097.70	9602.87	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2710.90	8403.79	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2744.00	8506.40	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	2803.30	8690.23	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3176.30	9846.53	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3489.50	10817.45	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	246.81	740.43	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	249.55	748.65	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	256.90	770.70	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1141.80	3425.40	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1121.10	3363.30	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	873.95	2621.85	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2614.00	7842.00	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2613.30	7839.90	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2839.80	8519.40	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3483.20	10449.60	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3325.70	9977.10	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	2780.50	8341.50	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3540.50	10621.50	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3550.00	10650.00	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3183.40	9550.20	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3693.50	11080.50	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3551.20	10653.60	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3833.60	11500.80	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3798.00	11394.00	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3440.50	10321.50	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3632.40	10897.20	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	2751.50	8254.50	FALSE	spill
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3421.20	10263.60	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3314.30	9942.90	TRUE	

Check the 10% rule: 23.69% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
1	1	—	102.0	10991.36	10516.5	-680.3	102.0	24.14163	
2	2	—	94.5	10220.08	9745.2	91.0	94.5	22.44757	
3	3	—	88.7	9623.95	9149.1	687.1	88.7	21.13822	
4	1	-6.00	0.2	494.28	19.4	9816.8	0.2	1.085646	
5	2	-6.00	-0.5	428.04	-46.9	9883.0	-0.5	0.940155	
6	3	-6.00	0.0	477.93	3.0	9833.1	0.0	1.049734	
7	1	cold R1881	-7.01	547.119	72.2	9763.9	0.7	1.201702	
8	2	cold R1881	-7.01	589.31	114.4	9721.7	1.1	1.294371	
9	3	cold R1881	-7.01	-0.4	437.503	-37.4	9873.5	-0.4	0.96094
10	1	cold R1881	-8.01	13.7	1883.312	1408.4	13.7	4.136541	
11	2	cold R1881	-8.01	11.5	1663.274	1188.4	11.5	3.653246	
12	3	cold R1881	-8.01	12.2	1736.403	1261.5	12.2	3.813867	
13	1	cold R1881	-9.01	53.0	5935.88	5461.0	53.0	13.03768	
14	2	cold R1881	-9.01	63.0	6969.42	6494.5	63.0	15.30776	
15	3	cold R1881	-9.01	56.8	6332.99	5858.1	56.8	13.9099	
16	1	cold R1881	-10.01	88.5	9602.87	9128.0	88.5	21.09192	
17	2	cold R1881	-10.01	76.9	8403.79	7928.9	76.9	18.45824	
18	3	cold R1881	-10.01	77.9	8506.4	8031.5	77.9	18.68361	
19	1	cold R1881	-11.01	79.7	8690.23	8215.3	79.7	19.08738	
20	2	cold R1881	-11.01	90.9	9846.53	9371.6	90.9	21.6271	
21	3	cold R1881	-11.01	100.3	10817.45	10342.6	100.3	23.75965	
22	1	Weak Positive	-3	2.6	740.43	265.5	2.6	1.626294	
23	2	Weak Positive	-3	2.7	748.65	273.8	2.7	1.644349	
24	3	Weak Positive	-3	2.9	770.7	295.8	2.9	1.69278	
25	1	Weak Positive	-4	28.6	3425.4	2950.5	28.6	7.523611	
26	2	Weak Positive	-4	28.0	3363.3	2888.4	28.0	7.387214	
27	3	Weak Positive	-4	20.8	2621.85	2147.0	20.8	5.75868	
28	1	Weak Positive	-5	71.4	7842	7367.1	71.4	17.22431	
29	2	Weak Positive	-5	71.4	7839.9	7365.0	71.4	17.2197	
30	3	Weak Positive	-5	78.0	8519.4	8044.5	78.0	18.71217	
31	1	Weak Positive	-6	96.7	10449.6	9974.7	96.7	22.95169	
32	2	Weak Positive	-6	92.2	9977.1	9502.2	92.2	21.91389	
33	3	Weak Positive	-6	76.3	8341.5	7866.6	76.3	18.32142	
34	1	Weak Positive	-7	98.4	10621.5	10146.6	98.4	23.32926	
35	2	Weak Positive	-7	98.7	10650	10175.1	98.7	23.39186	
36	3	Weak Positive	-7	88.0	9550.2	9075.3	88.0	20.97623	
37	1	Weak Positive	-8	102.9	11080.5	10605.6	102.9	24.33741	
38	2	Weak Positive	-8	98.7	10653.6	10178.7	98.7	23.39976	
39	3	Weak Positive	-8	106.9	11500.8	11025.9	106.9	25.26057	
40	1	Weak Positive	-9	105.9	11394	10919.1	105.9	25.02599	
41	2	Weak Positive	-9	95.5	10321.5	9846.6	95.5	22.67033	
42	3	Weak Positive	-9	101.1	10897.2	10422.3	101.1	23.93481	
43	1	Weak Positive	-10						
44	2	Weak Positive	-10	94.9	10263.6	9788.7	94.9	22.54316	
45	3	Weak Positive	-10	91.8	9942.9	9468.0	91.8	21.83877	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: 23.69% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	138.19	428.39	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	158.98	492.84	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	151.80	470.58	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	141.40	438.34	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	153.47	475.76	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	138.48	429.29	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	411.80	1276.58	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	357.76	1109.06	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	348.47	1080.26	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1511.30	4685.03	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1541.10	4777.41	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1568.60	4862.66	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3091.20	9582.72	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3115.60	9658.36	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3194.00	9901.40	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3649.20	11312.52	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3582.40	11105.44	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3694.00	11451.40	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3684.30	11421.33	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3701.30	11474.03	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3550.80	11007.48	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3563.00	11045.30	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3601.20	11163.72	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3254.50	10088.95	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	138.78	430.22	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	158.31	490.76	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	155.57	482.27	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	94.19	291.99	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	151.91	470.92	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	122.19	378.79	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	182.72	566.43	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	167.93	520.58	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	138.35	428.89	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	429.10	1330.21	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	466.55	1446.31	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	468.73	1453.06	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1784.30	5531.33	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1837.30	5695.63	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1813.00	5620.30	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3474.60	10771.26	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3368.30	10441.73	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3179.30	9855.83	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3621.80	11227.58	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3702.90	11478.99	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3677.70	11400.87	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3653.50	11325.85	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3680.70	11410.17	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3608.10	11185.11	TRUE	

