Validation data is presented for the quantitation and confirmation ion transitions.

3.0 MATERIALS

Equivalent equipment and materials may be substituted unless otherwise specified. Note any specification in the following descriptions before making substitutions. Substitutions should only be made *if equivalency/suitability has been verified with acceptable control and fortification recovery data.*

3.1 Equipment

Instrumentation

LC system, Agilent 1200 with temperature controlled autosampler (Agilent Technologies, Wilmington, DE)

Mass Spectrometer System, API 5000 triple quadrupole mass spectrometer using a Turbo Ion Spray (Applied Biosystems/MDS Sciex, Foster City, CA)

VWR brand Vortex Geni 2 Mixer, Cat. No. 58815-178 (VWR Scientific Co., Bridgeport, NJ)

Biohit Proline Electronic Pipettors, Variable Volume with Tip Ejector, Vanguard, 5.0-100 µL Cat. No. 53495-200, 50-1000 µL Cat. No. 53495-205 and 0.10-5.0 mL Cat. No. 53495-290 (VWR Scientific Co., Bridgeport, NJ)

Chromatographic Supplies

HPLC Column: 3.0 mm i.d. × 50 mm, MacMod ACE C18-PFP analytical column Part # ACE-1110-0503 (MacMod, Chadds Ford, PA)

HPLC Vials, Target DP Amber Kit, T/S/T Septa, 100 PK, Part # 5182-0556 (Agilent Technologies, Wilmington, DE)

Low Flow Mixer Assembly, Part# 411-0050 (Analytical Scientific Instruments)

Labware

Pyrex Brand Single Metric Scale Graduated Cylinders, 10-mL and 100-mL capacity, Cat. No. 24709-715 and 24709-748, respectively (VWR Scientific Co., Bridgeport, NJ)

VWR brand Disposable Pasteur Pipettes, Borosilicate Glass, 9 in, Cat. No. 53283-914 equipped with 2 mL, 13 X 32 mm rubber bulbs, Cat. No. 56310-240 (VWR Scientific Co., Bridgeport, NJ)

Centrifuge tubes, Polystyrene 50-mL capacity, Cat. No. 21008-939 (VWR Scientific Co., Bridgeport, NJ)

Centrifuge tubes, Polystyrene 15-mL capacity, Cat. No. 21008-930 (VWR Scientific Co., Bridgeport, NJ)

Miscellaneous

6 Port Electrically Actuated Valve, Valco Instruments Co. Inc., PN 1384 (Alltech, Deerfield, IL)

Carbon Steel Balls, 1/4 inch, Catalog No. 00073254 (MSC Industrial Supply, Melville, NY)

Genogrinder : Spex SamplePrep Model number 2000

3.2 *Reagents and Standards*

Equivalent reagents may be substituted for those listed below. To determine if impurities in substituted reagents interfere with analyses, appropriate amounts of the solvents should be taken through the entire method using the chromatographic conditions specified in this report.

Acetone - EM Omni Solv®, HPLC-grade acetone, #AX0116-1 (EM Science, Gibbstown, NJ)

Ammonium Carbonate - Baker Analyzed®, #0650-01 (J. T. Baker Inc., Danvers, MA)

Ethyl Acetate - EM Omni Solv®, HPLC-grade ethyl acetate, #EX0241-1 (EM Science, Gibbstown, NJ)

Formic Acid - Guaranteed Reagent 98% minimum, #FX0440-5 (EM Science, Gibbstown, NJ)

Hexanes - EM Omni Solv®, #HX0296-1 (EM Science, Gibbstown, NJ).

Methanol - EM Omni Solv®, HPLC-grade methanol, #MX0488-1 (EM Science, Gibbstown, NJ)

Water - EM Omni Solv®, HPLC-grade water, #WX0004-1 (EM Science, Gibbstown, NJ)

IN-B5363-000, Purity 100%, prepared by DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company

IN-JW212-002, Purity 93.7%, prepared by DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company

Pyrithiobac sodium – DPX-PE350-4, Purity 98.7%, prepared by DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company

3.3 *Safety and Health*

No unusually hazardous materials are used in this method. All appropriate material safety data sheets should be read and followed, and proper personal protective equipment used. An MSDS sheet for the analytes is available from DuPont Soil Protection, Global Technology Division, E. I. du Pont de Nemours and Company.

