UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF PESTICIDE PROGRAMS
ENVIRONMENTAL CHEMISTRY LABORATORY
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December 12, 2006

MEMORANDUM

SUBJECT: XDE-742 (DP# 332342)

FROM: Joseph Ferrario, Branch Chief
BEAD/Environmental Chemistry Laboratory

TO: Cara Dzubow ECM Gatekeeper
EISB 7507P

The EFED/Environmental Fate and Effects Division has requested an Environmental Chemistry Method Review on XDE-742 and its metabolites in water using the method submitted by Dow AgroSciences LLC in accordance with the registration of the above mentioned analyte and its degradates, MRID No.469085-01. The method and independent laboratory validation data was reviewed and the conclusions included in the attached Environmental Chemistry Method Review Report.

The following report includes an overview of the method and the method completeness, statements of adherence to EPA regulations, a presentation of results and a discussion of problems found in the registrant method and those discovered by the independent laboratory. A statement of method acceptability is also included.

If you have any questions concerning this report, please contact Elizabeth Flynt at (228) 688-2410 or me at (228) 688-3212.

Attachments
cc: Dr. Christian Byrne, QA Officer
BEAD/Environmental Chemistry Laboratory

Elizabeth C. Flynt
BEAD/ECL

XDE-742 in water/108702/DowAgroSciences LLC/62719

ENVIRONMENTAL CHEMISTRY METHOD REVIEW REPORT

Data Requirement: PMRA Data Code: NA
EPA DP Barcode 332342
OECD Data Point: NA
EPA Guideline: ECM Method Review

Test material:
Common name: XDE-742
Chemical name: XDE-742, 7-OH-XDE-742, ADTP metabolite of XDE-742, ATSA metabolite, sulfinic acid metabolite, and sulfonic acid metabolite.
IUPAC: See Appendix A

Primary Evaluator: Elizabeth Flynt **Date:** 11/17/06
Elizabeth Flynt, Chemist

Peer Reviewer: Charles Kennedy **Date:** 12/06/06
Charles Kennedy, Chemist

QA Officer: Christian Byrne **Date:** 12/06/06
Dr. Christian Byrne, QA Officer

ANALYTICAL METHOD: 469085-01, D.D. Shackelford, February 15, 2006, "*Determination of Residues of XDE-742 and its Metabolites in Drinking Water, Ground Water, and Surface Water by Liquid Chromatography with Tandem Mass Spectrometry.*" The unpublished study was conducted by the Indianapolis Regulatory Laboratories of Dow AgroSciences LLC of 9330 Zionsville Road, Indianapolis, Indiana 46268-1054. Pages 1 -100. The study is Dow AgroSciences No. 051039.

EXECUTIVE SUMMARY

The method is applicable for the quantitative determination of residues of XDE-742 and its five major metabolites in drinking water, ground water, and surface water. The method was created by DowAgroSciences LLC in Indianapolis, Indiana in accordance with EPA's Good Laboratory Practice Standards, Title 40 Code of Federal Regulations Part 160. An independent laboratory validation was submitted with this method. It was entitled, "*Independent Laboratory Validation of Dow AgroSciences LLC Method GRM 05.19-Determination of Residues of XDE-742 and its Metabolites in Drinking Water, Ground Water, and Surface Water by Liquid Chromatography with Tandem Mass Spectrometry Detection.*" The laboratory that performed the validation was PTRL of Europe GmbH of Ulm, Germany. The independent validation was for the parent XDE-742 only. After a thorough review, the ECB finds this method and its validation data acceptable for the parent only, due to the omission of an independent validation for the degradates.

Method Summary: Residues of XDE-742 and its metabolites are analyzed without need for prior extraction, concentration or cleanup. The parent compound, XDE-742 and its 7-OH-XDE-742, ADTP and ATSA metabolites are analyzed directly by liquid

chromatography with positive-ion electrospray tandem mass spectrometry (LC/MS/MS). The XDE-742 sulfinic acid and sulfonic acid metabolites are analyzed by liquid chromatography with negative-ion electrospray tandem mass spectrometry.