		Values for analysis by nonlinear regression								
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot		
46	1	Unknown 1	-3.91733	-0.5	428.389	-46.5	9882.6	-0.5	0.940921	
47	2	Unknown 1	-3.91733	0.2	492.838	17.9	9818.2	0.2	1.082478	
48	3	Unknown 1	-3.91733	0.0	470.58	-4.3	9840.5	0.0	1.033591	
49	1	Unknown 1	-4.01424	-0.4	438.34	-36.6	9872.7	-0.4	0.962778	
50	2	Unknown 1	-4.01424	0.0	475.757	0.9	9835.3	0.0	1.044961	
51	3	Unknown 1	-4.01424	-0.4	429.288	-45.6	9881.7	-0.4	0.942896	
52	1	Unknown 1	-5.01424	7.8	1276.58	801.7	9034.5	7.8	2.803904	
53	2	Unknown 1	-5.01424	6.2	1109.056	634.2	9202.0	6.2	2.435951	
54	3	Unknown 1	-5.01424	5.9	1080.257	605.4	9230.8	5.9	2.372696	
55	1	Unknown 1	-6.01424	40.8	4685.03	4210.1	5626.0	40.8	10.29029	
56	2	Unknown 1	-6.01424	41.7	4777.41	4302.5	5533.6	41.7	10.49319	
57	3	Unknown 1	-6.01424	42.6	4862.66	4387.8	5448.4	42.6	10.68044	
58	1	Unknown 1	-7.01424	88.3	9582.72	9107.8	728.3	88.3	21.04766	
59	2	Unknown 1	-7.01424	89.1	9658.36	9183.5	652.7	89.1	21.2138	
60	3	Unknown 1	-7.01424	91.4	9901.4	9426.5	409.6	91.4	21.74762	
61	1	Unknown 1	-8.01424	105.1	11312.52	10837.6	-1001.5	105.1	24.84703	
62	2	Unknown 1	-8.01424	103.1	11105.44	10630.5	-794.4	103.1	24.39219	
63	3	Unknown 1	-8.01424	106.5	11451.4	10976.5	-1140.4	106.5	25.15207	
64	1	Unknown 1	-9.01424	106.2	11421.33	10946.4	-1110.3	106.2	25.08602	
65	2	Unknown 1	-9.01424	106.7	11474.03	10999.1	-1163.0	106.7	25.20177	
66	3	Unknown 1	-9.01424	102.1	11007.48	10532.6	-696.4	102.1	24.17703	
67	1	Unknown 1	-10.01424	102.5	11045.3	10570.4	-734.3	102.5	24.2601	
68	2	Unknown 1	-10.01424	103.7	11163.72	10688.8	-852.7	103.7	24.5202	
69	3	Unknown 1	-10.01424	93.2	10088.95	9614.1	222.1	93.2	22.15956	
70	1	Unknown 2	-3.31527	-0.4	430.218	-44.7	9880.8	-0.4	0.944939	
71	2	Unknown 2	-3.31527	0.2	490.761	15.9	9820.3	0.2	1.077916	
72	3	Unknown 2	-3.31527	0.1	482.267	7.4	9828.8	0.1	1.05926	
73	1	Unknown 2	-4.01424	-1.8	291.989	-182.9	10019.0	-1.8	0.64133	
74	2	Unknown 2	-4.01424	0.0	470.921	-4.0	9840.1	0.0	1.03434	
75	3	Unknown 2	-4.01424	-0.9	378.789	-96.1	9932.2	-0.9	0.831979	
76	1	Unknown 2	-5.01424	0.9	566.432	91.5	9744.6	0.9	1.244122	
77	2	Unknown 2	-5.01424	0.4	520.583	45.7	9790.5	0.4	1.143418	
78	3	Unknown 2	-5.01424	-0.4	428.885	-46.0	9882.1	-0.4	0.942011	
79	1	Unknown 2	-6.01424	8.3	1330.21	855.3	8980.8	8.3	2.921698	
80	2	Unknown 2	-6.01424	9.4	1446.305	971.4	8864.7	9.4	3.176691	
81	3	Unknown 2	-6.01424	9.5	1453.063	978.2	8858.0	9.5	3.191534	
82	1	Unknown 2	-7.01424	49.0	5531.33	5056.4	4779.7	49.0	12.14911	
83	2	Unknown 2	-7.01424	50.6	5695.63	5220.7	4615.4	50.6	12.50999	
84	3	Unknown 2	-7.01424	49.9	5620.3	5145.4	4690.7	49.9	12.34453	
85	1	Unknown 2	-8.01424	99.9	10771.26	10296.4	-460.2	99.9	23.65819	
86	2	Unknown 2	-8.01424	96.7	10441.73	9966.8	-130.7	96.7	22.93441	
87	3	Unknown 2	-8.01424	91.0	9855.83	9380.9	455.2	91.0	21.64753	
88	1	Unknown 2	-9.01424	104.3	11227.58	10752.7	-916.5	104.3	24.66046	
89	2	Unknown 2	-9.01424	106.7	11478.99	11004.1	-1168.0	106.7	25.21266	
90	3	Unknown 2	-9.01424	106.0	11400.87	10926.0	-1089.8	106.0	25.04108	
91	1	Unknown 2	-10.01424	105.2	11325.85	10851.0	-1014.8	105.2	24.87631	
92	2	Unknown 2	-10.01424	106.1	11410.17	10935.3	-1099.1	106.1	25.06151	
93	3	Unknown 2	-10.01424	103.9	11185.11	10710.2	-874.1	103.9	24.56718	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Check the 10% rule: 23.69% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2443.30	7574.23	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2460.50	7627.55	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2350.00	7285.00	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2028.90	6289.59	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2224.80	6896.88	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2158.20	6690.42	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2579.00	7994.90	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2601.10	8063.41	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2574.90	7982.19	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3467.30	10748.63	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3597.20	11151.32	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	2883.60	8939.16	FALSE	spill
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3644.40	11297.64	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3641.90	11289.89	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3606.20	11179.22	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3767.50	11679.25	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3646.80	11305.08	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3681.20	11411.72	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3726.40	11551.84	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3650.10	11315.31	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3744.50	11607.95	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3609.50	11189.45	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3642.90	11292.99	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3536.50	10963.15	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	134.18	415.96	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	137.58	426.50	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	130.17	403.53	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	718.12	2226.17	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	752.90	2333.99	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	747.64	2317.68	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	2936.80	9104.08	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	3018.70	9357.97	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	3132.40	9710.44	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3528.10	10937.11	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3516.10	10899.91	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3679.40	11406.14	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3654.20	11328.02	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3651.30	11319.03	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3749.30	11622.83	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3775.10	11702.81	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3645.40	11300.74	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3708.30	11495.73	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3808.40	11806.04	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3615.70	11208.67	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3656.70	11335.77	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3714.90	11516.19	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3844.20	11917.02	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3702.20	11476.82	TRUE	

		Values for analysis by nonlinear regression						
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICR)	Ratio Total binding/ Hot
94	1	Unknown 3	-3.31527					
95	2	Unknown 3	-3.31527					
96	3	Unknown 3	-3.31527					
97	1	Unknown 3	-4.01424	56.4	6289.59	5814.7	4021.4	56.4 13.81457
98	2	Unknown 3	-4.01424	62.3	6896.88	6422.0	3414.2	62.3 15.14843
99	3	Unknown 3	-4.01424	60.3	6690.42	6215.5	3620.6	60.3 14.69496
100	1	Unknown 3	-5.01424	72.9	7994.9	7520.0	2316.1	72.9 17.56015
101	2	Unknown 3	-5.01424	73.6	8063.41	7588.5	2247.6	73.6 17.71062
102	3	Unknown 3	-5.01424	72.8	7982.19	7507.3	2328.8	72.8 17.53223
103	1	Unknown 3	-6.01424	99.6	10748.63	10273.7	-437.6	99.6 23.60849
104	2	Unknown 3	-6.01424	103.5	11151.32	10676.4	-840.3	103.5 24.49296
105	3	Unknown 3	-6.01424					
106	1	Unknown 3	-7.01424	105.0	11297.64	10822.7	-986.6	105.0 24.81434
107	2	Unknown 3	-7.01424	104.9	11289.89	10815.0	-978.9	104.9 24.79732
108	3	Unknown 3	-7.01424	103.8	11179.22	10704.3	-868.2	103.8 24.55424
109	1	Unknown 3	-8.01424	108.7	11679.25	11204.4	-1368.2	108.7 25.65252
110	2	Unknown 3	-8.01424	105.0	11305.08	10830.2	-994.0	105.0 24.83069
111	3	Unknown 3	-8.01424	106.1	11411.72	10936.8	-1100.7	106.1 25.06491
112	1	Unknown 3	-9.01424	107.4	11551.84	11076.9	-1240.8	107.4 25.37267
113	2	Unknown 3	-9.01424	105.1	11315.31	10840.4	-1004.3	105.1 24.85315
114	3	Unknown 3	-9.01424	108.0	11607.95	11133.1	-1296.9	108.0 25.49591
115	1	Unknown 3	-10.01424	103.9	11189.45	10714.6	-878.4	103.9 24.57671
116	2	Unknown 3	-10.01424	104.9	11292.99	10818.1	-982.0	104.9 24.80413
117	3	Unknown 3	-10.01424	101.7	10963.15	10488.3	-652.1	101.7 24.07966
118	1	Unknown 4	-3.01424	-0.6	415.958	-58.9	9895.1	-0.6 0.913618
119	2	Unknown 4	-3.01424	-0.5	426.498	-48.4	9884.5	-0.5 0.936768
120	3	Unknown 4	-3.01424	-0.7	403.527	-71.4	9907.5	-0.7 0.886314
121	1	Unknown 4	-3.71321	17.0	2226.172	1751.3	8084.9	17.0 4.889605
122	2	Unknown 4	-3.71321	18.0	2333.99	1859.1	7977.0	18.0 5.126419
123	3	Unknown 4	-3.71321	17.9	2317.684	1842.8	7993.3	17.9 5.090604
124	1	Unknown 4	-4.71321	83.7	9104.08	8629.2	1207.0	83.7 19.99637
125	2	Unknown 4	-4.71321	86.2	9357.97	8883.1	953.1	86.2 20.55402
126	3	Unknown 4	-4.71321	89.6	9710.44	9235.5	600.6	89.6 21.32819
127	1	Unknown 4	-5.71321	101.5	10937.11	10462.2	-626.1	101.5 24.02247
128	2	Unknown 4	-5.71321	101.1	10899.91	10425.0	-588.9	101.1 23.94076
129	3	Unknown 4	-5.71321	106.0	11406.14	10931.2	-1095.1	106.0 25.05266
130	1	Unknown 4	-6.71321	105.3	11328.02	10853.1	-1017.0	105.3 24.88107
131	2	Unknown 4	-6.71321	105.2	11319.03	10844.1	-1008.0	105.2 24.86133
132	3	Unknown 4	-6.71321	108.1	11622.83	11147.9	-1311.8	108.1 25.5286
133	1	Unknown 4	-7.71321	108.9	11702.81	11227.9	-1391.8	108.9 25.70427
134	2	Unknown 4	-7.71321	105.0	11300.74	10825.8	-989.7	105.0 24.82115
135	3	Unknown 4	-7.71321	106.9	11495.73	11020.8	-1184.7	106.9 25.24943
136	1	Unknown 4	-8.71321	109.9	11806.04	11331.1	-1495.0	109.9 25.931
137	2	Unknown 4	-8.71321	104.1	11208.67	10733.8	-897.6	104.1 24.61893
138	3	Unknown 4	-8.71321	105.3	11335.77	10860.9	-1024.7	105.3 24.89809
139	1	Unknown 4	-9.71321	107.1	11516.19	11041.3	-1205.2	107.1 25.29437
140	2	Unknown 4	-9.71321	111.0	11917.02	11442.1	-1606.0	111.0 26.17476
141	3	Unknown 4	-9.71321	106.7	11476.82	11001.9	-1165.8	106.7 25.2079

