Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

TITLE: Surface water and groundwater analysis using aryl hydrocarbon and endocrine receptor biological assays and liquid chromatography-high resolution mass spectrometry in Susquehanna County, PA

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Results – Target Anthropogenic Organic Chemicals

Table ESI1. Normalized peak area ratios of compounds confirmed in the target screening process. For each detected compound, the ratio of analyte peak area to the isotope labelled internal standard peak area was normalized to the maximum ratio detected in any of the samples. This allows for the comparison of the abundance of each compound across samples, where 1.0 represents the maximum concentration detected. NF represents compounds that were not found.

Sample*	Adrenalone	Atrazine-2-hydroxy	Benzo-phenone	Bis(2-ethylhexyl) phthalate	Caffeine	Carbamaz-epine	Coumarin	DEET	Diethyl phthalate	Metoprolol	Para-xanthine/ Theo-phylline	Tributyl phosphate	Tris(2-chloro-ethyl)-phosphate
1W	0.40	NF	0.91	0.02	0.03	1.00	0.09	0.06	0.32	NF	0.01	0.35	0.33
2W	0.03	NF	0.34	0.01	0.07	0.65	0.04	0.02	0.11	NF	NF	0.03	0.31
3W	0.08	NF	0.09	0.03	0.07	0.67	0.09	0.02	0.49	NF	0.01	0.05	0.25
4W	0.03	NF	0.06	0.02	0.03	0.77	0.06	0.03	0.38	NF	NF	0.04	0.27
5SP	0.01	NF	NF	0.00	0.04	0.28	0.06	0.01	0.13	NF	NF	0.01	0.04
6W	0.00	NF	0.08	0.00	0.02	0.22	0.03	0.03	0.20	NF	NF	0.15	0.06
6P	0.02	0.07	0.32	0.00	0.33	0.17	0.50	0.02	0.28	0.22	0.37	0.02	0.16
7W	0.00	NF	NF	0.01	0.04	0.28	0.05	0.01	0.28	NF	NF	0.03	0.09
8W	1.00	NF	NF	0.01	0.70	0.35	0.10	0.02	0.24	NF	0.05	0.02	0.11
9W	0.00	NF	NF	0.01	0.07	0.36	0.03	0.01	0.14	NF	0.01	0.01	0.19
10W	0.00	NF	NF	0.01	0.21	0.31	0.04	0.01	0.19	NF	0.02	0.01	0.08
10P	0.01	0.02	1.00	0.00	0.10	0.09	0.32	0.03	0.54	0.05	0.07	0.02	0.06
11W	0.00	NF	0.11	0.21	0.11	0.35	0.06	0.04	0.50	NF	0.01	0.20	0.16
12W	0.01	0.00	0.06	0.00	0.07	0.42	0.02	0.01	0.09	0.00	0.02	0.02	0.05
13W	0.01	0.01	0.07	0.02	0.24	0.72	0.11	0.03	0.41	NF	0.05	0.03	0.15
13P	0.01	0.02	0.17	0.00	0.13	0.12	0.22	0.03	0.32	0.05	0.08	0.03	0.04
14W	NF	NF	NF	0.01	0.06	0.24	0.04	0.01	0.12	NF	NF	0.02	0.03
14P	0.03	0.08	0.77	0.01	0.46	0.17	1.00	0.19	0.54	0.26	0.46	1.00	0.27
14C	0.01	0.47	0.06	0.00	0.11	0.14	0.09	0.01	0.18	0.04	0.06	0.01	0.06
15W	0.00	0.01	NF	0.00	0.03	0.22	0.02	0.01	0.04	NF	NF	0.02	0.13
16W	0.01	NF	0.08	0.19	0.07	0.24	0.05	0.01	0.25	NF	0.01	0.05	0.13
16C	0.00	0.29	0.08	0.01	0.04	0.04	0.09	0.01	0.31	NF	0.01	0.04	0.11
17W	0.00	0.00	NF	0.00	0.05	0.13	0.01	0.00	0.03	NF	0.02	0.01	0.06

