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

3.1.1 *Instrumentation*

LC system, HP1200 with temperature controlled autosampler (Agilent Technologies, Wilmington, DE)

Mass Spectrometer System, API 5000 triple quadrupole mass spectrometer using a Turbo Ion Spray and Analyst version 1.4 software (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)

Evaporator - N-Evap® Model 111 laboratory sample evaporator/nitrogen manifold fitted with Teflon®-coated needles (Organomation Associates, South Berlin, MA). This unit is attached to a dry, clean nitrogen source.

3.1.2 *Solid-Phase Extraction Equipment*

Visiprep 12 port SPE vacuum manifold, PN 5-7030 (Supelco, Bellefonte, PA)

3.1.2.1 *Solid-Phase Extraction Supplies:*

Oasis® HLB cartridge, 0.5g/12cc, PN 186000116 (Waters, Milford, MA) - **Do not substitute**

Solid Phase Extraction Plastic Reservoir – 75-mL size, Catalog No. 1213-1012 (Varian, Harbor City, CA)

Reservoir Adapters – Catalog No. 1213-1003 (Varian, Harbor City, CA)

3.1.3 *Chromatographic Supplies*

HPLC Column: 2.0 mm i.d. × 15 cm, Varian Polaris 3-µm C18-A, analytical column Part # 002001-150X020, Serial #9652004 (Lake Forest, CA)

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)

3.1.4 *Labware*

Wide mouth centrifuge bottle, 125-mL high density, Cat. No. 414004-112 (VWR Scientific Co., Bridgeport, NJ)

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, Pyrex Brand 15-mL capacity, Cat. No. 21048-027 (VWR Scientific Co., Bridgeport, NJ)

Centrifuge tubes, Pyrex Brand Conical Centrifuge Tubes with Standard Taper Stopper, 50-mL capacity, Cat. No. 21048-050 (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)

3.1.5 *Miscellaneous*

Syringe filter - Acrodisc PTFE 0.2 µm, 13-mm diameter Filter Unit, Cat. No. 28143-985 (VWR Scientific Co., Bridgeport, NJ)

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

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.

Acetic Acid - Baker Analyzed® glacial acetic acid, #9524-00 (J. T. Baker, Inc. Danvers, MA)

Ammonium Hydroxide Solution - 28-30%, #AX-1303-13 (EM Science, Gibbstown, NJ)

Acetonitrile (ACN) - EM Omni Solv®, HPLC-grade acetonitrile, #AX0142-1 (EM Science, Gibbstown, NJ)

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)

Phosphoric acid - EM Omni Solv®, #PX0995-6 (EM Science, Gibbstown, NJ)

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

Metsulfuron methyl (DPX-T6376), GLP characterized material used (Dash 265, 98.9% pure) for sample analysis, prepared by DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company

IN-A4098 reference substance (Dash 005, 98.7% pure) used for sample analysis: Analytical standard grade reagent (DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company)

IN-D5119 reference substance (Dash 001, 99.5% pure) used for sample analysis: Analytical standard grade reagent (DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company)

IN-NC148 reference substance (Dash 001, 77.0% pure) used for sample analysis: Analytical standard grade reagent (DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company)

IN-B5685 reference substance (Dash 017, 99.8% pure) used for sample analysis: Analytical standard grade reagent (DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company)

IN-00581 reference substance (product #24093-1, lot number 07028EU, 99.9% pure) used for sample analysis: Analytical standard grade reagent (Sigma-Aldrich)

IN-B5067 reference substance (Dash 005, 89.4% pure) used for sample analysis: Analytical standard grade reagent (DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company)

IN-F5438 reference substance (Dash 002, 97.4% pure) used for sample analysis: Analytical standard grade reagent (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 Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company.

4.0 METHOD

4.1 Principles of the Analytical Method

The analytes were concentrated from the water samples onto a Waters Oasis SPE. The SPE cartridge was washed prior to the elution of the analytes. The eluate volume was reduced under a flow of nitrogen and the final volume was adjusted using aqueous buffer. Detection and quantitative analysis was performed using LC/MS/MS analysis.

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 weekly and stored at room temperature unless stated otherwise:

0.01 M ammonium formate (pH=3.5) - Add 0.63 g of ammonium formate to a volume of 900 mL of EM Science water. Mix the resulting solution to homogeneity and dilute to 1000 mL. Adjust the pH of the solution to 3.5 using concentrated formic acid.

1.0 M ammonium hydroxide. Add 6.9 mL of ammonium hydroxide solution (28-30% NH_3) to a volume of 93.1 mL of EM Science water. Mix the resulting solution to homogeneity.