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	262.97	815.21	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	267.11	828.04	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	282.08	874.45	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	701.14	2173.53	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	701.17	2173.63	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	734.27	2276.24	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2673.50	8287.85	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3064.30	9499.33	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3040.40	9425.24	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3751.90	11630.89	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3637.70	11276.87	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3237.90	10037.49	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3120.80	9674.48	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3660.50	11347.55	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3624.20	11235.02	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3675.40	11393.74	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3715.90	11519.29	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3744.60	11608.26	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3583.10	11107.61	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3604.80	11174.88	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3726.30	11551.53	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3677.00	11398.70	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3730.00	11563.00	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3705.40	11486.74	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3612.00	11197.20	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3613.60	11202.16	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3703.50	11480.85	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	149.96	449.88	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	150.69	452.07	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	182.40	547.20	TRUE	
172	1	none	Hot	—	—	—	30	—	—	—	—	—	—	45120.00	45120.00	TRUE	
173	2	none	Hot	—	—	—	30	—	—	—	—	—	—	46984.00	46984.00	TRUE	
174	3	none	Hot	—	—	—	30	—	—	—	—	—	—	44109.00	44109.00	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	—	46225.00	46225.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	—	44550.00	44550.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	—	46184.00	46184.00	TRUE	

Check the 10% rule: **23.69%** If the ratio of EtOH / Hot is > 10% then there are problems with the assay

Values for analysis by nonlinear regression									
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
142	1	Unknown 5	-3.31527	3.3	815.207	340.3	9495.8	3.3	1.790536
143	2	Unknown 5	-3.31527	3.4	828.041	353.1	9483.0	3.4	1.818724
144	3	Unknown 5	-3.31527	3.9	874.448	399.5	9436.6	3.9	1.920654
145	1	Unknown 5	-4.01424	16.5	2173.534	1698.6	8137.5	16.5	4.77399
146	2	Unknown 5	-4.01424	16.5	2173.627	1698.7	8137.4	16.5	4.774194
147	3	Unknown 5	-4.01424	17.5	2276.237	1801.3	8034.8	17.5	4.999569
148	1	Unknown 5	-5.01424	75.8	8287.85	7813.0	2023.2	75.8	18.20359
149	2	Unknown 5	-5.01424	87.5	9499.33	9024.4	811.7	87.5	20.8645
150	3	Unknown 5	-5.01424	86.8	9425.24	8950.3	885.8	86.8	20.70177
151	1	Unknown 5	-6.01424	108.2	11630.89	11156.0	-1319.9	108.2	25.5463
152	2	Unknown 5	-6.01424	104.8	11276.87	10802.0	-965.8	104.8	24.76872
153	3	Unknown 5	-6.01424	92.7	10037.49	9562.6	273.5	92.7	22.04653
154	1	Unknown 5	-7.01424	89.2	9674.48	9199.6	636.6	89.2	21.24921
155	2	Unknown 5	-7.01424	105.4	11347.55	10872.7	-1036.5	105.4	24.92397
156	3	Unknown 5	-7.01424	104.4	11235.02	10760.1	-924.0	104.4	24.6768
157	1	Unknown 5	-8.01424	105.9	11393.74	10918.8	-1082.7	105.9	25.02542
158	2	Unknown 5	-8.01424	107.1	11519.29	11044.4	-1208.3	107.1	25.30118
159	3	Unknown 5	-8.01424	108.0	11608.26	11133.4	-1297.2	108.0	25.4966
160	1	Unknown 5	-9.01424	103.1	11107.61	10632.7	-796.6	103.1	24.39696
161	2	Unknown 5	-9.01424	103.8	11174.88	10700.0	-863.8	103.8	24.54471
162	3	Unknown 5	-9.01424	107.4	11551.53	11076.6	-1240.5	107.4	25.37199
163	1	Unknown 5	-10.01424	105.9	11398.7	10923.8	-1087.7	105.9	25.03631
164	2	Unknown 5	-10.01424	107.5	11563	11088.1	-1252.0	107.5	25.39719
165	3	Unknown 5	-10.01424	106.8	11486.74	11011.8	-1175.7	106.8	25.22969
166	1	—	—	104.0	11197.2	10722.3	-886.2	104.0	24.59374
167	2	—	—	104.0	11202.16	10727.3	-891.1	104.0	24.60463
168	3	—	—	106.7	11480.85	11006.0	-1169.8	106.7	25.21675
169	1	-6.00	-0.2	449.88	-25.0	9861.2	-0.2	0.988125	
170	2	-6.00	-0.2	452.07	-22.8	9859.0	-0.2	0.992935	
171	3	-6.00	0.7	547.2	72.3	9763.8	0.7	1.20188	
172	1			45120	44645.1				
173	2			46984	46509.1				
174	3			44109	43634.1				
175	1			46225	45750.1				
176	2			44550	44075.1				
177	3			46184	45709.1				

Prism data															
standard curve				weak positive				CR42341				CR42346			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-6.0	0.18795	-0.45446	0.02939	-3	2.5752	2.6549	2.8688	-3.9	-0.4511	0.1740	-0.0419	-3.3	-0.4333	0.1538	0.0714
-6.0	-0.24265	-0.22141	0.70119	-4	28.6150	28.0127	20.8219	-4.0	-0.3546	0.0083	-0.4424	-4.0	-1.7739	-0.0386	-0.9321
-7.0	0.70041	1.10959	-0.36269	-5	71.4487	71.4283	78.0184	-5.0	7.7750	6.1503	5.8710	-5.0	0.8877	0.4430	-0.4463
-8.0	13.65927	11.52527	12.23450	-6	96.7381	92.1557	76.2930	-6.0	40.8313	41.7272	42.5540	-6.0	8.2951	9.4210	9.4866
-9.0	52.96249	62.98612	56.81380	-7	98.4053	98.6817	88.0154	-7.0	88.3308	89.0644	91.4215	-7.0	49.0390	50.6325	49.9019
-10.0	88.52624	76.89714	77.89229	-8	102.8568	98.7166	106.9330	-8.0	105.1070	103.0987	106.4539	-8.0	99.8577	96.6618	90.9795
-11.0	79.67514	90.88934	100.30566	-9	105.8972	95.4958	101.0791	-9.0	106.1623	106.6734	102.1486	-9.0	104.2832	106.7215	105.9639
				-10		94.9342	91.8240	-10.0	102.5154	103.6639	93.2404	-10.0	105.2363	106.0541	103.8714

