Supporting information for

Identification of Degradation Products of Sea-Dumped Chemical Warfare Agent-Related Phenylarsenic Chemicals in Marine Sediment

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TABLE OF Contents

Table of Contents 1

Table S-1 List of current target phenylarsenic CWAs in sediment analysis 2

Table S-2 Concentrations of current target chemicals detected in sediment samples quantitated in CHEMSEA, MODUM and DAIMON projects. 3

Figure S-1 Total ion chromatogram for sediment sample #1 3

Figure S-2 Extracted ion chromatograms for sediment sample #6 containing methylated phenylarsenicals and target chemicals 4

Figure S-3 Total ion chromatogram and spectrum for diphenylthioarsinic acid 5

Figure S-4 Total ion chromatogram and spectrum for methyldiphenylarsine sulfide 5

Figure S-5 Total ion chromatogram and spectrum for 10-methyl-5H-phenarsazinine-10-sulfide 6

Figure S-6 Total ion chromatogram and spectrum for dimethylphenylarsine sulfide 6

Figure S-7 Total ion chromatogram and spectrum for triphenylarsine sulfide 7

Table S-3 Detected fragments and their relative abundance for all detected sulfur containing chemicals 8

Figure S-8 Extracted ion chromatogram for sediment sample #8 containing sulfur-containing phenylarsenic chemicals and target chemicals 9

Figure S-9 Extracted ion chromatogram for sediment sample #8 containing sulfur-containing phenylarsenic chemical and target chemical 10

Figure S-10 Spectrum for hydroxyphenarsazinic acid 10

Figure S-11 Extracted ion chromatogram and spectra for two isomers of hydroxydiphenylarsinic acid 11

Figure S-12 Extracted ion chromatogram and spectra for two isomers of hydroxytriphenylarsine oxide 12

TABLE S-1 LIST OF CURRENT TARGET PHENYLARSENIC CWAS IN SEDIMENT ANALYSIS

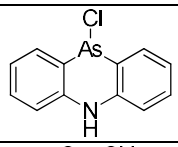
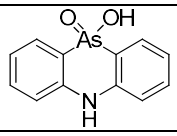
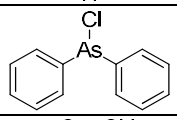
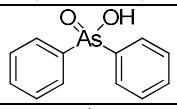
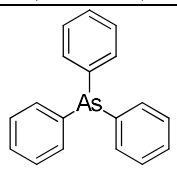
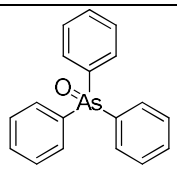
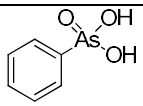
Chemical (acronym)	Structure
Adamsite (DM)	
5,10-Dihydrophen-arsazin-10-ol 10-oxide	
Clark I (DA)	
Diphenylarsinic acid (DPA)	
Triphenylarsine (TPA)	
Triphenylarsine oxide (TPAO)	
Phenylarsonic acid (PAA)	

TABLE S-2 CONCENTRATIONS OF CURRENT TARGET CHEMICALS DETECTED IN SEDIMENT SAMPLES QUANTITATED IN CHEMSEA, MODUM AND DAIMON PROJECTS.

		concentration [µg/kg] in dry in weight			
Sample ID	**Project**	**DMox**	**DPA**	**TPAO**	**PAA**
#1	CHEMSEA	22	1300	190	N.A.*
#2	CHEMSEA	5.2	1300	180	N.A.*
#3	CHEMSEA	30	210	67	N.A.*
#4	MODUM	3.4	15	1900	120
#5	MODUM	N.D.**	N.D.**	N.D.**	N.D.**
#6	DAIMON	79 ± 30	120	300	180
#7	DAIMON	N.D.**	N.D.**	N.D.**	N.D.**
#8	DAIMON	12	83	310	246
#9	DAIMON	151	1100	195	2641
#10	CHEMSEA	37	2104	310	37
#11	CHEMSEA	9.2	2302	321	9.2
#12	CHEMSEA	53	369	121	53
#13	DAIMON	13	86	321	255
#14	DAIMON	144	95	138	191