4.0 METHOD

4.1 *Principles of the Analytical Method*

Pyrithiobac sodium was extracted from soil samples using a solution of acetone: aqueous ammonium carbonate. The extracts were partitioned using an ethyl acetate: hexane partition. The extracts were diluted and analyzed using reversed phase liquid chromatography (LC) and electrospray mass spectrometry/mass spectrometry (MS/MS).

4.2 *Analytical Procedure*

4.2.1 *Glassware and Equipment Cleaning*

Glassware should be scrubbed with a brush using a laboratory soap solution, rinsed two to five times with tap water, rinsed with distilled or deionized water and finally rinsed with acetone or another suitable solvent and allowed to air dry prior to each use.

4.2.2 *Preparation of Solutions*

The following solutions should be prepared monthly and stored at room temperature unless stated otherwise:

Mobile Phase A : 0.05% aqueous formic acid solution - Add 500 µL of formic acid to 1000 mL of water and mix the resulting solution to homogeneity.

0.1 M Aqueous Ammonium Carbonate Add 9.6 g of ammonium carbonate to a volume of 900 mL of EM science water. Mix the resulting solution to homogeneity and dilute to 1000 mL.

90:10 Acetone: 0.1 M Aqueous Ammonium Carbonate - Combine 900-mL of acetone and 100-mL of 0.1 M aqueous ammonium carbonate. Mix the resulting solution to homogeneity.

50:50 Acetone: 0.1 M Aqueous Ammonium Carbonate - Combine 500-mL of acetone and 500-mL of 0.1 M aqueous ammonium carbonate. Mix the resulting solution to homogeneity.

20:80 Acetone: 0.1 M Aqueous Ammonium Carbonate - Combine 200-mL of acetone and 800-mL of 0.1 M aqueous ammonium carbonate. Mix the resulting solution to homogeneity.

4.2.3 *Preparation and Stability of Stock Standard*

Use Class A volumetric flasks when preparing standard solutions.

Prepare standard stock solutions for IN-B5363, IN-JW212 and pyrithiobac sodium accurately weighing 10 ± 0.01 mg into individual 100-mL volumetric flask using an analytical balance. Record the accurate weight of the standard. Dissolve the standards in approximately 50 mL of HPLC-grade methanol. After dissolving, bring the solution to a volume of 100 mL using HPLC-grade methanol and invert the volumetric flask to mix the solution to homogeneity. The standard solutions are stable for approximately 6 months when stored in a freezer at approximately -20°C immediately after each use. The concentration of each analyte in solution is 100 µg/mL.

4.2.4 *Preparation and Stability of Intermediate and Fortification Standards*

Use Class A volumetric flasks when preparing standard solutions.

Prepare a 1.0-µg/mL IN-B5363, IN-JW212 and pyrithiobac sodium intermediate standard in methanol by pipetting 1.00 mL of each 100.0-µg/mL stock standard into a

100-mL volumetric flask. Dilute the standard to approximately 50-mL with methanol and mix to homogeneity. Bring to volume with methanol and mix to homogeneity.

Prepare a 0.10-µg/mL IN-B5363, IN-JW212 and pyrithiobac sodium standard in methanol by pipetting 1.00 mL of the 1.0-µg/mL standard into a 10-mL volumetric flask. Dilute the standard to approximately 5-mL with methanol and mix to homogeneity. Bring to volume with methanol and mix to homogeneity.

Alternate or additional solutions may be prepared as needed. All standard solutions prepared in with methanol are stable for approximately 6 months if stored in a freezer at approximately -20°C immediately after each use.

4.2.5 *Preparation and Stability of Calibration Standards*

Prepare the calibration standards as showed in the table below. (Alternative or additional standards may be prepared as needed):

Standard Used	Volume Transferred (µL)	Volume of Water Added (µL)	Final Concentration (ng/mL)
0.10 µg/mL	75	925	7.5
0.10 µg/mL	50	950	5.0
0.10 µg/mL	10	990	1.0
7.5 ng/mL	100	900	0.75
5.0 ng/mL	100	900	0.50
1.0 ng/mL	100	900	0.10

During method validation these standard solutions were freshly prepared with each sample set and stored approximately 4°C prior to use. The standards have shown stability for 2 weeks. Each of the calibration standards was vortex mixed for 30 seconds prior to analysis.