METHOD ACCEPTABILITY/DEFICIENCIES/CLARIFICATIONS

This method and independent laboratory validation are presented in a very complete package. Almost all elements requested in the OPPTS Harmonized Guidelines are present with one exception. The ILV validation of the method was performed only for the parent compound, XDE-742, not for the degradates. Based on the parameters set in the Ecological Effects Test Guidelines, OPPTS 850.7100, Data Reporting for Environmental Chemistry Methods; "Public Draft." (U.S. Environmental Protection Agency. Office of Prevention, Pesticides, and Toxic Substances (7101). U.S. Government Printing Office: Washington, DC, 1996, EPA-712-C-96-348) ECB finds this method acceptable as submitted for the parent XDE-742 only.

COMPLIANCE

Signed and dated statements that this method was conducted in accordance with the requirements for Good Laboratory Practice Standards, 40 CFR 160 were present in the method. Also present was a statement of non-confidentiality on the basis of the method falling within the scope of FIFRA Section 10 (d)(1)(A), (B), or (C).]

A. BACKGROUND INFORMATION

XDE-742 is a technical herbicide with the active ingredient pyroxsulam. It has been submitted to EPA for registration for use in the control of annual grass and broadleaf weeds in winter wheat.

TABLE A.1. Test Compound Nomenclature

Compound XDE-742	Chemical Structure * See Appendix A
Common name	XDE-742
Company experimental name	XDE-742
IUPAC name	N-(5,7-dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide
CAS Name	*N*-(5,7-dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide
CAS #	422556-08-9

MATERIALS AND METHODS

B.1. Principle of Method

The Dow AgroScience method for XDE-742 utilizes direct injection of the fortified water sample on a liquid chromatograph with tandem mass spectrometery using positive and negative electrospray. Prior to analysis, AmQuel+Plus is added to the water samples to stabilize residues prior to analysis.

TABLE B.1.1.	**Summary Parameters for the Analytical Method Used for the Quantitation of Chemical Residues in Matrices Studied**
Method ID	ECM0227W1-W6
Analyte(s)	XDE-742, 7-OH-XDE-742, ADTP metab., ATSA metab., sulfinic acid metab., sulfonic acid metab.
Extraction solvent/technique	Fortify 9 ml of water sample plus 100 µl of AmQuel+Plus and dilute with 1 ml of acetonitrile.
Cleanup strategies	None
Instrument/Detector	Spark Holland Pharma MDS//Sciex API 4000 LC/MS/MS System,

C. RESULTS AND DISCUSSION

C.1. Recovery Results Summary

TABLE C.1.1. Recovery Results from Method Validation of [matrices]

Matrix	Spiking Level (conc. units)	% Recoveries	Relative Standard Deviation
*	*	*	*

* See Appendix B

C.1.2. Method Characteristics

TABLE C.1.2. Method Characteristics

Analyte	XDE-742 (Pyroxsulam)
Limit of Quantitation	0.05 µg/L
Limit of Detection (LOD)	0.015 µg/L
Accuracy/Precision at LOQ	See Appendix B
Reliability of the Method/ [ILV]	The independent laboratory validated the method successfully
Linearity	All analytes displayed linearity over the test range 0.015 to 10 ng/ml. The coefficient of variations in all analytes ranged from 0.9972 to 0.9999
Specificity	The method is very specific for all analytes by nature of the method of detection (LC/MS/MS).

C.2. Independent Laboratory Validation (ILV)

The ILV was conducted in accordance with the *OPPTS 850.7100 Guidelines.*

TABLE C.2.1. Recovery Results Obtained by an Independent Laboratory Validation of the Method for the Determination of XDE-742 in Water