*N.A. = not analysed, N.D. = not detected

FIGURE S-1 TOTAL ION CHROMATOGRAM FOR SEDIMENT SAMPLE #1

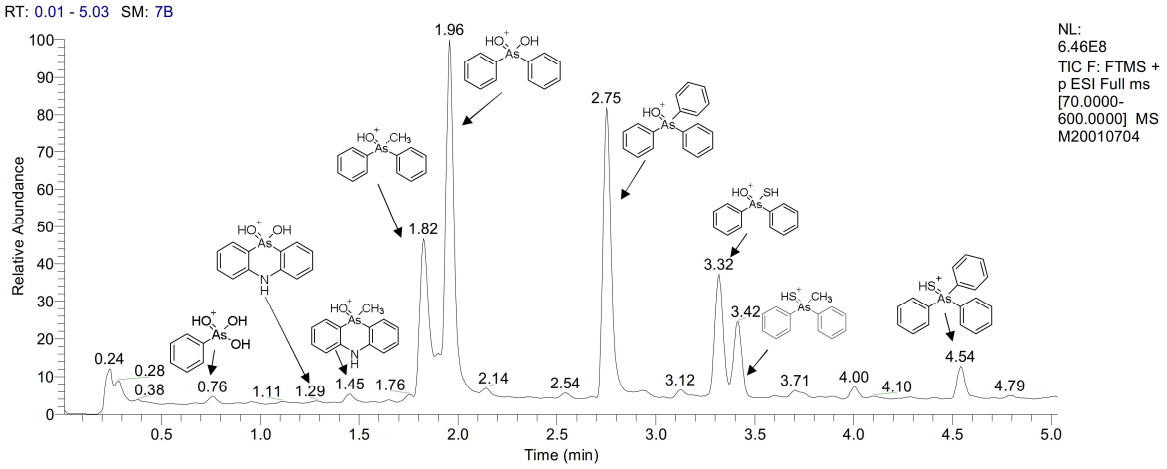
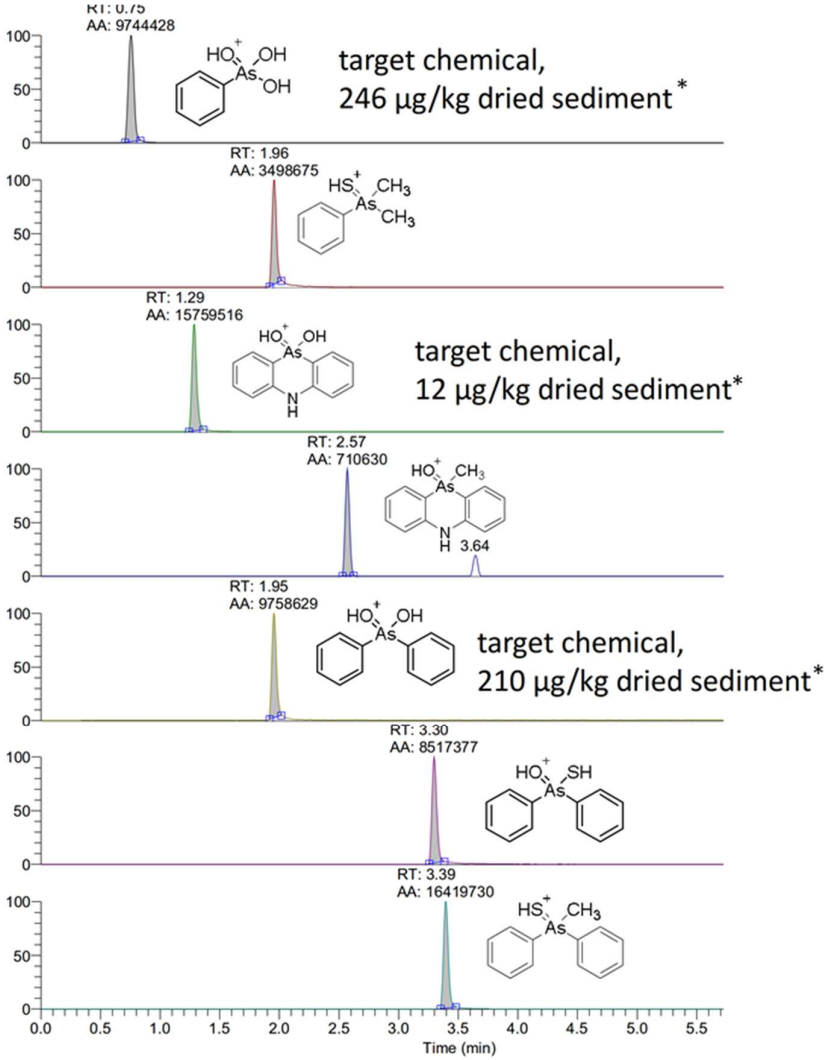


FIGURE S-2 EXTRACTED ION CHROMATOGRAMS FOR SEDIMENT SAMPLE #6 CONTAINING METHYLATED PHENYLARSENICALS AND TARGET CHEMICALS



* Concentrations of target chemicals have been quantified previously using LC-MS/MS method from the same sediment sample.