4.2.6 *Source of Samples*

Soil control samples were obtained from a field test site located in Chesapeake Farms, Maryland and Toulon, Illinois. The soil characteristics are shown in the following table:

Soil Name	Country	Type	% Clay	% Sand	% Silt	pH_w	OM (%)	Notebook
Sassafras	USA	Sandy Loam	7	58	35	6	1	2004-072
Tama	USA	Silty Clay	42.8	5.2	52	6.5	4.6	2007-018

4.2.7 *Storage and Preparation of Samples*

All samples should be stored frozen at approximately -20°C. Samples were ground in a Hobart Mixer or Cuisinart®. The samples were stored in a -20°C freezer prior to

analysis. Careful and complete grinding is necessary to assure homogeneity. No additional purification was performed prior to sample processing.

4.2.8 *Sample Fortification Procedure*

Fortifications were made directly to the 10.0-g soil sample after weighing the sample. Fortified samples were prepared using a 1.0-µg/mL standard solution.

Fortification Level (mg/kg)	Volume of Standard (mL)
0.0010	0.010
0.010	0.10

4.2.9 *Analyte Extraction and Purification Procedures*

1. Accurately measure 10.0-g (± 1%) of soil sample into a 50-mL plastic centrifuge tubes. Fortify samples if necessary and allow the fortification to dry in a fume hood for approximately 15-minutes. Cap and shake the samples vigorously.
2. Add two 1/4" steel balls and 20-mL of 90:10 acetone: 0.1 M aqueous ammonium carbonate to each sample.
3. Place samples on a genogrinder and homogenize for 3 minutes at a rate of approximately 1200 strokes per minute.
4. Centrifuge the samples for 10 minutes to drive the particulates to the bottom of the tube at a rate of approximately 3000 RPM.
5. Transfer the supernatants into a clean 50-mL centrifuge tubes. Re-extract the samples a second time using 10-mL of 50:50 acetone: 0.1 M aqueous ammonium carbonate. Combining the two extracts into the same 50-mL centrifuge tube.
6. Re-extract the samples a third time using 10-mL of 20:80 acetone: 0.1 M aqueous ammonium carbonate. Combining the three extracts and adjust the volume of the extracts from each sample to 50-mL using 20:80 acetone: 0.1 M ammonium carbonate. Mix the extract using a vortex mixer for approximately 30 seconds.
7. Pipette 10-mL of each extract into a clean glass 14-mL centrifuge tubes. Evaporate the extract to approximately 4-mL nitrogen in an N-Evap at approximately 30°C. Add 1-mL of ethyl acetate and 1-mL of hexane to each sample extract. Mix the extract using a vortex mixer for approximately 30 seconds. Centrifuge the extract for 5 minutes at a rate of approximately 3000 RPM using a pipette discard the upper ethyl acetate: hexane layer.
8. Place the samples on the N-Evap for an additional 15 minutes to remove any ethyl acetate or hexane that might remain after the partition step. The volume should be approximately 3.5-mL.
9. Dilute the extracts to 4-mL using water and mix the extract using a vortex mixer. Transfer an aliquot of each extract into an auto-sampler vial and analyze using LC/MS/MS.

Extracts will be stable for approximately 2 days if stored at 8°C.

4.3 Instrumentation for the Method

4.3.1 Chromatography

Reversed-phase chromatography was used to separate pyrithiobac sodium from co-extracts. A MacMod C18-PFP column was selected. Alternative chromatographic conditions can be used, provided the analytical method is validated and provides acceptable recoveries as defined by regulatory method guidelines.

To accommodate the low flow rate the solvent mixing chamber (Agilent part no. G1312-87330) is replaced with a low flow mixer assembly from Analytical Scientific Instruments (ASI part no. 411-0050). This reduces the volume of the mixing chamber from 450 to 50 microliters.