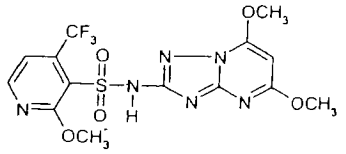
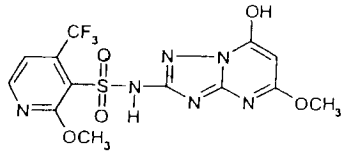
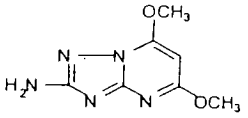
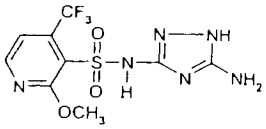
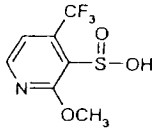
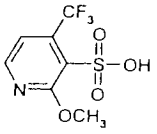
		Drinking Water		Surface Water	
		XDE-742, 435 m/z ->		XDE-742, 435 m/z ->	
		195 m/z	82 m/z	195 m/z	82 m/z
LOQ 0.05 µg/L	Average (n =5)	81%	80%	81%	84%
	RSD (n = 5)	6%	5%	7%	8%
	CI (n=5, P=95%)	6%	5%	7%	9%
10xLOQ 0.5 µg/L	Average (n =5)	105%	102%	96%	97%
	RSD (n = 5)	8%	9%	2%	1%
	CI (n=5, P=95%)	11%	11%	2%	2%

RSD: Relative standard deviation CI: Confidence interval

D. CONCLUSION

The method presented has been thoroughly studied and validated by both the registrant and the independent laboratories. It was validated in a number of different matrices successfully. ECB considers it acceptable to support the registration studies that it was used for.

Appendix A . Identity and Structures of XDE-742 and Its Metabolites

Common Name of Compound	Structural Formula and Chemical Name (IUPAC)
XDE-742 Molecular Formula: $C_{14}H_{13}F_3N_6O_5S$ Formula Weight: 434.4 g/mole Nominal Mass: 434 CAS Number 422556-08-9	 *N*-(5,7-dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide
7-OH-XDE-742 Molecular Formula: $C_{13}H_{11}F_3N_6O_5S$ Formula Weight: 420.3 g/mole Nominal Mass: 420 CAS Number NA	 *N*-(7-hydroxy-5-methoxy[1,2,4]triazolo[1,5-*a*]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide
ADTP metabolite of XDE-742 Molecular Formula: $C_7H_9N_5O_2$ Formula Weight: 195.2 g/mole Nominal Mass: 195 CAS Number NA	 5,7-dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-amine
ATSA metabolite of XDE-742 Molecular Formula: $C_9H_9F_3N_6O_3S$ Formula Weight: 338.27 g/mol Nominal Mass: 338 CAS Number NA	 *N*-(5-amino-1H-1,2,4-triazol-3-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide
sulfinic acid metabolite of XDE-742 Molecular Formula: $C_7H_6F_3NO_3S$ Formula Weight: 241.19 g/mol Nominal Mass: 241 CAS Number NA	 2-methoxy-4-(trifluoromethyl)pyridine-3-sulfinic acid
sulfonic acid metabolite of XDE-742 Molecular Formula: $C_7H_6F_3NO_4S$ Formula Weight: 257.19 g/mol Nominal Mass: 257 CAS Number NA	 2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonic acid

Appendix B. - LODs, LOQs, and Recoveries

Calculated Limits of Detection and Quantitation for the Determination of XDE-742 (Quantitation Ion, Q1/Q3 *m/z* 435.1/195.1) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0462	0.0010	0.0031	0.0105	6
ground water	0.050	0.0464	0.0011	0.0033	0.0110	6
surface water	0.050	0.0479	0.0024	0.0072	0.0240	6

Calculated Limits of Detection and Quantitation for the Determination of XDE-742 (Confirmation Ion, Q1/Q3 *m/z* 435.1/82.0) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0482	0.0029	0.0086	0.0285	6
ground water	0.050	0.0479	0.0019	0.0057	0.0189	6
surface water	0.050	0.0491	0.0017	0.0051	0.0171	6

Calculated Limits of Detection and Quantitation for the Determination of 7-OH-XDE-742 (Quantitation Ion, Q1/Q3 *m/z* 420.9/181.0) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0525	0.0016	0.0049	0.0164	6
ground water	0.050	0.0458	0.0018	0.0053	0.0176	6
surface water	0.050	0.0502	0.0039	0.0116	0.0385	6