1:10 (v/v) phosphoric acid solution. Add 10 mL of phosphoric acid into 90 mL of water. Mix the resulting solution to homogeneity.

Solution A - Basic Acetonitrile - Add 20 mL of 1.0 M ammonium hydroxide to 980 mL of acetonitrile and mix the resulting solution to homogeneity. This solution may be prepared monthly.

Injection Solvent -- 0.005 M aqueous ammonium acetate. Add 0.385 g of ammonium acetate to a volume of 900 mL of EM Science water. Mix the resulting solution to homogeneity and dilute to 1000 mL. Adjust the pH of the solution to 6.5 using the 1:10 (v/v) phosphoric acid solution (approximately 1-3 drops will be required).

Mobile Phase A : 0.02 M aqueous formic acid solution - Add 920 µL of formic acid to 1000 mL of water mix the resulting solution to homogeneity.

Mobile Phase B: Methanol

4.2.3 *Preparation and Stability of Stock Standards*

Use Class A volumetric flasks when preparing standard solutions.

Prepare standard stock solutions by accurately weighing 10.00 ± 0.1 mg of each analyte into individual 100-mL volumetric flask using an analytical balance. Record the accurate weight of the standard. Dissolve the standards in approximately 10 mL of HPLC-grade methanol. If the standard does not dissolve add 5 mL of DMSO and place in a sonication bath or for 10-minutes. After dissolving, bring the solutions to a volume of 100 mL using HPLC-grade methanol and invert the volumetric flask to mix the solutions to homogeneity. These standard solutions are stable for approximately 3-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 Fortification Standards*

Use Class A volumetric flasks when preparing standard solutions.

Prepare a 10.0-µg/mL metsulfuron-methyl, IN-A4098, IN-D5119, IN-00581, IN-NC148, IN-B5685, IN-B5067, and IN-F5438 fortification standard in methanol by pipetting 1.00 mL of each of the 100.0-µg/mL stock standards into a 10-mL volumetric flask. Bring to volume using HPLC-grade methanol and mix to homogeneity.

Prepare a 1.0-µg/mL metsulfuron-methyl, IN-A4098, IN-D5119, IN-00581, IN-NC148, IN-B5685, IN-B5067, and IN-F5438 fortification standard in methanol by pipetting 1.00 mL of the 10.0-µg/mL fortification standard into a 10-mL volumetric flask. Bring to volume using HPLC-grade methanol and mix to homogeneity.

Prepare a 0.10-µg/mL metsulfuron-methyl, IN-A4098, IN-D5119, IN-00581, IN-NC148, IN-B5685, IN-B5067, and IN-F5438 fortification standard in methanol by pipetting 1.00 mL of the 1.00-µg/mL fortification standard into a 10-mL volumetric flask. Bring to volume using HPLC-grade methanol and mix to homogeneity.

Alternate or additional solutions may be prepared as needed. All standard solutions prepared in methanol are stable for approximately 3 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 by pipetting volumes of the 1.00-µg/mL and 0.10-µg/mL standard solutions shown in the following table into separate 10.0-mL volumetric flasks (alternative or additional standards may be prepared as needed):

DESIRED STANDARD CONCENTRATION (NG/ML)	VOLUME OF 1.00-µG/ML STANDARD REQUIRED (ML)	VOLUME OF 0.10-µG/ML STANDARD REQUIRED (ML)
15	0.150	-
10	0.100	-
5.0	0.050	-
1.0	-	0.100
0.50	-	0.050
0.25	-	0.025

Add the appropriate amount of injection solution to the volumetric flasks to dilute to 10.00 mL. These standard solutions should be freshly prepared with each sample set and stored approximately 4°C prior to use. Each of the calibration standards was vortexed for 30 seconds prior to injection.

4.2.6 *Source of Samples*

Water control samples were obtained from local water sources. All water sources are provided in the table below. Bottled water was purchased from a local grocery store.

ORIGIN	LOCATION
White Clay Creek	Newark, Delaware
Kemblesville Well	Kemblesville, Pennsylvania
Tap Water	Stine-Haskell Research Center, Newark Delaware

All samples were refrigerated until use. GLP characterization data for the White Clay Creek Water (surface water) is provided in Appendix 5.

4.2.7 *Storage and Preparation of Samples*

Water samples should be stored at approximately 4°C. The water samples were shaken by hand prior to use to ensure homogeneity. No additional filtration or purification was performed prior to sample processing.