SYSTEM:	Agilent 1200 HPLC			
COLUMN:	3.0 mm i.d. × 50 mm, MacMod ACE C18-PFP			
COLUMN TEMPERATURE:	40°C			
SAMPLE TEMPERATURE	4°C			
INJECTION VOLUME:	0.025 mL			
FLOW RATE:	0.600 mL/min			
CONDITIONS:	A: 0.05% aqueous formic acid			
	B: Methanol			
	Time	%A	%B	Flow (mL/Min.)
	0.0	90	10	0.60
	2.0	90	10	0.60
	5.0	1	99	0.60
	7.0	1	99	0.60
	8.0	90	10	0.60
	15.0	90	10	0.60
IN-B5363 RETENTION TIME:	2.1 minutes			
IN-JW212 RETENTION TIME:	6.2 minutes			
DPX-PE350 RETENTION TIME:	6.9 minutes			
TOTAL RUN TIME:	15.0 min			

A six-port electronically activated switching valve was used to direct the flow to waste prior to and following the elution of the compounds of interest. The use of this valve reduces source contamination and enables additional samples to be analyzed prior to source cleaning. The valve switching times are given in the following table.

TIME (MINUTES)	COLUMN ELUATE FLOW
0.0-1.2	Waste
1.2-8.2	MS source
8.2-End	Waste

4.3.2 *LC/MS/MS Analysis*

The quantitative analysis of pyrithiobac sodium was performed using an Applied Biosystem API 5000 LC/MS/MS system. Quantitative analysis was based on the integration of a single ion transition. A summary of the experimental conditions is provided in the following table:

Period 1 Analytes	Ions Monitored	Declustering Potential (DP)	Collision Energy (CE)	Exit Potential (CXP)
IN-B5363	**157.1→ 68.0 AMU**	**56**	**31**	**10**
	157.1→ 58.0 AMU	61	33	10
Time:	0-4.0 minutes			
Ion Mode:	Positive			
Turbopray Voltage:	5500 V			
Source Temperatures:	700 C			
CUR:	30			
CAD:	4			
GS1:	40			
GS2:	50			
Dwell	0.15 Seconds			
Period 2 Analyte	**Ions Monitored**	**Declustering Potential (DP)**	**Collision Energy (CE)**	**Exit Potential (CXP**
IN-JW212	**313.0→ 196.0 AMU**	**66**	**39**	**22**
	313.0→ 295.0 AMU	66	21	14
Pyrithiobac Sodium	**327.0→ 308.9 AMU**	**71**	**25**	**22**
	329.0→ 139.1 AMU	71	41	24
	329.0→ 83.0 AMU	71	59	32
Time:	4.0-15.0 minutes			
Ion Mode:	Positive			
Turbospray Voltage:	5500 V			
Source Temperatures:	700 C			
CUR:	30			
CAD:	4			
GS1:	40			
GS2:	50			
Dwell	0.15 Seconds			

A complete list of the experimental parameters is given in Appendix 3. A typical LC/MS and LC/MS/MS full scan spectrum of IN-B5363, IN-JW212 and pyrithiobac sodium is shown in Figure 1.

The instrument was operated in MS/MS-(MRM) positive ion mode for quantitative analysis. Peak area was used for quantitation. **Quantitation was performed using the ion transition displayed in bold face print.** The other transitions were used to confirm any detected residues.

4.3.3 *Calibration Procedure and Sample Analysis*

A 0.050-ng/mL chromatographic standard should be analyzed prior to the start of analyses to establish that the instrument is working properly. If a signal-to-noise ratio of approximately 5-10 to 1 is not attained, the instrument must be tuned or cleaned prior to sample analysis. Operating parameters must be tailored to the particular instrument used, especially if it is to be an alternate vendor's instrument, and should be checked daily. Note that some ion channels other than those used for development of this method may need to be added or eliminated when utilizing this method on other instrumentation. Each ion channel used for sample analysis/quantitation must be checked to insure it is free of interference. The control will be used to demonstrate that baseline interference is less than signal-to-noise 3:1. Begin each sample set by injecting a minimum of 2 calibration standards. The first injection should always be disregarded.