17P	0.01	0.27	0.28	0.01	0.09	0.08	0.31	0.07	0.59	NF	0.04	0.09	0.17
18W	0.02	0.00	NF	0.03	0.07	0.15	0.01	0.01	0.08	NF	0.03	0.01	0.06
19W	0.01	NF	NF	0.00	0.06	0.29	0.03	0.01	0.11	NF	NF	0.02	0.06
19P	0.00	0.01	0.14	0.00	0.09	0.06	0.11	0.02	0.29	0.00	0.04	0.03	0.06
20W	0.00	NF	NF	0.01	0.06	0.30	0.04	0.01	0.16	NF	0.01	0.01	0.12
21W	0.00	NF	NF	0.01	0.07	0.37	0.03	0.01	0.13	NF	NF	0.01	0.08
22W	0.01	NF	0.01	0.00	0.09	0.30	0.01	0.01	0.03	NF	0.03	0.01	0.15
22SP	0.00	NF	0.01	0.00	0.06	0.27	0.03	0.01	0.14	NF	0.03	0.01	0.06
23W	0.00	NF	0.03	0.01	0.32	0.37	0.02	0.01	0.09	0.01	0.08	0.01	0.04
24W	0.00	NF	0.01	0.04	0.07	0.24	0.01	0.00	0.09	NF	0.04	0.01	0.02
24C	0.03	1.00	0.08	0.05	0.55	0.21	0.10	0.01	0.19	0.25	0.71	0.02	0.17
25W	0.02	0.02	0.06	0.01	0.04	0.17	0.05	0.03	0.36	0.01	0.01	0.02	0.13
26W	0.03	0.00	0.05	0.01	0.11	0.24	0.04	0.01	0.13	0.00	0.03	0.01	0.20
27W	0.05	NF	0.10	0.13	0.06	0.17	0.06	0.02	0.37	NF	0.01	0.02	0.14
27P	0.02	0.01	0.17	0.00	0.34	0.08	0.08	1.00	0.35	0.27	0.42	0.01	0.10
28W	0.09	NF	0.16	0.00	0.10	0.25	0.02	0.02	0.10	0.02	0.07	0.01	0.13
28C	0.00	0.02	0.09	0.03	0.15	0.16	0.07	0.02	0.41	0.03	0.11	0.02	0.13
30W	0.01	NF	0.05	0.05	0.26	0.20	0.01	0.01	0.08	0.01	0.03	0.01	0.19
31W	0.01	NF	0.08	0.03	0.21	0.20	0.03	0.01	0.19	NF	0.02	0.02	0.16
31C	0.01	0.08	0.08	0.01	0.42	0.14	0.05	0.01	0.27	0.29	0.37	0.01	0.10
32W	0.02	0.00	0.04	0.02	0.39	0.25	0.01	0.01	0.12	0.01	0.07	0.01	0.15
32C	0.00	0.13	0.05	0.00	0.14	0.18	0.03	0.01	0.20	0.11	0.09	0.01	0.12
33W	0.00	0.00	0.14	0.05	0.09	0.26	0.05	0.01	0.40	NF	0.02	0.03	0.25
33P1	0.04	0.04	0.67	1.00	1.00	0.06	0.30	0.05	1.00	0.34	1.00	0.05	0.26
33P2	0.02	0.02	0.34	0.22	0.32	0.05	0.29	0.04	0.45	0.11	0.26	0.05	0.42
34W	0.02	NF	0.05	0.01	0.05	0.26	NF	0.00	0.07	NF	NF	0.01	0.29
34L	0.02	0.15	0.22	0.01	0.36	0.09	0.13	0.09	0.70	0.06	0.16	0.04	0.31
35SP	0.00	0.05	0.10	0.01	0.07	0.18	0.02	0.01	0.14	NF	0.01	0.01	0.13
36W	0.01	0.00	0.10	0.05	0.16	0.30	0.04	0.01	0.17	NF	0.02	0.03	0.27
37SP	0.03	0.01	0.10	0.01	0.05	0.21	0.04	0.01	0.16	NF	NF	0.01	0.11

*Samples were coded by water source and site number. W= Well; SP= Spring; P= Pond; C=Creek; L=Lake

Results – Suspect HFF Additives

Table ESI2. Normalized intensities of compounds confirmed in the suspect screening process. The intensities of each analyte peak were normalized based on the intensities of the isotope labelled internal standards in each of the samples. This allows for the comparison of the abundance of each compound across samples, where higher peak area represents higher abundance. NF represents compounds that were not found.