FIGURE S-3 TOTAL ION CHROMATOGRAM AND SPECTRUM FOR DIPHENYLTHIOARSINIC ACID

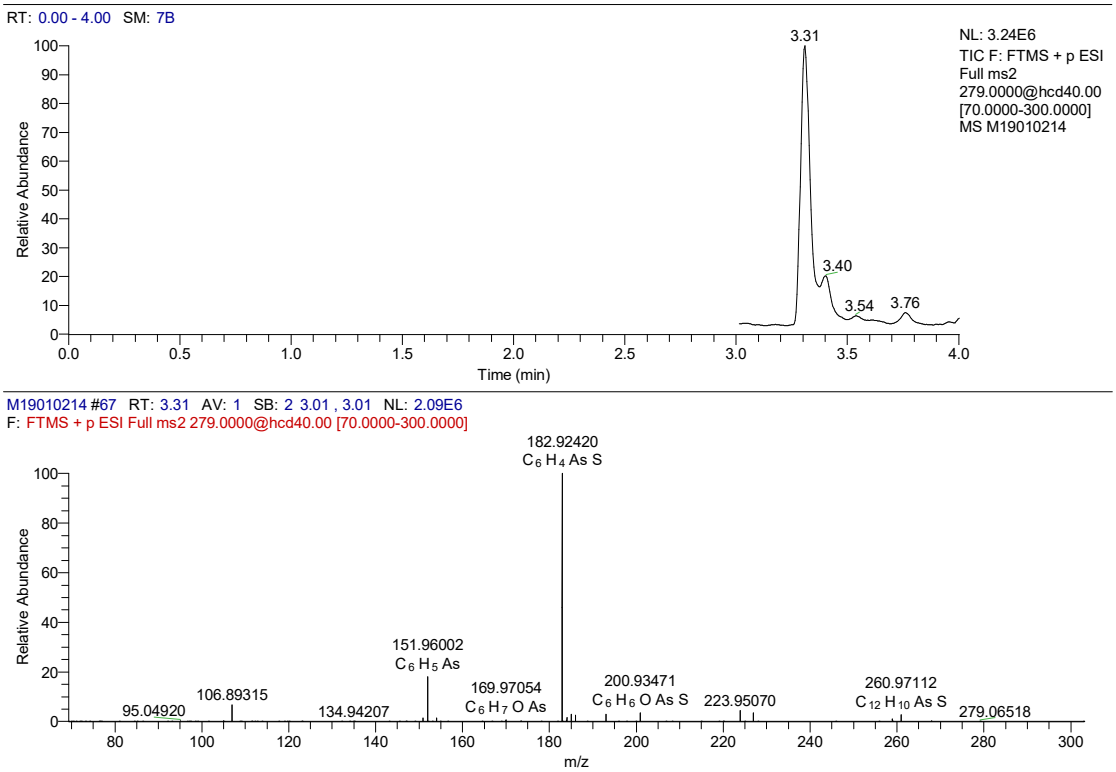


FIGURE S-4 TOTAL ION CHROMATOGRAM AND SPECTRUM FOR METHYLDIPHENYLARSINE SULFIDE