4.4 Calculations

4.4.1 *Methods*

Average Response Factor (RF_{Avg}) was calculated as follows:

$$RF_{Ave} = \frac{(\text{Conc. A} \div \text{Area A}) + (\text{Conc. B} \div \text{Area B}) + (\text{Conc. C} \div \text{Area C}) + (\text{Conc. D} \div \text{Area D}) + (\text{Conc. E} \div \text{Area E})}{\text{Total Number of Standards Injected}}$$

µg/g (ppm) found was calculated as follows:

$$\text{ppm Found} = \frac{(\text{Peak Area}) \times (RF_{Ave}) \times (\textit{Aliquot}\ \text{Factor}) \times (\text{Final Volume})}{(\text{Sample Weight})}$$

In the event a peak was detected in the control, a corrected peak area was used to calculate ppm found for freshly fortified samples. The corrected peak area is the area of the fortified sample minus the area of the control sample.

The percent recovery found was calculated as follows:

$$\%\ \text{Recovery} = \frac{\mu\text{g/g Found}}{\mu\text{g/g Fortified}} \times \frac{100}{1}$$

4.4.2 *Example*

For a Tama soil sample fortified with pyrithiobac sodium at 0.0010 ppm [Date analyzed 18-Feb-13, LOQ 1], the concentration found was calculated as follows:

Average Response Factor was calculated as follows:

$$RF_{Ave} = \frac{\begin{array}{c}(0.10\,ng/mL \div 214000\,AC) + (0.50\,ng/mL \div 1090000\,AC) + (0.75\,ng/mL \div 1600000\,AC) \\ + (1.0\,ng/mL \div 2110000\,AC) + (5.0\,ng/mL \div 8970000\,AC) + (7.5\,ng/mL \div 12000000\,AC)\end{array}}{6}$$

(AC ≡ Area Counts)

$RF_{Avg} = 5.08517e^{-7}$ ng/mL/AC

ng/g (ppb) found was calculated as follows:

$$\text{ppm Found} = \frac{(924000\,AC) \times (5.08517e-7\,ng/mL/AC) \times 5 \times 4.0\,mL)}{(10\,g)}$$

ng/g Found = 0.940 = 0.940 µg/kg

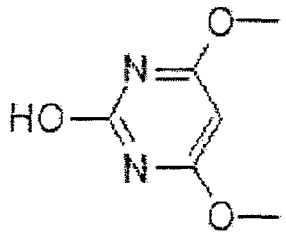
The percent recovery found was calculated as follows:

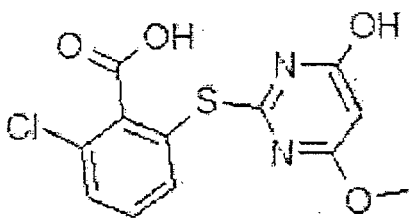
$$\%\,\text{Recovery} = \frac{0.940\,\mu g/kg}{1.0\,\mu g/kg} \times \frac{100}{1}$$

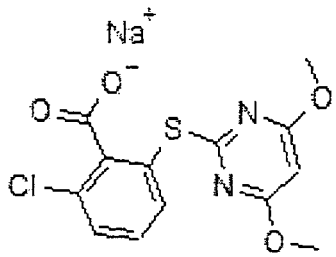
Recovery = 94%

(percent recoveries are rounded to the nearest whole number in Table, without rounding the concentration found)

APPENDIX 1 STRUCTURE OF PYRITHIOBAC SODIUM AND METABOLITES

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-B5363
FORMULA	$C_6H_8N_2O_3$
MOLECULAR WEIGHT	156.14
MONOISOTOPIC WEIGHT	156.05

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-JW212
FORMULA	$C_{12}H_9N_2O_4ClS$
MOLECULAR WEIGHT	313.74
MONOISOTOPIC WEIGHT	311.99

COMMON NAME	PYRITHIOBAC SODIUM
STRUCTURE	
DPX NUMBER	DPX-PE350
FORMULA	$C_{13}H_{10}N_2O_4ClS\text{-}Na$
MOLECULAR WEIGHT	348.74
MONOISOTOPIC WEIGHT	347.99

APPENDIX 3 EXPERIMENTAL CONDITIONS

File Information for Sample 8 (LOQ 1 Soil) of 02182013PE350andMetsInTamaSoilVal2.wiff