Calculated Limits of Detection and Quantitation for the Determination of 7-OH-XDE-742 (Confirmation Ion, Q1/Q3 *m/z* 420.9/148.1) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0496	0.0036	0.0107	0.0356	6
ground water	0.050	0.0485	0.0033	0.0100	0.0333	6
surface water	0.050	0.0520	0.0024	0.0071	0.0236	6

Calculated Limits of Detection and Quantitation for the Determination of ADTP (Quantitation Ion, Q1/Q3 *m/z* 196.2/115.1) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0486	0.0023	0.0070	0.0232	6
ground water	0.050	0.0471	0.0018	0.0054	0.0180	6
surface water	0.050	0.0481	0.0030	0.0089	0.0298	6

Calculated Limits of Detection and Quantitation for the Determination of ADTP (Confirmation Ion, Q1/Q3 *m/z* 196.2/163.9) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0473	0.0030	0.0089	0.0296	6
ground water	0.050	0.0451	0.0028	0.0084	0.0279	6
surface water	0.050	0.0494	0.0029	0.0087	0.0289	6

Calculated Limits of Detection and Quantitation for the Determination of ATSA (Quantitation Ion, Q1/Q3 *m/z* 339.0/99.1) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0558	0.0010	0.0029	0.0095	6
ground water	0.050	0.0565	0.0021	0.0063	0.0211	6
surface water	0.050	0.0559	0.0029	0.0086	0.0288	6

Calculated Limits of Detection and Quantitation for the Determination of ATSA (Confirmation Ion, Q1/Q3 *m/z* 339.0/57.2) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0523	0.0056	0.0169	0.0565	6
ground water	0.050	0.0542	0.0049	0.0148	0.0495	6
surface water	0.050	0.0516	0.0052	0.0155	0.0515	6

Calculated Limits of Detection and Quantitation for the Determination of Sulfinic Acid (Quantitation Ion, Q1/Q3 *m/z* 239.9/175.8) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0475	0.0034	0.0102	0.0340	6
ground water	0.050	0.0463	0.0033	0.0100	0.0332	6
surface water	0.050	0.0471	0.0034	0.0101	0.0338	6

Calculated Limits of Detection and Quantitation for the Determination of Sulfinic Acid (Confirmation Ion, Q1/Q3 *m/z* 239.9/155.7) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0435	0.0043	0.0130	0.0434	6
ground water	0.050	0.0398	0.0023	0.0070	0.0235	6
surface water	0.050	0.0464	0.0039	0.0118	0.0394	6

Calculated Limits of Detection and Quantitation for the Determination of Sulfonic Acid (Quantitation Ion, Q1/Q3 *m/z* 255.7/149.0) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0444	0.0054	0.0161	0.0535	6
ground water	0.050	0.0433	0.0046	0.0137	0.0455	6
surface water	0.050	0.0461	0.0036	0.0108	0.0361	6

Calculated Limits of Detection and Quantitation for the Determination of Sulfonic Acid (Confirmation Ion, Q1/Q3 *m/z* 255.7/79.7) in Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (µg/L)	Standard Deviation (*s*)	Limit of Detection (3*s*)	Limit of Quantitation (10*s*)	Number of Samples (n)
drinking water	0.050	0.0531	0.0045	0.0134	0.0445	6
ground water	0.050	0.0467	0.0069	0.0206	0.0687	6
surface water	0.050	0.0467	0.0075	0.0225	0.0751	6

Recovery Summary of the XDE-742 (Quantitation Ion, Q1/Q3 *m/z* 435.1/195.1) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	92	89 - 94	2.1	2.3	6
	5.00	100	98 - 103	1.9	1.9	6
	0.050 - 5.00	96	89 - 103	4.3	4.5	12
ground water	0.050	93	89 - 96	2.2	2.4	6
	5.00	99	97 - 101	1.4	1.4	6
	0.050 - 5.00	96	89 - 101	3.8	4.0	12
surface water	0.050	96	90 - 102	4.8	5.0	6
	5.00	100	95 - 104	3.1	3.1	6
	0.050 - 5.00	98	90 - 104	4.5	4.6	12