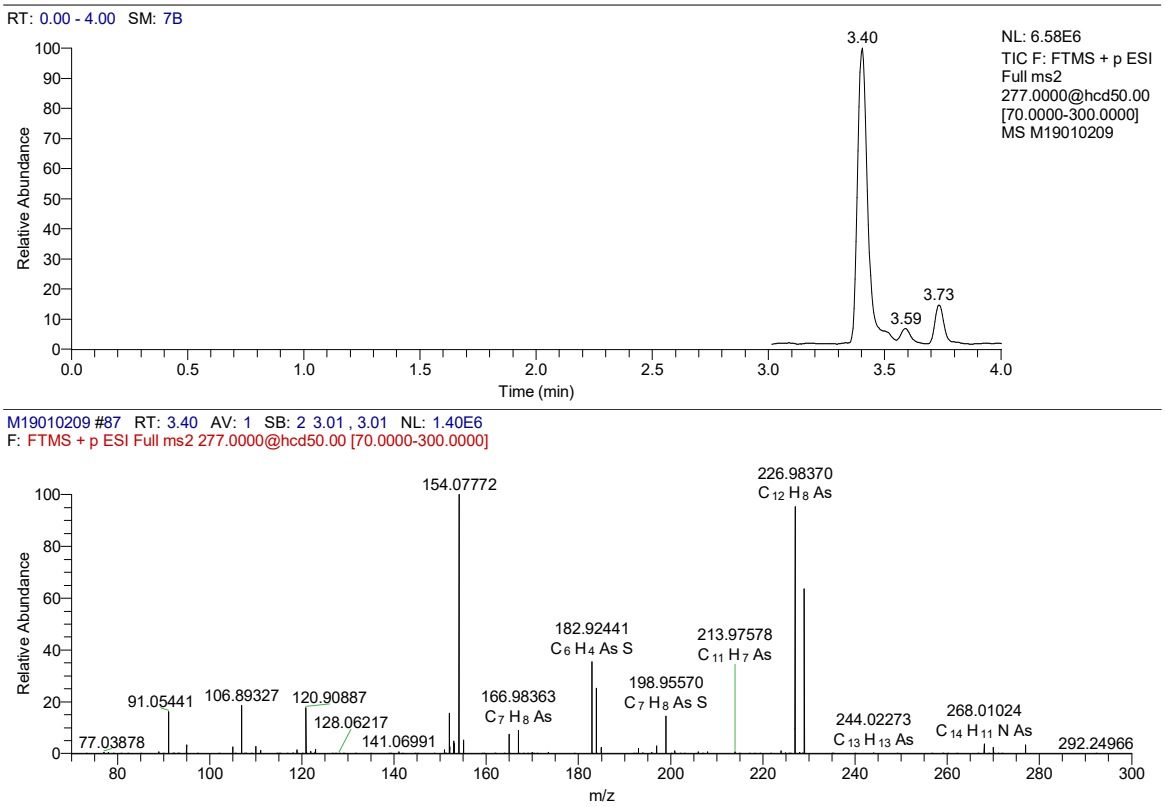


FIGURE S-5 TOTAL ION CHROMATOGRAM AND SPECTRUM FOR 10-METHYL-5H-PHENARSAZININE-10-SULFIDE

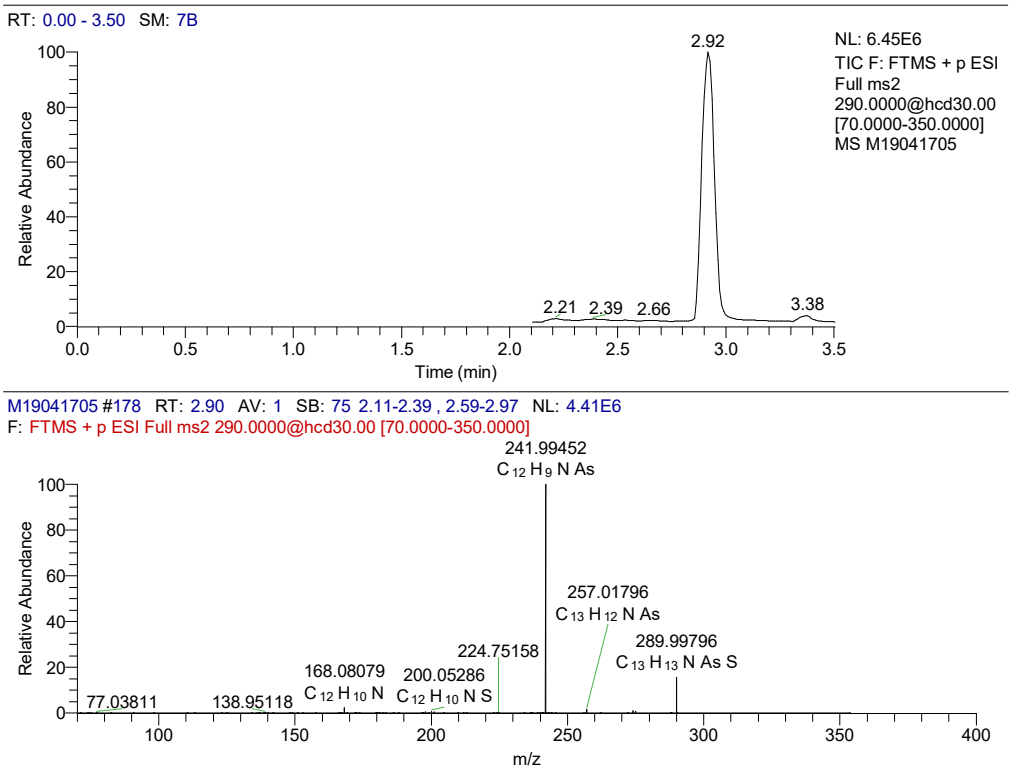


FIGURE S-6 TOTAL ION CHROMATOGRAM AND SPECTRUM FOR DIMETHYLPHENYLARSINE SULFIDE