File Name: 02182013PE350andMetsInTamaSoilVal2.wiff

File Path: D:\Analyst Data\Projects\11272012PE350InSoil\2012_11_27\Data\

Original Name: 02182013PE350andMetsInTamaSoilVal2.wiff

Software Version:Analyst 1.5.1

Log Information from Devices at Start of acquisition:

AutoSampler	Agilent 1200 G1367B
Firmware Version	A.06.02
Serial Number	DE64555947
Linked Pump G1312A	DE63056839
Injection Volume used	25.00 µl

Time from start =0.0000 min	Pump	Agilent 1200 G1312A
Firmware Version	A.06.02	
Serial Number	DE63056839	

Time from start =0.0000 min	AutoSampler	Agilent 1200 G1367B
Start of Run -	Temperature	
Tray Temperature	4.02 C	

Time from start =0.0000 min	Column Oven	Agilent 1200 G1316A
Firmware Version	A.06.02	
Serial Number	DE63060334	
Switching Valve	Installed	
Time from start =0.0000 min	Mass Spectrometer	API 5000
Config Table Version	01	
Firmware Version	M401402 B4T0301 M3L1417 B3T0300	
Component Name	Triple Quadrupole LC/MS/MS Mass Spectrometer	
Component ID	API 5000	
Manufacturer	AB Sciex Instruments	
Model	API 5000	
Serial Number	AG13130610	
Time from start =0.0000 min	Mass Spectrometer	API 5000
Start of Run -	Detailed Status	
Vacuum Status	At Pressure	
Vacuum Gauge (10e-5 Torr)	1.8	
Backing Pump	Ok	
Interface Turbo Pump	Normal	
Analyzer Turbo Pump	Normal	
Sample Introduction Status	Ready	
Source/Ion Path Electronics	On	

Source Type	Turbo Spray
Source Temperature (at setpoint)	700.0 C
Source Exhaust Pump	Ok
Interface Heater	Ready

Acquisition Info

Acquisition Method:	\01142013PE350InSoilwMets2Period.dam
Acquisition Path:	D:\Analyst Data\Projects\11272012PE350InSoil\2012_11_27\Acquisition Methods\
First Sample Started:	Monday, February 18, 2013 11:14:39 AM
Last Sample Finished:	Tuesday, February 19, 2013 9:58:46 AM
Sample Acq Time:	Monday, February 18, 2013 1:04:51 PM
Sample Acq Duration:	15min0sec
Number of Scans:	0
Periods in File:	2
Batch Name:	\02182013PE350andMetsInTamaSoilVal2.dab
Batch Path:	D:\Analyst Data\Projects\11272012PE350InSoil\2012_11_27\Batch\
Software Version:	Analyst 1.5.1
Set Name:	02182013PE350andMetsInTamaSoilVal2
Sample Name	LOQ 1 Soil
Autosampler Vial:	12

Agilent LC Pump Method Properties

Pump Model: Agilent 1200 Binary Pump

Minimum Pressure (psi):	0.0
Maximum Pressure (psi):	5801.0
Dead Volume (µl):	40.0
Maximum Flow Ramp (ml/min²):	100.0
Maximum Pressure Ramp (psi/sec):	290.0
Max Flow Ramp Up (ml/min²):	100.0
Max Flow Ramp Dn (ml/min²):	100.0

Step Table:

Step	Total Time(min)	Flow Rate(µl/min)	A (%)	B (%)
0	0.00	600	90.0	10.0
1	2.00	600	90.0	10.0
2	5.00	600	1.0	99.0
3	7.00	600	1.0	99.0
4	8.00	600	90.0	10.0
5	15.00	600	90.0	10.0

Left Compressibility:	50.0
Right Compressibility:	115.0
Left Dead Volume (µl):	40.0
Right Dead Volume (µl):	40.0

Left Stroke Volume (µl):	-1.0
Right Stroke Volume (µl):	-1.0
Left Solvent: A2	
Right Solvent: B2	

Agilent Autosampler Properties

Autosampler Model:	Agilent 1200 High Performance Autosampler
Syringe Size (µl):	100
Injection Volume (µl):	25.00
Draw Speed (µl/min):	200.0
Eject Speed (µl/min):	200.0
Needle Level (mm):	0.00
Temperature Control	Enabled
Setpoint (4 - 40 C):	4
Wash is not used	