Recovery Summary of the XDE-742 (Confirmation Ion, Q1/Q3 *m/z* 435.1/82.0) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation, (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	96	88 - 105	5.7	5.9	6
	5.00	96	94 - 98	1.7	1.7	6
	0.050 - 5.00	96	88 - 105	4.0	4.2	12
ground water	0.050	96	92 - 101	3.8	4.0	6
	5.00	95	94 - 97	1.2	1.3	6
	0.050 - 5.00	96	92 - 101	2.7	2.8	12
surface water	0.050	98	94 - 102	3.4	3.5	6
	5.00	96	92 - 100	3.2	3.3	6
	0.050 - 5.00	97	92 - 102	3.4	3.5	12

Recovery Summary of the 7-OH-XDE-742 (Quantitation Ion, Q1/Q3 *m/z* 420.9/181.0) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	105	100 - 110	3.3	3.1	6
	5.00	101	99 - 104	2.1	2.1	6
	0.050 - 5.00	103	99 - 110	3.3	3.2	12
ground water	0.050	92	87 - 96	3.5	3.8	6
	5.00	99	97 - 101	1.7	1.8	6
	0.050 - 5.00	95	87 - 101	4.7	4.9	12
surface water	0.050	100	92 - 108	7.7	7.7	6
	5.00	105	99 - 113	6.1	5.8	6
	0.050 - 5.00	103	92 - 113	7.1	6.9	12

Recovery Summary of the 7-OH-XDE-742 (Confirmation Ion, Q1/Q3 *m/z* 420.9/148.1) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	99	91 - 108	7.1	7.2	6
	5.00	101	98 - 104	2.2	2.2	6
	0.050 - 5.00	100	91 - 108	5.1	5.1	12
ground water	0.050	97	88 - 106	6.7	6.9	6
	5.00	100	97 - 101	1.6	1.6	6
	0.050 - 5.00	98	88 - 106	4.8	4.9	12
surface water	0.050	104	98 - 110	4.7	4.5	6
	5.00	105	99 - 113	6.0	5.7	6
	0.050 - 5.00	104	98 - 113	5.2	4.9	12

Recovery Summary of the ADTP (Quantitation Ion, Q1/Q3 *m/z* 196.2/115.1) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	97	88 - 101	4.6	4.8	6
	5.00	100	96 - 104	3.4	3.4	6
	0.050 - 5.00	99	88 - 104	4.1	4.2	12
ground water	0.050	94	90 - 100	3.6	3.8	6
	5.00	98	94 - 100	1.9	2.0	6
	0.050 - 5.00	96	90 - 100	3.3	3.4	12
surface water	0.050	96	88 - 102	6.0	6.2	6
	5.00	101	97 - 105	3.3	3.3	6
	0.050 - 5.00	99	88 - 105	5.4	5.4	12

Recovery Summary of the ADTP (Confirmation Ion, Q1/Q3 *m/z* 196.2/163.9) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	95	85 - 103	5.9	6.2	6
	5.00	100	97 - 104	3.4	3.4	6
	0.050 - 5.00	97	85 - 104	5.4	5.6	12
ground water	0.050	90	83 - 97	5.6	6.2	6
	5.00	98	94 - 100	2.5	2.6	6
	0.050 - 5.00	94	83 - 100	5.6	6.0	12
surface water	0.050	99	90 - 105	5.8	5.9	6
	5.00	100	95 - 103	2.9	2.9	6
	0.050 - 5.00	99	90 - 105	4.4	4.4	12

Recovery Summary of the ATSA (Quantitation Ion., Q1/Q3 *m/z* 339.0/99.1) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	112	109 - 114	1.9	1.7	6
	5.00	99	96 - 100	1.6	1.6	6
	0.050 - 5.00	105	96 - 114	7.0	6.7	12
ground water	0.050	113	109 - 118	4.2	3.7	6
	5.00	98	96 - 100	1.1	1.1	6
	0.050 - 5.00	105	96 - 118	8.5	8.0	12
surface water	0.050	112	106 - 119	5.8	5.1	6
	5.00	98	93 - 101	2.9	3.0	6
	0.050 - 5.00	105	93 - 119	8.5	8.1	12