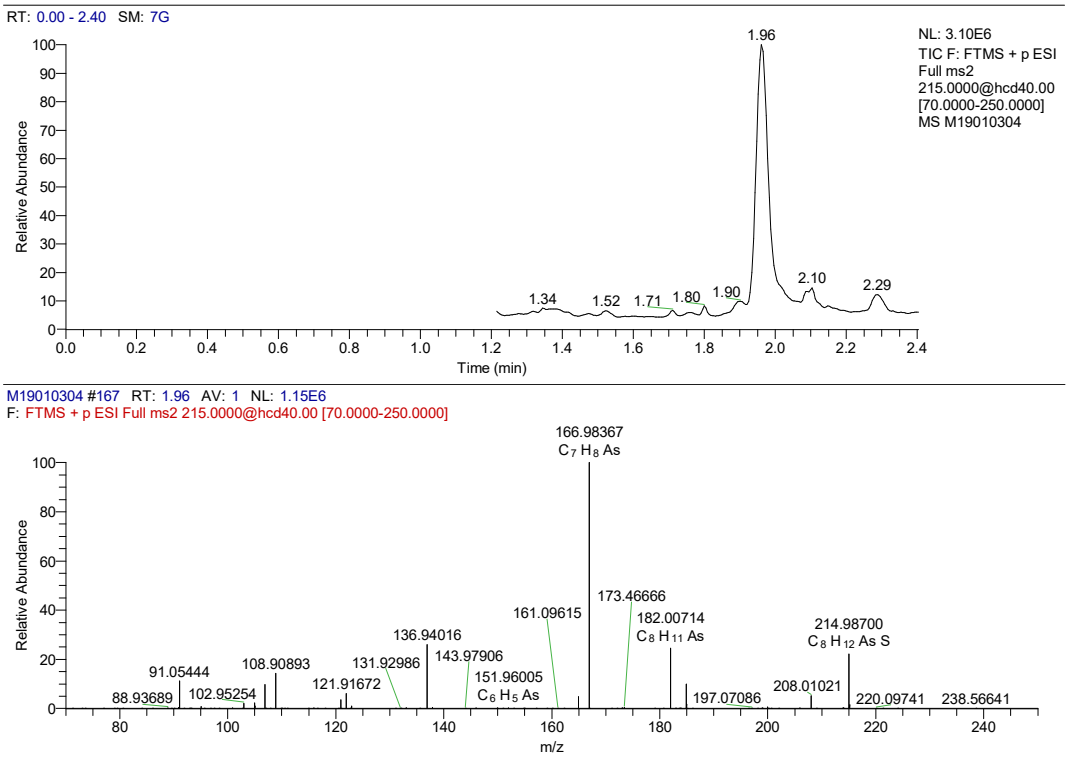


FIGURE S-7 TOTAL ION CHROMATOGRAM AND SPECTRUM FOR TRIPHENYLARSINE SULFIDE

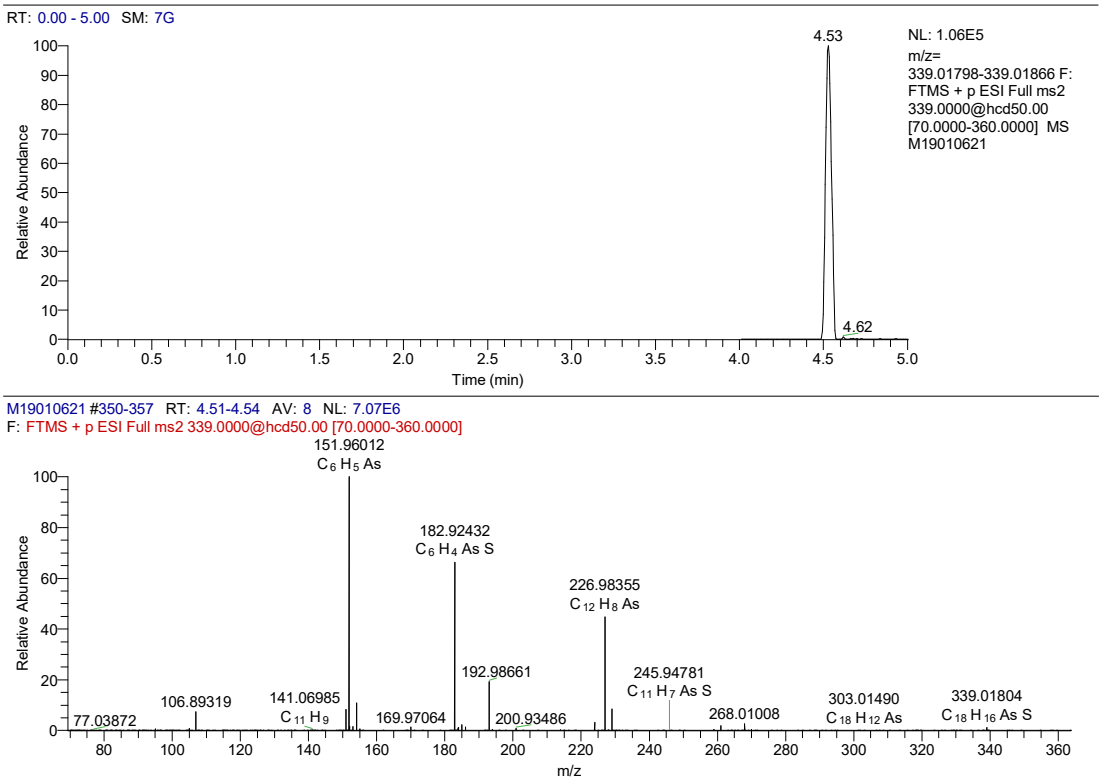
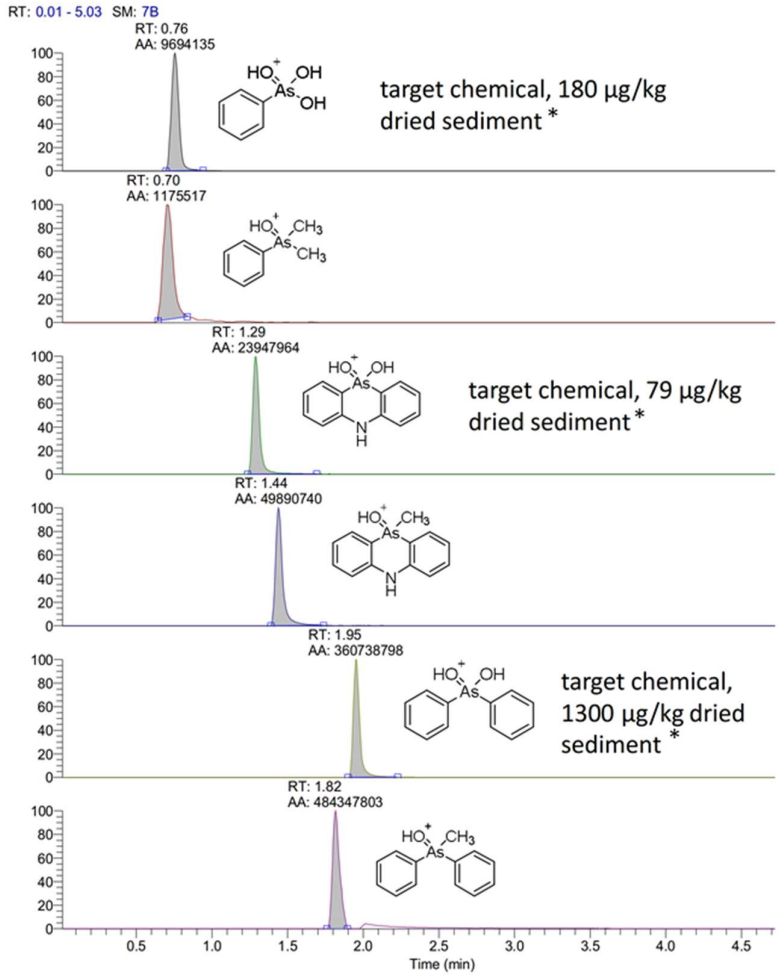