4.2.8 *Sample Fortification Procedure*

All fortifications were made directly to the water following the measurement of the sample.

Fortified 100-mL samples were prepared using a 1.00-µg/mL and 0.10-µg/mL fortification standard solution.

Fortification Level (µg/L)	Volume of Standard (mL)	Spiking standards Concentration (µg/mL)
0.050	0.050	0.10
0.50	0.050	1.00

The total amount of acetonitrile applied to the water should be less than 0.50 mL.

4.2.9 *Analyte Extraction and Purification Procedures*

1. Accurately measure 100.0 mL (± 1%) of water into a 125-mL polycarbonate Erlenmeyer flask. Fortify sample if necessary. Cap and shake the samples vigorously.
2. Add 1 mL of 0.01 M ammonium formate (pH=3.5) and 50 µL of concentrated formic acid (98%) to each sample and shake vigorously.
3. Using an adapter, place a 75-mL reservoir above a 20-cc, 0.5-g Oasis HLB cartridge and attach it to an SPE manifold. Precondition the cartridge with 10 mL of methanol, discard the conditioning solution. **Do not let the cartridge go to dryness**. Then condition the cartridge with 10 mL of HPLC grade water. **Do not let the cartridge go to dryness**.
4. Load the sample into the 75-mL reservoir. Using vacuum, pull the sample through the Oasis cartridges at a flow rate of 2-10 mL/min until the flow begins. Once the flow is started remove the vacuum and allow the sample to pass through using a gravity flow. Use vacuum to dry the cartridge for 1 minute. Discard the eluate.
5. Wash the cartridge with 10 mL of hexane. Use vacuum to dry the cartridge for 3 minutes. Discard the eluate.
6. Elute the analytes with 20 mL of Solution A. Load Solution A onto the cartridge, vacuum or positive pressure may be required to start the flow but should be turned off once the flow has started. Once the dripping has stopped, use a small amount of vacuum to empty the remaining liquid in the cartridge into a centrifuge tube. Collect the eluate in a 50-mL centrifuge tube.
7. Adjust the volume of the eluate to 20 mL using Solution A. Transfer a 10-mL aliquot of the extract into a 15-mL centrifuge tube.
8. Evaporate the extract to approximately 3.0 mL using a flow of nitrogen in an N-Evap at approximately 30°C. Pipette 0.250 mL of water into the centrifuge tube and continue evaporating until the volume reaches approximately 0.25 mL. Adjust the final volume to 2.5 mL using the injection solution. Vortex the centrifuge tube and filter an aliquot of the extract using a disposable syringe through a 0.2-µm Acrodisc filter into an HPLC vial. Analyze the solution by LC/MS/MS as described in the following section.

Extracts will be stable for approximately 24 hours if stored at 4°C.

4.3 Instrumentation for the Method

4.3.1 Chromatography

Reversed-phase chromatography was used to separate metsulfuron methyl and metabolites from co-extracts. The column choice reflected experimental results indicating preferred separation from co-extracts. Alternative chromatographic conditions can be used, provided the analytical method is validated and provides acceptable recoveries as defined by regulatory method guidelines.

For this method the HPLC is operating at a flow rate of 0.40 mL/min. To accommodate the low flow rates 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.

The chromatographic condition for the analysis of metsulfuron methyl and metabolites used is presented in the following table.

SYSTEM:	Agilent 1200 HPLC
COLUMN:	2.0 mm i.d. × 15 cm, 3 μm Polaris C18
COLUMN TEMPERATURE:	40°C
SAMPLE TEMPERATURE	8°C
INJECTION VOLUME:	0.025 mL
FLOW RATE:	0.40 mL/min
CONDITIONS:	A: 0.02 M aqueous Formic Acid B: Methanol

Time	%A	%B	Flow (mL/Min.)
0.0	98	2	0.40
1.0	98	2	0.40
3.5	70	30	0.40
12.0	20	80	0.40
12.5	2	98	0.40
15.0	2	98	0.40
15.2	98	2	0.40
25.0	98	2	0.40

ANALYTE:	Approximate Retention time:
IN-A4098 RETENTION TIME:	4.2 minutes
IN-D5119 RETENTION TIME:	6.8 minutes
IN-00581 RETENTION TIME:	7.5 minutes
IN-NC148 RETENTION TIME:	8.5 minutes
IN-B5685 RETENTION TIME:	8.7 minutes
IN-B5067 RETENTION TIME:	9.8 minutes
IN-F5438 RETENTION TIME:	10.3 minutes
DPX-T6576 RETENTION TIME:	12.0 minutes
TOTAL RUN TIME:	25 minutes

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
0.0-3.0	Waste
3.0-13.0	MS source
13.0-End	Waste

4.3.2 *LC/MS/MS Analysis*

The quantitative analysis of metsulfuron methyl and metabolites was performed using an Applied Biosystem API 5000 LC/MS/MS system. Quantitative analysis was based on the integration of a single ion transition. The system parameters were adjusted while a solution of each analyte was infused directly into the ion source. The solution composition was 50% methanol/50% water, so that it would approximate the composition of the mobile phase at the retention time of the analyte. The solution concentration was approximately 2 µg/mL.