Recovery Summary of the ATSA (Confirmation Ion, Q1/Q3 *m/z* 339.0/57.2) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	105	90 - 119	11.3	10.8	6
	5.00	97	94 - 100	2.6	2.7	6
	0.050 - 5.00	101	90 - 119	8.8	8.7	12
ground water	0.050	108	92 - 118	9.9	9.1	6
	5.00	97	95 - 98	1.1	1.1	6
	0.050 - 5.00	103	92 - 118	9.1	8.9	12
surface water	0.050	103	89 - 117	10.3	10.0	6
	5.00	96	91 - 100	3.0	3.1	6
	0.050 - 5.00	100	89 - 117	8.1	8.1	12

Recovery Summary of the Sulfinic Acid (Quantitation Ion, Q1/Q3 *m/z* 239.9/175.8) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	95	83 - 101	6.8	7.1	6
	5.00	95	90 - 100	3.5	3.7	6
	0.050 - 5.00	95	83 - 101	5.1	5.4	12
ground water	0.050	93	84 - 102	6.6	7.2	6
	5.00	92	86 - 101	5.1	5.5	6
	0.050 - 5.00	92	84 - 102	5.6	6.1	12
surface water	0.050	94	84 - 102	6.8	7.2	6
	5.00	94	87 - 101	6.2	6.6	6
	0.050 - 5.00	94	84 - 102	6.2	6.6	12

Recovery Summary of the Sulfinic Acid (Confirmation Ion, Q1/Q3 *m/z* 239.9/155.7) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	87	79 - 101	8.7	10.0	6
	5.00	91	88 - 93	1.8	2.0	6
	0.050 - 5.00	89	79 - 101	6.4	7.1	12
ground water	0.050	80	71 - 84	4.7	5.9	6
	5.00	93	88 - 97	3.3	3.6	6
	0.050 - 5.00	86	71 - 97	8.0	9.3	12
surface water	0.050	93	84 - 106	7.9	8.5	6
	5.00	89	81 - 95	4.5	5.1	6
	0.050 - 5.00	91	81 - 106	6.5	7.1	12

Recovery Summary of the Sulfonic Acid (Quantitation Ion, Q1/Q3 *m/z* 255.7/149.0) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	89	77 - 107	10.7	12.1	6
	5.00	93	89 - 98	3.5	3.7	6
	0.050 - 5.00	91	77 - 107	8.0	8.7	12
ground water	0.050	87	72 - 100	9.1	10.5	6
	5.00	94	89 - 98	3.2	3.4	6
	0.050 - 5.00	90	72 - 100	7.4	8.2	12
surface water	0.050	92	83 - 99	7.2	7.8	6
	5.00	92	87 - 98	4.5	4.9	6
	0.050 - 5.00	92	83 - 99	5.7	6.2	12

Recovery Summary of the Sulfonic Acid Confirmation Ion, Q1/Q3 *m/z* 255.7/79.7) from Water

Sample Matrix	Fortification Level (µg/L)	Average Recovery (Percent)	Recovery Range (Percent)	Standard Deviation (Percent)	Relative Std. Dev. (Percent)	Number of Samples (n)
drinking water	0.050	106	94 - 116	8.9	8.4	6
	5.00	95	91 - 98	2.7	2.9	6
	0.050 - 5.00	101	91 - 116	8.5	8.5	12
ground water	0.050	93	72 - 113	13.7	14.7	6
	5.00	93	91 - 95	1.6	1.7	6
	0.050 - 5.00	93	72 - 113	9.3	10.0	12
surface water	0.050	93	76 - 114	15.0	16.1	6
	5.00	95	91 - 100	3.6	3.8	6
	0.050 - 5.00	94	76 - 114	10.5	11.1	12