TABLE S-3 DETECTED FRAGMENTS AND THEIR RELATIVE ABUNDANCE FOR ALL DETECTED SULFUR CONTAINING CHEMICALS

Fragment ion *[m/z]*	Relative abundance [%]	Fragment ion *[m/z]*	Relative abundance [%]
Diphenylarsinothio acid		**Methyldiphenylarsine sulfide**	
260.97112	2.72	277.00259	2.81
226.98339	3.80	228.99913	65.12
200.93470	3.82	226.98365	100.00
182.92415	100.00	198.95566	14.36
151.96002	17.20	182.92439	33.95
		166.98361	8.52
		154.07769	99.37
		91.05440	14.34
Fragment ion *[m/z]*	Relative abundance [%]	Fragment ion *[m/z]*	Relative abundance
10-methyl-5H-phenarsazinine-10-sulfide			
289.99822	15.79		
241.99471	100.0		
168.08095	2.34		
Fragment ion *[m/z]*	Relative abundance [%]	Fragment ion *[m/z]*	Relative abundance
Dimethylphenylarsine sulfide		**Triphenylarsine sulfide**	
214.98699	24.06	339.01804	1.24
184.94008	10.48	303.01490	0.05
182.00715	24.74	228.99910	8.67
166.98366	100	226.98355	44.72
136.94016	26.25	213.97569	0.76
102.95235	2.15	182.92432	67.31
91.05444	11.13	154.07751	10.79
		151.96012	100

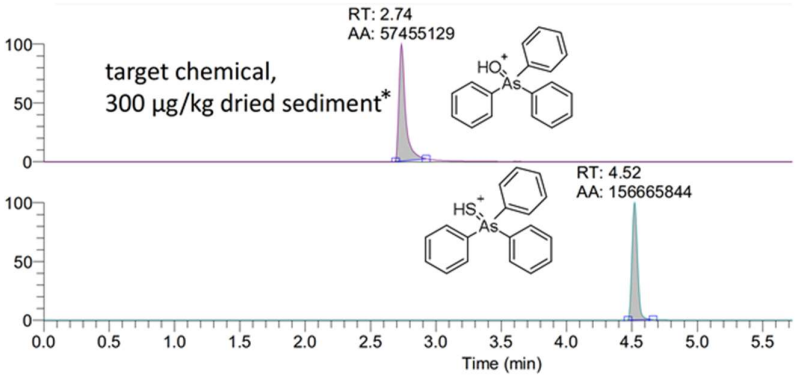
MS/HRMS data for 10-hydroxy-5H-phenarsazinine-10-sulfide is not available due to disturbing high matrix background.

FIGURE S-8 EXTRACTED ION CHROMATOGRAM FOR SEDIMENT SAMPLE #8 CONTAINING SULFUR-CONTAINING PHENYLARSENIC CHEMICALS AND TARGET CHEMICALS



* Concentrations of target chemicals have been quantified previously using LC-MS/MS method from the same sediment sample.

FIGURE S-9 EXTRACTED ION CHROMATOGRAM FOR SEDIMENT SAMPLE #8 CONTAINING SULFUR-CONTAINING PHENYLARSENIC CHEMICAL AND TARGET CHEMICAL



* Concentrations of target chemical have been quantified previously using LC-MS/MS method from the same sediment sample.