Automatic Delay Volume Reduction	Not Used
Equilibration Time (sec):	2
Enable Vial/Well Bottom Sensing	No
Use Custom Injector Program	Yes

Contents of Custom Injector Program

1: DRAW def. amount from sample	def. speed	def. offset
2: INJECT		

3: WAIT 1.20 min.
4: CONTACT A CLOSED
5: WAIT 0.10 min.
6: CONTACT A OPEN
7: WAIT 8.00 min.
8: CONTACT B CLOSED
9: WAIT 0.10 min.
10: CONTACT B OPEN

Agilent Column Oven Properties

Left Temperature (°C):	40.00
Right Temperature (°C):	40.00
Temperature Tolerance +/- (°C):	1.00
Start Acquisition Tolerance +/- (°C):	0.50
Time Table (Not Used)	
Column Switching Valve	Installed
Position for first sample in the batch:	Right

Use same position for all samples in the batch

Period 1:

Scans in Period:	775
Relative Start Time:	0.00 msec
Experiments in Period:	1

Period 1 Experiment 1:

Scan Type:	MRM (MRM)
Scheduled MRM:	No
Polarity:	Positive
Scan Mode:	N/A
Ion Source:	Turbo Spray
Resolution Q1:	Unit
Resolution Q3:	Unit
Intensity Thres.:	0.00 cps
Settling Time:	0.0000 msec
MR Pause:	5.0070 msec
MCA:	No
Step Size:	0.00 Da

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
157.116	68.008	150.00	DP	56.00	56.00	IN-B5363
			CE	31.00	31.00	

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
157.116	58.031	150.00	DP	61.00	61.00	IN-B5363
			CE	33.00	33.00	

Parameter Table (Period 1 Experiment 1)

CAD: 4.00
CUR: 30.00
GS1: 40.00
GS2: 50.00
IS: 5500.00
TEM: 700.00
ihe: ON
EP 10.00
CXP 10.00

Period 2:

Scans in Period:	388
Relative Start Time:	4.00 min
Experiments in Period:	1

Period 2 Experiment 1:

Scan Type:	MRM (MRM)
Scheduled MRM:	No
Polarity:	Positive
Scan Mode:	N/A
Ion Source:	Turbo Spray
Resolution Q1:	Unit

Resolution Q3:	*Unit*
Intensity Thres.:	0.00 cps
Settling Time:	0.0000 msec
MR Pause:	5.0070 msec
MCA:	No
Step Size:	0.00 Da

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
313.040	196.025	150.00	DP	66.00	66.00	IN-JW212
			CE	39.00	39.00	
			CXP	14.00	14.00	

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
313.040	295.025	150.00	DP	66.00	66.00	IN-JW212
			CE	21.00	21.00	
			CXP	22.00	22.00	

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
329.044	139.100	150.00	DP	71.00	71.00	DPX-PE350
			CE	41.00	41.00	
			CXP	24.00	24.00	

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
329.044	83.024	150.00	DP	71.00	71.00	DPX-PE350
		CE	59.00	59.00		
		CXP	32.00	32.00		

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start	Stop	ID
327.044	308.952	150.00	DP	71.00	71.00	DPX-PE350
		CE	25.00	25.00		
		CXP	22.00	22.00		

Parameter Table(Period 2 Experiment 1)

CAD: 4.00
CUR: 30.00
GS1: 40.00
GS2: 50.00
IS: 5500.00
TEM: 700.00
ihe: ON
EP 10.00

Resolution tables

Quad 1 Positive Unit

Last Modification Date Time: October 22, 2012 10:34:12

Quad 3 Positive Unit

Last Modification Date Time: October 22, 2012 10:30:13

Calibration tables

Quad 1 Positive Unit Resolution

Last Modification Date Time: October 22, 2012 10:27:30

Quad 3 Positive Unit Resolution

Last Modification Date Time: October 22, 2012 10:30:18

Instrument Parameters:

Detector Parameters (Positive):

CEM 2300.0

DF -400.0

Keyed Text:

File was created with the software version: Analyst 1.5.1