CR42347				CR42355				CR42369			
conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-3.3				-3.0	-0.5716	-0.4694	-0.6922	-3.3	3.3004	3.4249	3.8750
-4.0	56.3929	62.2826	60.2803	-3.7	16.9844	18.0301	17.8720	-4.0	16.4739	16.4748	17.4700
-5.0	72.9316	73.5960	72.8083	-4.7	83.6888	86.1511	89.5695	-5.0	75.7727	87.5221	86.8035
-6.0	99.6382	103.5436		-5.7	101.4662	101.1054	106.0150	-6.0	108.1947	104.7613	92.7413
-7.0	104.9627	104.8875	103.8142	-6.7	105.2573	105.1702	108.1165	-7.0	89.2207	105.4468	104.3554
-8.0	108.6637	105.0349	106.0691	-7.7	108.8922	104.9928	106.8839	-8.0	105.8947	107.1123	107.9752
-9.0	107.4280	105.1341	107.9722	-8.7	109.8934	104.0998	105.3325	-9.0	103.1197	103.7721	107.4250
-10.0	103.9134	104.9176	101.7187	-9.7	107.0823	110.9697	106.7005	-10.0	105.9428	107.5363	106.7967

Competitive Assay of a known Weak Positive
180 Assay Tubes

Please return by eMail to n.a.Holter@pnl.gov

Provide information in all blue cells in column O

If the DPM value for a tube was judged unreliable,

Include the DPM value in column O

Change the "TRUE" in column Q to "FALSE"

Provide a reason in column R

Columns T and U contain values to be analyzed
 by nonlinear regression software

Provide information in all blue cells in
 this column

Laboratory Code:		
Run identification:	516	
Assay start date:	10/27/2005	
Tracer lot number:	3559-507	
Specific activity on day of assay:	79.62	Ci/mmole
Cytosol vial or lot identification:	051905	
Protein (cytosol):	1000	micro gram per tube
Standard Curve IC50:	1.44E-09	M
Weak Positive, Max Concentration:	3.00E-02	M
Weak Positive IC50:	3.69E-05	M
RBA:	3.91222E-05	
Max Concentration, Unknown 1:	3.75E-03	M 5e-3)
IC50, Unknown 1:	7.10E-07	CR42341
RBA, Unknown 1:	0.20349%	
Max Concentration, Unknown 2:	1.50E-02	M (example 5e-3)
IC50, Unknown 2:	9.14E-08	CR42346
RBA, Unknown 2:	1.58004%	
Max Concentration, Unknown 3:	1.50E-02	M (example 5e-3)
IC50, Unknown 3:	7.43E-05	CR42347
RBA, Unknown 3:	0.00194%	
Max Concentration, Unknown 4:	3.00E-02	M (example 5e-3)
IC50, Unknown 4:	6.44E-05	CR42355
RBA, Unknown 4:	0.00224%	
Max Concentration, Unknown 5:	1.50E-02	M (example 5e-3)
IC50, Unknown 5:	3.14E-05	CR42369
RBA, Unknown 5:	0.00459%	
volume of ethanol counted:	2	mL
multiply DPM in sample by :	3.1	

protocol calls for counting decanted EtOH supernate
 reflects 100ul of reaction mixture processed

Column O, Rows 10 through 28 will contain output parameters

working volume

3.1E+02 uL

from the nonlinear regression software.

and the maximum concentration for the weak positive

Summary values				
	n	Mean	SD	
EtOH	6	11063.7	149.74	Total Binding, solvent control, tubes
Hot	6	44030.3	408.33	Total hot R1881 added to each tube
NSB	6	415.2	32.13	Nonspecific Binding
Specific EtOH	6	10648.5	149.74	

Assay Characterization Values	
EtOH / Hot	0.25 less than 0.1?
NSB / EtOH	0.04 around 0.25 ?

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
1	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3564.40	11049.64	TRUE	
2	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3535.10	10958.81	TRUE	
3	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3576.80	11088.08	TRUE	
4	1	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	138.90	416.70	TRUE	
5	2	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	148.89	446.67	TRUE	
6	3	Inert R1881	NSB		E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	149.74	449.22	TRUE	
7	1	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	251.41	779.37	TRUE	
8	2	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	191.35	593.19	TRUE	
9	3	Inert R1881	S	1	E-1-S1	3.00E-06	300	30	10	50	310	9.7E-08	100	172.14	533.63	TRUE	
10	1	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	609.46	1889.33	TRUE	
11	2	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	581.85	1803.74	TRUE	
12	3	Inert R1881	S	2	E-1-S2	3.00E-07	300	30	10	50	310	9.7E-09	100	605.40	1876.74	TRUE	
13	1	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2219.90	6881.69	TRUE	
14	2	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2236.70	6933.77	TRUE	
15	3	Inert R1881	S	3	E-1-S3	3.00E-08	300	30	10	50	310	9.7E-10	100	2228.40	6908.04	TRUE	
16	1	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	2620.80	8124.48	TRUE	
17	2	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3302.50	10237.75	TRUE	
18	3	Inert R1881	S	4	E-1-S4	3.00E-09	300	30	10	50	310	9.7E-11	100	3176.80	9848.08	TRUE	
19	1	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3443.00	10673.30	TRUE	
20	2	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3472.80	10765.68	TRUE	
21	3	Inert R1881	S	5	E-1-S5	3.00E-10	300	30	10	50	310	9.7E-12	100	3496.00	10837.60	TRUE	
22	1	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	307.05	921.15	TRUE	
23	2	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	310.47	931.41	TRUE	
24	3	Weak Positive	P	1	E-1-P1	3.00E-02	300	30	10	50	300	1.0E-03	100	293.96	881.88	TRUE	
25	1	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1184.60	3553.80	TRUE	
26	2	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1106.10	3318.30	TRUE	
27	3	Weak Positive	P	2	E-1-P2	3.00E-03	300	30	10	50	300	1.0E-04	100	1168.30	3504.90	TRUE	
28	1	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2831.60	8494.80	TRUE	
29	2	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2900.70	8702.10	TRUE	
30	3	Weak Positive	P	3	E-1-P3	3.00E-04	300	30	10	50	300	1.0E-05	100	2849.70	8549.10	TRUE	
31	1	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3517.90	10553.70	TRUE	
32	2	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3723.00	11169.00	TRUE	
33	3	Weak Positive	P	4	E-1-P4	3.00E-05	300	30	10	50	300	1.0E-06	100	3461.80	10385.40	TRUE	
34	1	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3464.90	10394.70	TRUE	
35	2	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3699.10	11097.30	TRUE	
36	3	Weak Positive	P	5	E-1-P5	3.00E-06	300	30	10	50	300	1.0E-07	100	3701.00	11103.00	TRUE	
37	1	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3241.30	9723.90	TRUE	
38	2	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3682.20	11046.60	TRUE	
39	3	Weak Positive	P	6	E-1-P6	3.00E-07	300	30	10	50	300	1.0E-08	100	3561.80	10685.40	TRUE	
40	1	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3805.60	11416.80	TRUE	
41	2	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3209.20	9627.60	TRUE	
42	3	Weak Positive	P	7	E-1-P7	3.00E-08	300	30	10	50	300	1.0E-09	100	3688.30	11064.90	TRUE	
43	1	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	2906.30	8718.90	TRUE	
44	2	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3502.50	10507.50	TRUE	
45	3	Weak Positive	P	8	E-1-P8	3.00E-09	300	30	10	50	300	1.0E-10	100	3454.20	10362.60	TRUE	