A summary of the experimental conditions for the analysis of metsulfuron methyl and metabolites is provided in the following table:

Period 1 Analytes	Ions Monitored	Declustering Potential (DP)	Collision Energy (CE)	Exit Potential (CXP)
IN-A4098	141.0→ 57.3 AMU	81	41	6
Time:	0-5 minutes			
Ion Mode:	Positive			
Turbospray Voltage:	5500 V			
Source Temperatures:	600°C			
CUR:	30			
CAD:	4			
GS1:	40			
GS2:	50			
Dwell	0.150 Seconds			

Period 2 Analyte	Ions Monitored	Degclusterin Potential (DP)	Collision Energy (CE)	Exit Potential (CXP)
IN-D5119	199.85→ 91.9 AMU	-60	-30	-17
IN-00581	181.9→ 42.0 AMU	-195	-56	-17
IN-NC148	341.8→ 181.9 AMU	-90	-30	-31
IN-B5685	257.3→ 42.0 AMU	-55	-52	-13
IN-B5067	366.1→ 125.1 AMU	-85	-24	-27
IN-F5438	366.1→ 155.9 AMU	-95	-28	-9
DPX-T6576	380.0→ 138.8 AMU	-80	-24	-17
Time:	5.0 – 25 minutes			
Ion Mode:	Negative			
Turbospray Voltage:	-4500 V			
Source Temperatures:	600°C			
CUR:	30			
CAD:	4			
GS1:	40			
GS2:	50			
Dwell	0.150** Seconds			

** Dwell for IN-D5119 was increased to 0.300 seconds to increase response

A complete list of the experimental parameters is given in Appendix 4. Additional ion transitions were added for confirmatory analysis, which are also provided in Appendix 4. A typical LC/MS and LC/MS/MS full scan spectrum of each analyte is shown in Figure 1 and Figure 2, respectively.

The instrument was operated in MS/MS-(MRM) positive and negative ion modes for quantitative analysis. Peak area was used for quantitation.

4.3.3 *Calibration Procedure and Sample Analysis*

A 0.25-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 for the least responsive analyte, 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:

$$RF_{Ave} = \frac{(\text{Conc. A} \div \text{Area A}) + (\text{Conc. B} \div \text{Area B}) + (\text{Conc. C} \div \text{Area C})}{3}$$

ppb found was calculated as follows:

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

In the event a peak was detected in the control, a corrected peak area was used to calculate ppb 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:

$$\%\ \text{Recovery} = \frac{(\text{ppb Found})}{(\text{Fortification level})} \text{ x } 100$$

4.4.2 *Example*

For a well water sample fortified with metsulfuron methyl at 0.05 µg/L (0.05 ppb) [Date Extracted 24-March-10, Well LOQ1], the concentration found was calculated as follows:

Average Response Factor was calculated as follows:

$$RF_{Ave} = \frac{\begin{array}{c}(0.25\ ng/mL \div 46700\ AC) + (0.50\ ng/mL \div 86900\ AC) + (1.0\ ng/mL \div 175000\ AC) \\ + (5.0\ ng/mL \div 919001\ AC) + (10.0\ ng/mL \div 1890000\ AC) + (15.0\ ng/mL \div 2730000\ AC)\end{array}}{6}$$

(AC ≡ Area Counts)

$RF_{Avg} = 5.50793e^{-6}$ ng/mL/AC

ppb found was calculated as follows[1]:

$$\text{ppb Found} = \frac{(176000\ AC) \times (5.50793e\text{-}6\ ng/mL/AC) \times (2.5\ mL) \times (2)}{(100\ mL)} \times \frac{1\ \mu g/L}{1\ ng/mL}$$

ppb Found = 0.0484698 µg/L

(ppb values are reported to two significant figures in Table 1 of this report. Rounding was performed using the Microsoft Excel rounding function)