FIGURE S-10 SPECTRUM FOR HYDROXYPHENARSAZINIC ACID

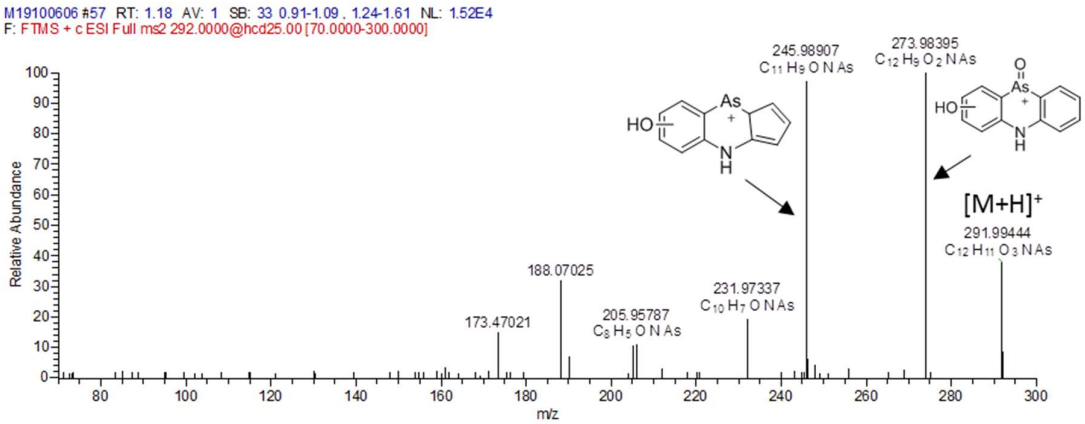


FIGURE S-11 EXTRACTED ION CHROMATOGRAM AND SPECTRA FOR TWO ISOMERS OF HYDROXYDIPHENYLARSINIC ACID