		Values for analysis by nonlinear regression						
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot
1	1	—	99.9	11049.64	10634.5	-401.1	99.9	25.09552
2	2	—	99.0	10958.81	10543.6	-310.3	99.0	24.88923
3	3	—	100.2	11088.08	10672.9	-439.6	100.2	25.18282
4	1	-6.00	0.0	416.7	1.5	10231.8	0.0	0.946393
5	2	-6.00	0.3	446.67	31.5	10201.8	0.3	1.01446
6	3	-6.00	0.0	449.22	34.0	10199.3	0.3	1.020251
7	1	cold R1881	-7.01	3.4	779.371	364.2	3.4	1.770077
8	2	cold R1881	-7.01	1.7	593.185	178.0	1.7	1.347219
9	3	cold R1881	-7.01	1.1	533.634	118.5	1.1	1.211969
10	1	cold R1881	-8.01	13.8	1889.326	1474.1	13.8	4.290965
11	2	cold R1881	-8.01	13.0	1803.735	1388.6	13.0	4.096574
12	3	cold R1881	-8.01	13.7	1876.74	1461.6	13.7	4.26238
13	1	cold R1881	-9.01	60.7	6881.69	6466.5	60.7	15.62943
14	2	cold R1881	-9.01	61.2	6933.77	6518.6	61.2	15.74771
15	3	cold R1881	-9.01	61.0	6908.04	6492.9	61.0	15.68927
16	1	cold R1881	-10.01	72.4	8124.48	7709.3	72.4	18.45201
17	2	cold R1881	-10.01	92.2	10237.75	9822.6	92.2	23.25158
18	3	cold R1881	-10.01	88.6	9848.08	9432.9	88.6	22.36658
19	1	cold R1881	-11.01	96.3	10673.3	10258.1	96.3	24.24079
20	2	cold R1881	-11.01	97.2	10765.68	10350.5	97.2	24.4506
21	3	cold R1881	-11.01	97.9	10837.6	10422.4	97.9	24.61394
22	1	Weak Positive	-3	4.8	921.15	506.0	4.8	2.09208
23	2	Weak Positive	-3	4.8	931.41	516.2	4.8	2.115383
24	3	Weak Positive	-3	4.4	881.88	466.7	4.4	2.002892
25	1	Weak Positive	-4	29.5	3553.8	3138.6	29.5	8.071254
26	2	Weak Positive	-4	27.3	3318.3	2903.1	27.3	7.536395
27	3	Weak Positive	-4	29.0	3504.9	3089.7	29.0	7.960194
28	1	Weak Positive	-5	75.9	8494.8	8079.6	75.9	19.29306
29	2	Weak Positive	-5	77.8	8702.1	8286.9	77.8	19.76387
30	3	Weak Positive	-5	76.4	8549.1	8133.9	76.4	19.41639
31	1	Weak Positive	-6	95.2	10553.7	10138.5	95.2	23.96916
32	2	Weak Positive	-6	101.0	11169	10753.8	101.0	25.3666
33	3	Weak Positive	-6	93.6	10385.4	9970.2	93.6	23.58692
34	1	Weak Positive	-7	93.7	10394.7	9979.5	93.7	23.60804
35	2	Weak Positive	-7	100.3	11097.3	10682.1	100.3	25.20376
36	3	Weak Positive	-7	100.4	11103	10687.8	100.4	25.21671
37	1	Weak Positive	-8	87.4	9723.9	9308.7	87.4	22.08455
38	2	Weak Positive	-8	99.8	11046.6	10631.4	99.8	25.08861
39	3	Weak Positive	-8	96.4	10685.4	10270.2	96.4	24.26827
40	1	Weak Positive	-9	103.3	11416.8	11001.6	103.3	25.9294
41	2	Weak Positive	-9	86.5	9627.6	9212.4	86.5	21.86583
42	3	Weak Positive	-9	100.0	11064.9	10649.7	100.0	25.13018
43	1	Weak Positive	-10	78.0	8718.9	8303.7	78.0	19.80203
44	2	Weak Positive	-10	94.8	10507.5	10092.3	94.8	23.86423
45	3	Weak Positive	-10	93.4	10362.6	9947.4	93.4	23.53514

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
46	1	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	166.14	515.03	TRUE	
47	2	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	166.94	517.51	TRUE	
48	3	Unknown 1	U1	1	E-1-U1	3.75E-03	300	30	10	50	310	1.2E-04	100	169.34	524.95	TRUE	
49	1	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	158.89	492.56	TRUE	
50	2	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	166.20	515.22	TRUE	
51	3	Unknown 1	U1	2	E-1-U1	3.00E-03	300	30	10	50	310	9.7E-05	100	173.07	536.52	TRUE	
52	1	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	383.01	1187.33	TRUE	
53	2	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	370.10	1147.31	TRUE	
54	3	Unknown 1	U1	3	E-1-U1	3.00E-04	300	30	10	50	310	9.7E-06	100	393.61	1220.19	TRUE	
55	1	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1657.60	5138.56	TRUE	
56	2	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1580.90	4900.79	TRUE	
57	3	Unknown 1	U1	4	E-1-U1	3.00E-05	300	30	10	50	310	9.7E-07	100	1468.10	4551.11	TRUE	
58	1	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3123.30	9682.23	TRUE	
59	2	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3100.40	9611.24	TRUE	
60	3	Unknown 1	U1	5	E-1-U1	3.00E-06	300	30	10	50	310	9.7E-08	100	3224.60	9996.26	TRUE	
61	1	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3174.70	9841.57	TRUE	
62	2	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	2894.80	8973.88	TRUE	
63	3	Unknown 1	U1	6	E-1-U1	3.00E-07	300	30	10	50	310	9.7E-09	100	3634.70	11267.57	TRUE	
64	1	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3713.20	11510.92	TRUE	
65	2	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	2856.90	8856.39	TRUE	
66	3	Unknown 1	U1	7	E-1-U1	3.00E-08	300	30	10	50	310	9.7E-10	100	3662.10	11352.51	TRUE	
67	1	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3389.50	10507.45	TRUE	
68	2	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3470.60	10758.86	TRUE	
69	3	Unknown 1	U1	8	E-1-U1	3.00E-09	300	30	10	50	310	9.7E-11	100	3486.50	10808.15	TRUE	
70	1	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	124.55	386.11	TRUE	
71	2	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	129.30	400.83	TRUE	
72	3	Unknown 2	U2	1	E-1-U2	1.50E-02	300	30	10	50	310	4.8E-04	100	104.27	323.24	TRUE	
73	1	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	152.97	474.21	TRUE	
74	2	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	129.21	400.55	TRUE	
75	3	Unknown 2	U2	2	E-1-U2	3.00E-03	300	30	10	50	310	9.7E-05	100	137.37	425.85	TRUE	
76	1	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	171.71	532.30	TRUE	
77	2	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	145.80	451.98	TRUE	
78	3	Unknown 2	U2	3	E-1-U2	3.00E-04	300	30	10	50	310	9.7E-06	100	160.36	497.12	TRUE	
79	1	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	436.29	1352.50	TRUE	
80	2	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	400.37	1241.15	TRUE	
81	3	Unknown 2	U2	4	E-1-U2	3.00E-05	300	30	10	50	310	9.7E-07	100	399.10	1237.21	TRUE	
82	1	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1753.60	5436.16	TRUE	
83	2	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1773.50	5497.85	TRUE	
84	3	Unknown 2	U2	5	E-1-U2	3.00E-06	300	30	10	50	310	9.7E-08	100	1783.10	5527.61	TRUE	
85	1	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3328.50	10318.35	TRUE	
86	2	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3255.70	10092.67	TRUE	
87	3	Unknown 2	U2	6	E-1-U2	3.00E-07	300	30	10	50	310	9.7E-09	100	3221.20	9985.72	TRUE	
88	1	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	2917.60	9044.56	TRUE	
89	2	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3470.10	10757.31	TRUE	
90	3	Unknown 2	U2	7	E-1-U2	3.00E-08	300	30	10	50	310	9.7E-10	100	3731.10	11566.41	TRUE	
91	1	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3603.60	11171.16	TRUE	
92	2	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3732.00	11569.20	TRUE	
93	3	Unknown 2	U2	8	E-1-U2	3.00E-09	300	30	10	50	310	9.7E-11	100	3684.70	11422.57	TRUE	