---

1 Aliquot factor was equal to 2 since 10-mL of extract was removed from a 20-mL volume (20 mL/10 mL = 2).

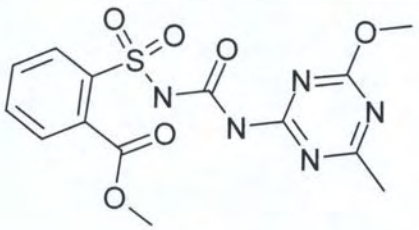
The percent recovery found was calculated as follows:

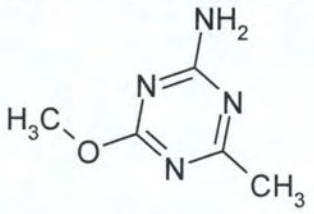
$$\% \text{ Recovery} = \frac{(0.0484698\ \mu g/L)}{(0.050\ \mu g/L)} \text{ x } 100$$

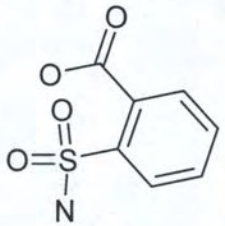
% Recovery = 96.9%

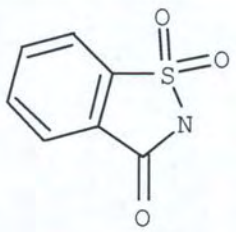
(percent recoveries are rounded to the nearest whole number in Table 1, without rounding the concentration or ppb found)

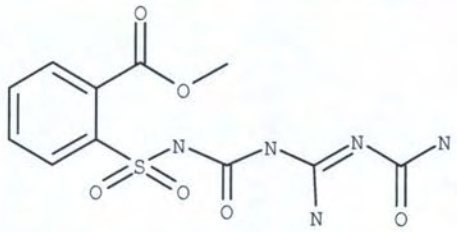
APPENDIX 1 STRUCTURE AND PROPERTIES OF METSULFURON-METHYL AND METABOLITES

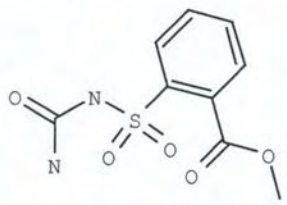
COMMON NAME	Metsulfuron-Methyl
STRUCTURE	
DPX NUMBER	DPX-T6376
TRADE NAMES	Ally, Escort
CAS CHEMICAL NAME	Methyl 2-[[[[(4-methoxy-6-methyl-1,2,3-triazin-2-yl)amino]carbonyl]amino]sulfonyl]benzoate
CAS NUMBER	74223-64-6
FORMULA	$C_{14}H_{15}N_5O_6S$
MOLECULAR WEIGHT	381.37
MONOISOTOPIC WEIGHT	381.07
PKA	3.3

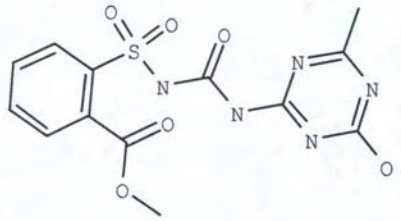
COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-A4098
FORMULA	$C_5H_8N_4O$
MOLECULAR WEIGHT	140.15
MONOISOTOPIC WEIGHT	140.07

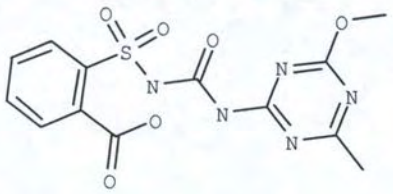
COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-D5119
FORMULA	$C_7H_7NO_4S$
MOLECULAR WEIGHT	201.20
MONOISOTOPIC WEIGHT	201.01

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-00581
FORMULA	$C_7H_5NO_3S$
MOLECULAR WEIGHT	183.19
MONOISOTOPIC WEIGHT	182.99

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-NC148
FORMULA	$C_{11}H_{13}N_5O_6S$
MOLECULAR WEIGHT	343.32
MONOISOTOPIC WEIGHT	343.06

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-B5685
FORMULA	$C_9H_{10}N_2O_5S$
MOLECULAR WEIGHT	258.25
MONOISOTOPIC WEIGHT	258.03

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-B5067
FORMULA	$C_{13}H_{13}N_5O_6S$
MOLECULAR WEIGHT	367.34
MONOISOTOPIC WEIGHT	367.06

COMMON NAME	None
STRUCTURE	
DPX NUMBER	IN-F5438
FORMULA	$C_{13}H_{13}N_5O_6S$
MOLECULAR WEIGHT	367.34
MONOISOTOPIC WEIGHT	367.06