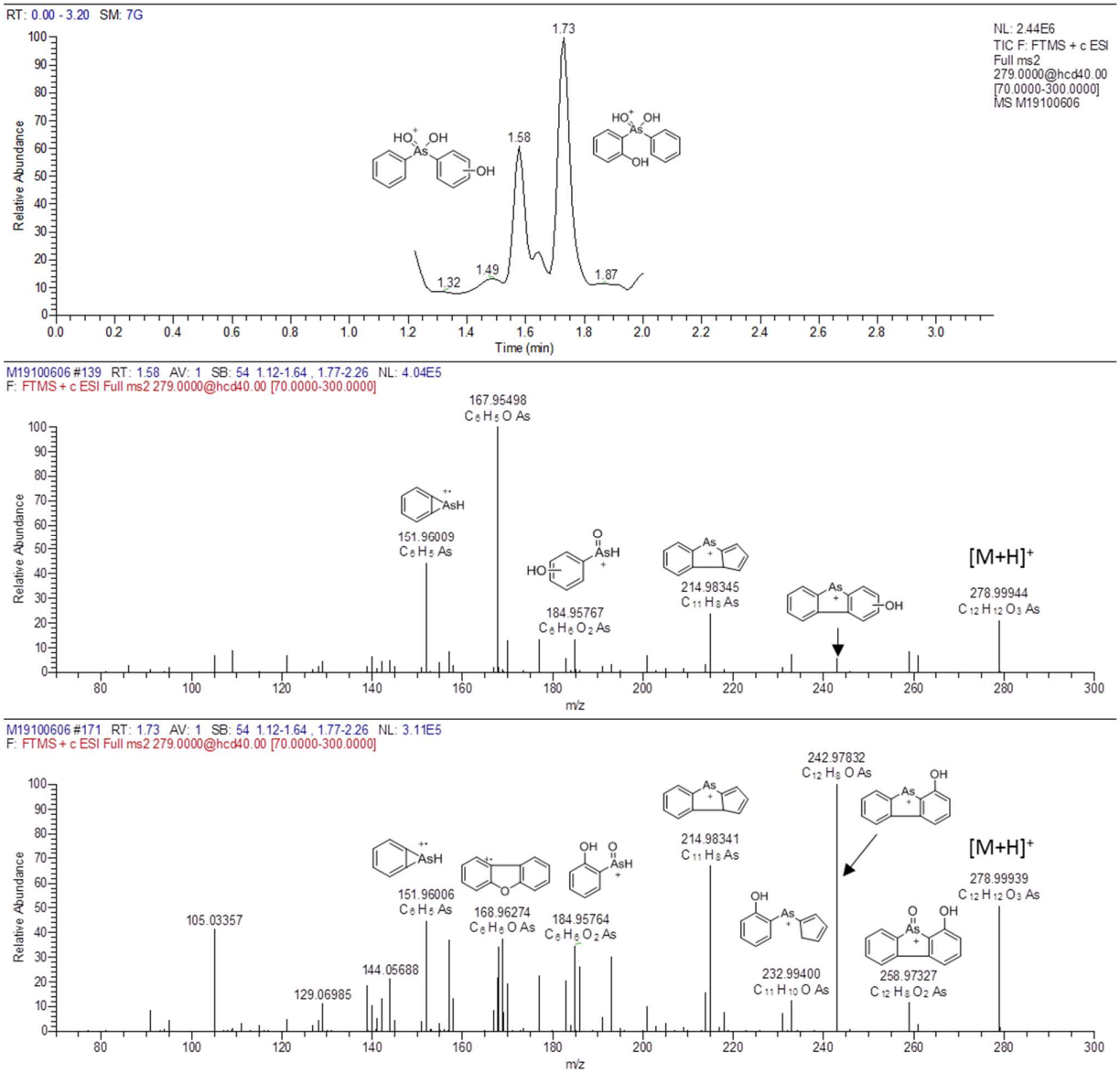
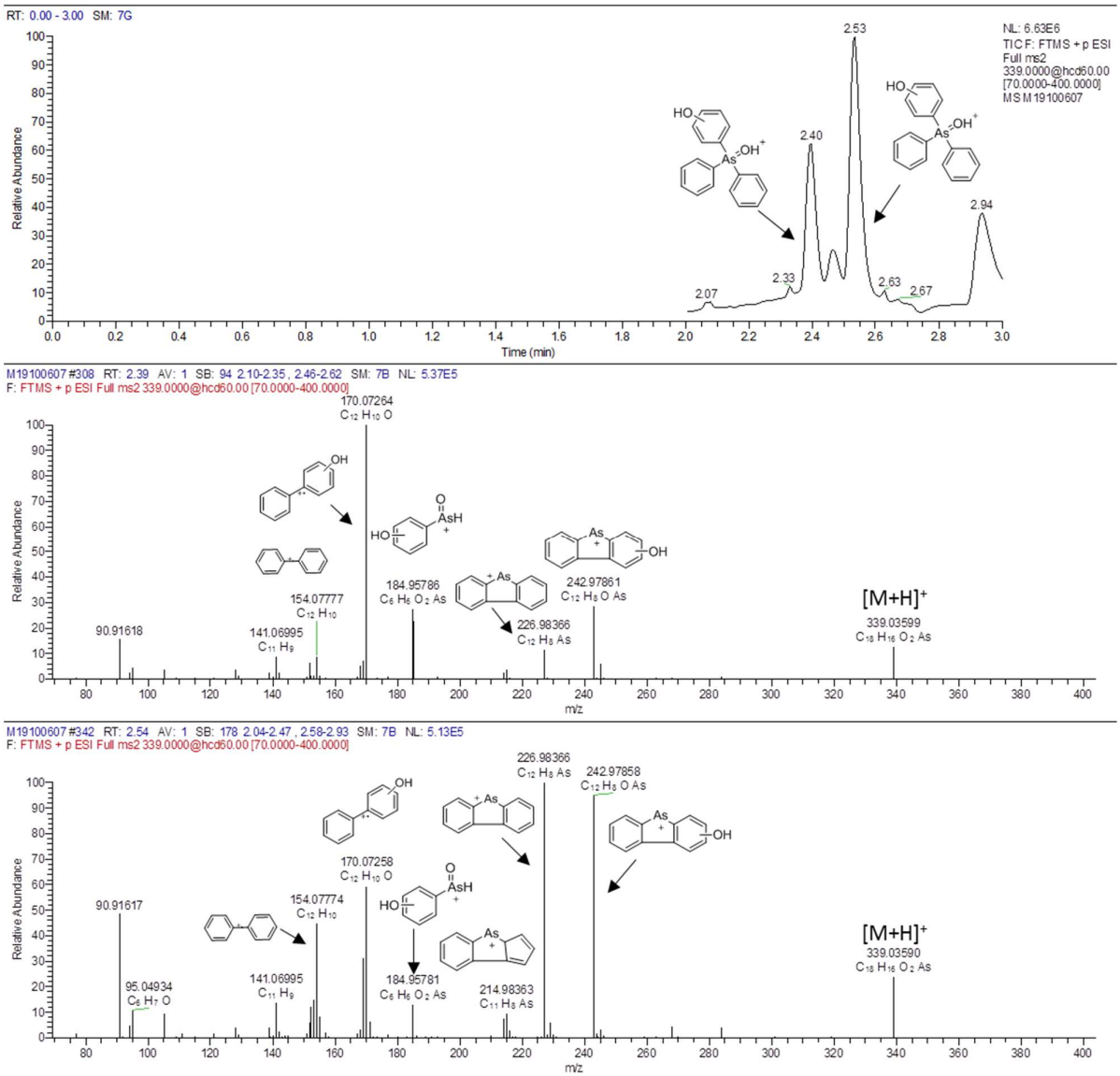



FIGURE S-12 EXTRACTED ION CHROMATOGRAM AND SPECTRA FOR TWO ISOMERS OF HYDROXYTRIPHENYLARSINE OXIDE