		Values for analysis by nonlinear regression											
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific E10H)	Ratio Total binding/ Hot					
46	1	Unknown 1	-3.91733	0.9	515.034	99.9	10133.5	0.9	1.169725				
47	2	Unknown 1	-3.91733	1.0	517.514	102.3	10131.0	1.0	1.175358				
48	3	Unknown 1	-3.91733	1.0	524.954	109.8	10123.6	1.0	1.192255				
49	1	Unknown 1	-4.01424	0.7	492.559	77.4	10156.0	0.7	1.118681				
50	2	Unknown 1	-4.01424	0.9	515.22	100.0	10133.3	0.9	1.170148				
51	3	Unknown 1	-4.01424	1.1	536.517	121.3	10112.0	1.1	1.218517				
52	1	Unknown 1	-5.01424	7.3	1187.331	772.2	9461.2	7.3	2.696621				
53	2	Unknown 1	-5.01424	6.9	1147.31	732.1	9501.2	6.9	2.605726				
54	3	Unknown 1	-5.01424	7.6	1220.191	805.0	9428.3	7.6	2.771251				
55	1	Unknown 1	-6.01424	44.4	5138.56	4723.4	5510.0	44.4	11.6705				
56	2	Unknown 1	-6.01424	42.1	4900.79	4485.6	5747.7	42.1	11.13049				
57	3	Unknown 1	-6.01424	38.8	4551.11	4135.9	6097.4	38.8	10.33631				
58	1	Unknown 1	-7.01424	87.0	9682.23	9267.1	966.3	87.0	21.98991				
59	2	Unknown 1	-7.01424	86.4	9611.24	9196.1	1037.3	86.4	21.82868				
60	3	Unknown 1	-7.01424	90.0	9996.26	9581.1	652.3	90.0	22.70312				
61	1	Unknown 1	-8.01424	88.5	9841.57	9426.4	806.9	88.5	22.3518				
62	2	Unknown 1	-8.01424	80.4	8973.88	8558.7	1674.6	80.4	20.38113				
63	3	Unknown 1	-8.01424	101.9	11267.57	10852.4	-619.1	101.9	25.59047				
64	1	Unknown 1	-9.01424	104.2	11510.92	11095.7	-862.4	104.2	26.14316				
65	2	Unknown 1	-9.01424	79.3	8856.39	8441.2	1792.1	79.3	20.11429				
66	3	Unknown 1	-9.01424	102.7	11352.51	10937.3	-704.0	102.7	25.78338				
67	1	Unknown 1	-10.01424	94.8	10507.45	10092.3	141.1	94.8	23.86412				
68	2	Unknown 1	-10.01424	97.1	10758.86	10343.7	-110.3	97.1	24.43511				
69	3	Unknown 1	-10.01424	97.6	10808.15	10393.0	-159.6	97.6	24.54705				
70	1	Unknown 2	-3.31527	-0.3	386.105	-29.1	10262.4	-0.3	0.876907				
71	2	Unknown 2	-3.31527	-0.1	400.83	-14.4	10247.7	-0.1	0.91035				
72	3	Unknown 2	-3.31527	-0.9	323.237	-91.9	10325.3	-0.9	0.734123				
73	1	Unknown 2	-4.01424	0.6	474.207	59.0	10174.3	0.6	1.077001				
74	2	Unknown 2	-4.01424	-0.1	400.551	-14.6	10248.0	-0.1	0.909716				
75	3	Unknown 2	-4.01424	0.1	425.847	10.7	10222.7	0.1	0.967167				
76	1	Unknown 2	-5.01424	1.1	532.301	117.1	10116.2	1.1	1.208942				
77	2	Unknown 2	-5.01424	0.3	451.98	36.8	10196.5	0.3	1.02652				
78	3	Unknown 2	-5.01424	0.8	497.116	81.9	10151.4	0.8	1.129031				
79	1	Unknown 2	-6.01424	8.8	1352.499	937.3	9296.0	8.8	3.071744				
80	2	Unknown 2	-6.01424	7.8	1241.147	826.0	9407.4	7.8	2.818845				
81	3	Unknown 2	-6.01424	7.7	1237.21	822.0	9411.3	7.7	2.809904				
82	1	Unknown 2	-7.01424	47.2	5436.16	5021.0	5212.4	47.2	12.3464				
83	2	Unknown 2	-7.01424	47.7	5497.85	5082.7	5150.7	47.7	12.48651				
84	3	Unknown 2	-7.01424	48.0	5527.61	5112.4	5120.9	48.0	12.5541				
85	1	Unknown 2	-8.01424	93.0	10318.35	9903.2	330.2	93.0	23.43464				
86	2	Unknown 2	-8.01424	90.9	10092.67	9677.5	555.8	90.9	22.92208				
87	3	Unknown 2	-8.01424	89.9	9985.72	9570.5	662.8	89.9	22.67918				
88	1	Unknown 2	-9.01424	81.0	9044.56	8629.4	1604.0	81.0	20.54166				
89	2	Unknown 2	-9.01424	97.1	10757.31	10342.1	-108.8	97.1	24.43159				
90	3	Unknown 2	-9.01424	104.7	11566.41	11151.2	-917.9	104.7	26.26919				
91	1	Unknown 2	-10.01424	101.0	11171.16	10756.0	-522.6	101.0	25.37151				
92	2	Unknown 2	-10.01424	104.7	11569.2	11154.0	-920.7	104.7	26.27552				
93	3	Unknown 2	-10.01424	103.4	11422.57	11007.4	-774.1	103.4	25.9425				

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triamcetonone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
94	1	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2428.00	7526.80	FALSE	precipitate in tube
95	2	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2511.80	7786.58	FALSE	precipitate in tube
96	3	Unknown 3	U3	1	E-1-U3	1.50E-02	300	30	10	50	310	4.8E-04	100	2478.00	7681.00	FALSE	precipitate in tube
97	1	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1971.20	6110.72	TRUE	
98	2	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	1647.90	5108.49	TRUE	
99	3	Unknown 3	U3	2	E-1-U3	3.00E-03	300	30	10	50	310	9.7E-05	100	2085.30	6464.43	TRUE	
100	1	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2380.80	7380.48	TRUE	
101	2	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2378.00	7371.80	TRUE	
102	3	Unknown 3	U3	3	E-1-U3	3.00E-04	300	30	10	50	310	9.7E-06	100	2614.30	8104.33	TRUE	
103	1	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3533.90	10955.09	TRUE	
104	2	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3393.30	10519.23	TRUE	
105	3	Unknown 3	U3	4	E-1-U3	3.00E-05	300	30	10	50	310	9.7E-07	100	3496.10	10837.91	TRUE	
106	1	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3395.10	10524.81	TRUE	
107	2	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3707.50	11493.25	TRUE	
108	3	Unknown 3	U3	5	E-1-U3	3.00E-06	300	30	10	50	310	9.7E-08	100	3638.80	11280.28	TRUE	
109	1	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3598.50	11155.35	TRUE	
110	2	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3814.30	11824.33	TRUE	
111	3	Unknown 3	U3	6	E-1-U3	3.00E-07	300	30	10	50	310	9.7E-09	100	3675.70	11394.67	TRUE	
112	1	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3770.30	11687.93	TRUE	
113	2	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3494.10	10831.71	TRUE	
114	3	Unknown 3	U3	7	E-1-U3	3.00E-08	300	30	10	50	310	9.7E-10	100	3747.10	11616.01	TRUE	
115	1	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3658.50	11341.35	TRUE	
116	2	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3445.00	10679.50	TRUE	
117	3	Unknown 3	U3	8	E-1-U3	3.00E-09	300	30	10	50	310	9.7E-11	100	3722.80	11540.68	TRUE	
118	1	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	141.45	438.50	TRUE	
119	2	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	123.49	382.82	TRUE	
120	3	Unknown 4	U4	1	E-1-U4	3.00E-02	300	30	10	50	310	9.7E-04	100	118.01	365.83	TRUE	
121	1	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	695.69	2156.64	TRUE	
122	2	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	752.37	2332.35	TRUE	
123	3	Unknown 4	U4	2	E-1-U4	6.00E-03	300	30	10	50	310	1.9E-04	100	737.32	2285.69	TRUE	
124	1	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	3005.20	9316.12	TRUE	
125	2	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	3106.10	9628.91	TRUE	
126	3	Unknown 4	U4	3	E-1-U4	6.00E-04	300	30	10	50	310	1.9E-05	100	2995.60	9286.36	TRUE	
127	1	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3749.20	11622.52	TRUE	
128	2	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3657.80	11339.18	TRUE	
129	3	Unknown 4	U4	4	E-1-U4	6.00E-05	300	30	10	50	310	1.9E-06	100	3643.20	11293.92	TRUE	
130	1	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3664.20	11359.02	TRUE	
131	2	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3669.90	11376.69	TRUE	
132	3	Unknown 4	U4	5	E-1-U4	6.00E-06	300	30	10	50	310	1.9E-07	100	3792.20	11755.82	TRUE	
133	1	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3727.40	11554.94	TRUE	
134	2	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3626.20	11241.22	TRUE	
135	3	Unknown 4	U4	6	E-1-U4	6.00E-07	300	30	10	50	310	1.9E-08	100	3638.80	11280.28	TRUE	
136	1	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3561.90	11041.89	TRUE	
137	2	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3710.00	11501.00	TRUE	
138	3	Unknown 4	U4	7	E-1-U4	6.00E-08	300	30	10	50	310	1.9E-09	100	3729.00	11559.90	TRUE	
139	1	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3767.40	11678.94	TRUE	
140	2	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3831.60	11877.96	TRUE	
141	3	Unknown 4	U4	8	E-1-U4	6.00E-09	300	30	10	50	310	1.9E-10	100	3696.90	11460.39	TRUE	

Check the 10% rule: 25.13% If the ratio of EtOH / Hot is > 10% then there are problems with the assay

		Values for analysis by nonlinear regression								
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EICR)	Ratio Total binding/ Hot		
94	1	Unknown 3	-3.31527							
95	2	Unknown 3	-3.31527							
96	3	Unknown 3	-3.31527							
97	1	Unknown 3	-4.01424	53.5	6110.72	5695.5	4537.8	53.5	13.87843	
98	2	Unknown 3	-4.01424	44.1	5108.49	4693.3	5540.0	44.1	11.60221	
99	3	Unknown 3	-4.01424	56.8	6464.43	6049.3	4184.1	56.8	14.68176	
100	1	Unknown 3	-5.01424	65.4	7380.48	6965.3	3268.0	65.4	16.76226	
101	2	Unknown 3	-5.01424	65.3	7371.8	6956.6	3276.7	65.3	16.74255	
102	3	Unknown 3	-5.01424	72.2	8104.33	7689.2	2544.2	72.2	18.40624	
103	1	Unknown 3	-6.01424	99.0	10955.09	10539.9	-306.6	99.0	24.88078	
104	2	Unknown 3	-6.01424	94.9	10519.23	10104.1	129.3	94.9	23.89087	
105	3	Unknown 3	-6.01424	97.9	10837.91	10422.7	-189.4	97.9	24.61464	
106	1	Unknown 3	-7.01424	94.9	10524.81	10109.6	123.7	94.9	23.90354	
107	2	Unknown 3	-7.01424	104.0	11493.25	11078.1	-844.7	104.0	26.10303	
108	3	Unknown 3	-7.01424	102.0	11280.28	10865.1	-631.8	102.0	25.61934	
109	1	Unknown 3	-8.01424	100.9	11155.35	10740.2	-506.8	100.9	25.3356	
110	2	Unknown 3	-8.01424	107.1	11824.33	11409.2	-1175.8	107.1	26.85496	
111	3	Unknown 3	-8.01424	103.1	11394.67	10979.5	-746.2	103.1	25.87914	
112	1	Unknown 3	-9.01424	105.9	11687.93	11272.8	-1039.4	105.9	26.54518	
113	2	Unknown 3	-9.01424	97.8	10831.71	10416.5	-183.2	97.8	24.60056	
114	3	Unknown 3	-9.01424	105.2	11616.01	11200.8	-967.5	105.2	26.38184	
115	1	Unknown 3	-10.01424	102.6	11341.35	10926.2	-692.8	102.6	25.75804	
116	2	Unknown 3	-10.01424	96.4	10679.5	10264.3	-31.0	96.4	24.25487	
117	3	Unknown 3	-10.01424	104.5	11540.68	11125.5	-892.2	104.5	26.21075	
118	1	Unknown 4	-3.01424	0.2	438.495	23.3	10210.0	0.2	0.995893	
119	2	Unknown 4	-3.01424	-0.3	382.819	-32.4	10265.7	-0.3	0.869444	
120	3	Unknown 4	-3.01424	-0.5	365.831	-49.3	10282.7	-0.5	0.830861	
121	1	Unknown 4	-3.71321	16.4	2156.639	1741.5	8491.9	16.4	4.898076	
122	2	Unknown 4	-3.71321	18.0	2332.347	1917.2	8316.2	18.0	5.297137	
123	3	Unknown 4	-3.71321	17.6	2285.692	1870.5	8362.8	17.6	5.191176	
124	1	Unknown 4	-4.71321	83.6	9316.12	8900.9	1332.4	83.6	21.15841	
125	2	Unknown 4	-4.71321	86.5	9628.91	9213.7	1019.6	86.5	21.86881	
126	3	Unknown 4	-4.71321	83.3	9286.36	8871.2	1362.2	83.3	21.09082	
127	1	Unknown 4	-5.71321	105.2	11622.52	11207.3	-974.0	105.2	26.39662	
128	2	Unknown 4	-5.71321	102.6	11339.18	10924.0	-690.7	102.6	25.75311	
129	3	Unknown 4	-5.71321	102.2	11293.92	10878.7	-645.4	102.2	25.65032	
130	1	Unknown 4	-6.71321	102.8	11359.02	10943.8	-710.5	102.8	25.79817	
131	2	Unknown 4	-6.71321	102.9	11376.69	10961.5	-728.2	102.9	25.8383	
132	3	Unknown 4	-6.71321	106.5	11755.82	11340.6	-1107.3	106.5	26.69937	
133	1	Unknown 4	-7.71321	104.6	11554.94	11139.8	-906.4	104.6	26.24314	
134	2	Unknown 4	-7.71321	101.7	11241.22	10826.0	-592.7	101.7	25.53063	
135	3	Unknown 4	-7.71321	102.0	11280.28	10865.1	-631.8	102.0	25.61934	
136	1	Unknown 4	-8.71321	99.8	11041.89	10626.7	-393.4	99.8	25.07792	
137	2	Unknown 4	-8.71321	104.1	11501	11085.8	-852.5	104.1	26.12063	
138	3	Unknown 4	-8.71321	104.7	11559.9	11144.7	-911.4	104.7	26.2544	
139	1	Unknown 4	-9.71321	105.8	11678.94	11263.8	-1030.4	105.8	26.52476	
140	2	Unknown 4	-9.71321	107.6	11877.96	11462.8	-1229.4	107.6	26.97677	
141	3	Unknown 4	-9.71321	103.7	11460.39	11045.2	-811.9	103.7	26.0284	

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)

Competitive Assay Tube Layout - One Test Chemical (Weak Positive)														Check the 10% rule:		If the ratio of EtOH / Hot is > 10% then there are problems with the assay	
Position	Replicate	Competitor	Competitor Code	Concentration Code	Labels on vials in set 1-1-E supplied by Battelle to laboratory "E"	Competitor Initial Concentration (M)	Cytosol (uL)	Tracer (Hot R1881) Volume (uL)	Competitor Volume (uL)	triancelenone Volume (uL)	Final Volume (uL)	Competitor Final Concentration (M)	Aliquot (uL)	DPM as sampled	corrected DPM for 2.0 mL	Use this value?	Notes to explain why "Use this value" is set to "FALSE"
142	1	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	267.71	829.90	TRUE	
143	2	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	265.55	823.21	TRUE	
144	3	Unknown 5	U5	1	E-1-U5	1.50E-02	300	30	10	50	310	4.8E-04	100	258.93	802.68	TRUE	
145	1	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	712.27	2208.04	TRUE	
146	2	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	559.36	1734.02	TRUE	
147	3	Unknown 5	U5	2	E-1-U5	3.00E-03	300	30	10	50	310	9.7E-05	100	698.28	2164.67	TRUE	
148	1	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3072.00	9523.20	TRUE	
149	2	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	3036.30	9412.53	TRUE	
150	3	Unknown 5	U5	3	E-1-U5	3.00E-04	300	30	10	50	310	9.7E-06	100	2956.00	9163.60	TRUE	
151	1	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3666.90	11367.39	TRUE	
152	2	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3802.70	11788.37	TRUE	
153	3	Unknown 5	U5	4	E-1-U5	3.00E-05	300	30	10	50	310	9.7E-07	100	3614.10	11203.71	TRUE	
154	1	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3468.90	10753.59	TRUE	
155	2	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3520.20	10912.62	TRUE	
156	3	Unknown 5	U5	5	E-1-U5	3.00E-06	300	30	10	50	310	9.7E-08	100	3582.00	11104.20	TRUE	
157	1	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3568.90	11063.59	TRUE	
158	2	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3530.90	10945.79	TRUE	
159	3	Unknown 5	U5	6	E-1-U5	3.00E-07	300	30	10	50	310	9.7E-09	100	3552.70	11013.37	TRUE	
160	1	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3140.50	9735.55	TRUE	
161	2	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3362.50	10423.75	TRUE	
162	3	Unknown 5	U5	7	E-1-U5	3.00E-08	300	30	10	50	310	9.7E-10	100	3499.50	10848.45	TRUE	
163	1	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3526.40	10931.84	TRUE	
164	2	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3537.80	10967.18	TRUE	
165	3	Unknown 5	U5	8	E-1-U5	3.00E-09	300	30	10	50	310	9.7E-11	100	3421.70	10607.27	TRUE	
166	1	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3613.20	11200.92	TRUE	
167	2	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3626.80	11243.08	TRUE	
168	3	ethanol	EtOH	0	—	—	300	30	10	50	310	—	100	3497.30	10841.63	TRUE	
169	1	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	134.35	403.05	TRUE	
170	2	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	120.57	361.71	TRUE	
171	3	Inert R1881	NSB	—	E-1-S0	1.00E-05	300	30	30	50	300	1.0E-06	100	137.91	413.73	TRUE	
172	1	DMSO	DMSO	—	—	—	300	30	30	50	300	—	100	3160.74	9482.22	TRUE	
173	2	DMSO	DMSO	—	—	—	300	30	30	50	300	—	100	3588.00	10764.00	TRUE	
174	3	DMSO	DMSO	—	—	—	300	30	30	50	300	—	100	3390.25	10170.75	TRUE	
175	1	none	Hot	—	—	—	30	—	—	—	—	—	100	43740.00	43740.00	TRUE	
176	2	none	Hot	—	—	—	30	—	—	—	—	—	100	44221.00	44221.00	TRUE	
177	3	none	Hot	—	—	—	30	—	—	—	—	—	100	44107.00	44107.00	TRUE	
178	1	none	Hot	—	—	—	30	—	—	—	—	—	100	44713.00	44713.00	TRUE	
179	2	none	Hot	—	—	—	30	—	—	—	—	—	100	43809.00	43809.00	TRUE	
180	3	none	Hot	—	—	—	30	—	—	—	—	—	100	43592.00	43592.00	TRUE	

		Values for analysis by nonlinear regression							
Position	Replicate	concentration (log)	percent bound	Usable DPM values	Specific Binding (Total - mean NSB)	Free DPM (mean total add - total bound)	Percent Binding (specific bound / mean specific EtOH)	Ratio Total binding/ Hot	
142	1	Unknown 5	-3.31527	3.9	829.901	414.7	9818.6	3.9	1.884839
143	2	Unknown 5	-3.31527	3.8	823.205	408.0	9825.3	3.8	1.869632
144	3	Unknown 5	-3.31527	3.6	802.683	387.5	9845.8	3.6	1.823023
145	1	Unknown 5	-4.01424	16.8	2208.037	1792.9	8440.5	16.8	5.014809
146	2	Unknown 5	-4.01424	12.4	1734.016	1318.8	8914.5	12.4	3.93823
147	3	Unknown 5	-4.01424	16.4	2164.668	1749.5	8483.8	16.4	4.916311
148	1	Unknown 5	-5.01424	85.5	9523.2	9108.0	1125.3	85.5	21.62873
149	2	Unknown 5	-5.01424	84.5	9412.53	8997.4	1236.0	84.5	21.37738
150	3	Unknown 5	-5.01424	82.2	9163.6	8748.4	1484.9	82.2	20.81202
151	1	Unknown 5	-6.01424	102.9	11367.39	10952.2	-718.9	102.9	25.81718
152	2	Unknown 5	-6.01424	106.8	11788.37	11373.2	-1139.9	106.8	26.77329
153	3	Unknown 5	-6.01424	101.3	11203.71	10788.5	-555.2	101.3	25.44544
154	1	Unknown 5	-7.01424	97.1	10753.59	10338.4	-105.1	97.1	24.42314
155	2	Unknown 5	-7.01424	98.6	10912.62	10497.4	-264.1	98.6	24.78432
156	3	Unknown 5	-7.01424	100.4	11104.2	10689.0	-455.7	100.4	25.21943
157	1	Unknown 5	-8.01424	100.0	11063.59	10648.4	-415.1	100.0	25.1272
158	2	Unknown 5	-8.01424	98.9	10945.79	10530.6	-297.3	98.9	24.85966
159	3	Unknown 5	-8.01424	99.5	11013.37	10598.2	-364.9	99.5	25.01314
160	1	Unknown 5	-9.01424	87.5	9735.55	9320.4	913.0	87.5	22.11101
161	2	Unknown 5	-9.01424	94.0	10423.75	10008.6	224.8	94.0	23.67402
162	3	Unknown 5	-9.01424	98.0	10848.45	10433.3	-199.9	98.0	24.63858
163	1	Unknown 5	-10.01424	98.8	10931.84	10516.7	-283.3	98.8	24.82797
164	2	Unknown 5	-10.01424	99.1	10967.18	10552.0	-318.7	99.1	24.90824
165	3	Unknown 5	-10.01424	95.7	10607.27	10192.1	41.2	95.7	24.09082
166	1	—	—	101.3	11200.92	10785.7	-552.4	101.3	25.4391
167	2	—	—	101.7	11243.08	10827.9	-594.6	101.7	25.53485
168	3	—	—	97.9	10841.63	10426.5	-193.1	97.9	24.62309
169	1	-6.00	—	-0.1	403.05	-12.1	10245.5	-0.1	0.915392
170	2	-6.00	—	-0.5	361.71	-53.5	10286.8	-0.5	0.821502
171	3	-6.00	—	0.0	413.73	-1.4	10234.8	0.0	0.939648
172	1	—	—	85.1	9482.22	9067.0	1166.3	85.1	21.53565
173	2	—	—	97.2	10764	10348.8	-115.5	97.2	24.44678
174	3	—	—	91.6	10170.75	9755.6	477.8	91.6	23.09942
175	1				43740	43324.8			
176	2				44221	43805.8			
177	3				44107	43691.8			
178	1				44713	44297.8			
179	2				43809	43393.8			
180	3				43592	43176.8			

Prism data															
standard curve				weak positive				CR42341				CR42346			
conce ntratio n (log)	Y1-SC	Y2-SC	Y3-SC	conce ntratio n (log)	y1-PC	y2-PC	y3-PC	conce ntratio n (log)	y1-U1	y2-U1	y3-U1	conce ntratio n (log)	y1-U1	y2-U1	y3-U1
-6.0	0.01427	0.29572	0.31967	-3	4.7516	4.8479	4.3828	-3.9	0.9377	0.9610	1.0309	-3.3	-0.2730	-0.1348	-0.8634
-6.0	-0.11391	-0.50214	-0.01362	-4	29.4747	27.2631	29.0155	-4.0	0.7267	0.9395	1.1395	-4.0	0.5543	-0.1374	0.1002
-7.0	3.42011	1.67164	1.11240	-5	75.8756	77.8223	76.3855	-5.0	7.2513	6.8754	7.5598	-5.0	1.0999	0.3456	0.7695
-8.0	13.84368	13.03990	13.72548	-6	95.2107	100.9889	93.6302	-6.0	44.3572	42.1243	38.8404	-6.0	8.8023	7.7566	7.7197
-9.0	60.72688	61.21596	60.97433	-7	93.7175	100.3156	100.3691	-7.0	87.0267	86.3600	89.9758	-7.0	47.1519	47.7313	48.0107
-10.0	72.39790	92.24358	88.58420	-8	87.4180	99.8395	96.4475	-8.0	88.5231	80.3746	101.9146	-8.0	93.0005	90.8811	89.8768
-11.0	96.33382	97.20136	97.87676	-9	103.3160	86.5137	100.0113	-9.0	104.1999	79.2713	102.7123	-9.0	81.0384	97.1228	104.7210
				-10	77.9801	94.7768	93.4160	-10.0	94.7763	97.1373	97.6002	-10.0	101.0092	104.7472	103.3702

CR42347					CR42355					CR42369				
conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1		conce ntratio n (log)	y1-U1	y2-U1	y3-U1	
-3.3					-3.0	0.2190	-0.3039	-0.4634		-3.3	3.8946	3.8318	3.6390	
-4.0	53.4867	44.0748	56.8084		-3.7	16.3540	18.0041	17.5659		-4.0	16.8367	12.3852	16.4294	
-5.0	65.4110	65.3295	72.2087		-4.7	83.5886	86.5260	83.3091		-5.0	85.5333	84.4940	82.1563	
-6.0	98.9801	94.8870	97.8797		-5.7	105.2479	102.5871	102.1621		-6.0	102.8520	106.8054	101.3149	
-7.0	94.9394	104.0340	102.0340		-6.7	102.7734	102.9393	106.4997		-7.0	97.0878	98.5813	100.3804	
-8.0	100.8607	107.1431	103.1082		-7.7	104.6133	101.6671	102.0340		-8.0	99.9990	98.8928	99.5274	
-9.0	105.8622	97.8214	105.1868		-8.7	99.7952	104.1067	104.6599		-9.0	87.5274	93.9903	97.9787	
-10.0	102.6075	96.3920	104.4794		-9.7	105.7778	107.6468	103.7254		-10.0	98.7618	99.0936	95.7137	