Sample*	Triethyl Phosphate	Diethyl-ene Glycol	Ethyl Aceto-acetate	Quinoline and Iso-quinoline	Quin-aldine	2-(Dibutyl-amino)-ethanol	Bio-polymer	Bio-polymer	Dimethyl Glutarate or Diethyl-ene Glycol Mono-acrylate	Tert-butyl Peroxy-benzoate	Dimethyl Adipate	Triton (octyl/non ylphenols)	Sorbitan Mono-oleate
1W	1.50E+06	3.50E+05	1.40E+06	NF	NF	2.00E+06	4.00E+05	NF	1.20E+07	1.70E+06	6.70E+06	6.70E+06	1.00E+07
2W	2.20E+06	3.70E+05	7.90E+05	NF	NF	1.00E+06	NF	NF	8.70E+06	1.20E+06	6.00E+06	5.80E+06	6.00E+06
3W	1.60E+06	NF	1.10E+06	NF	NF	5.70E+06	NF	NF	3.90E+06	1.50E+06	1.10E+07	2.70E+06	3.40E+07
4W	1.70E+06	4.00E+05	NF	NF	NF	8.80E+05	NF	NF	5.30E+06	1.30E+06	5.80E+06	3.50E+07	NF
5SP	1.30E+06	4.20E+05	9.60E+05	NF	NF	1.70E+06	NF	NF	4.80E+06	8.90E+05	4.50E+06	1.40E+06	9.00E+06
6W	2.60E+06	4.50E+05	1.20E+06	NF	NF	8.10E+05	NF	NF	8.00E+06	9.20E+05	2.40E+06	2.90E+06	9.90E+06
6P	1.40E+07	3.10E+05	1.10E+06	1.60E+06	6.70E+06	1.50E+06	4.40E+06	2.40E+06	1.10E+06	6.10E+06	1.30E+07	6.00E+06	1.40E+07
7W	7.80E+06	NF	8.20E+05	NF	NF	1.20E+06	NF	NF	1.60E+06	1.20E+06	1.40E+07	5.60E+07	NF
8W	2.60E+06	4.30E+05	8.30E+05	NF	NF	2.10E+06	9.20E+05	7.90E+05	5.10E+07	1.10E+06	6.80E+06	1.70E+06	5.40E+06
9W	NF	5.60E+05	NF	NF	NF	7.60E+05	NF	NF	5.80E+06	1.10E+06	2.30E+06	NF	7.30E+06
10W	NF	7.10E+05	5.80E+05	NF	NF	NF	4.50E+05	NF	7.40E+06	8.80E+05	2.50E+06	4.80E+06	NF
10P	3.20E+06	4.00E+05	7.90E+05	1.80E+06	5.20E+06	NF	1.40E+06	9.90E+05	6.00E+05	4.60E+06	1.10E+07	1.90E+07	NF
11W	1.00E+06	5.80E+05	NF	NF	NF	2.40E+06	NF	NF	1.40E+07	1.40E+06	1.80E+06	4.50E+06	NF
12W	1.40E+06	8.50E+05	4.90E+05	NF	NF	1.60E+06	3.70E+05	NF	2.80E+06	7.20E+05	2.40E+06	3.70E+07	NF
13W	3.50E+06	NF	6.60E+05	NF	NF	1.10E+06	1.00E+06	6.90E+05	8.30E+06	7.80E+05	3.90E+06	1.00E+07	5.10E+06
13P	1.40E+06	5.60E+05	6.30E+05	6.40E+06	8.40E+06	2.20E+06	1.20E+06	7.00E+05	NF	6.40E+06	4.10E+06	9.70E+06	NF
14W	1.60E+06	9.10E+05	4.90E+05	NF	NF	NF	NF	NF	2.90E+06	7.30E+05	2.50E+06	2.40E+06	3.20E+06
14P	4.20E+06	6.50E+05	3.20E+06	NF	NF	1.40E+06	6.40E+06	4.60E+06	8.40E+05	1.30E+07	3.00E+07	8.10E+06	NF
14C	1.80E+06	8.50E+05	7.50E+05	NF	NF	1.10E+07	9.50E+05	6.40E+05	8.00E+05	1.10E+06	7.40E+06	3.90E+07	NF
15W	NF	1.10E+06	5.00E+05	NF	3.30E+06	2.30E+06	NF	NF	9.30E+05	6.40E+05	1.80E+06	4.40E+06	7.90E+06
16W	7.00E+05	1.20E+06	NF	NF	NF	9.30E+05	NF	NF	NF	5.10E+05	1.70E+06	2.50E+06	3.40E+07
16C	2.80E+06	1.10E+06	6.90E+05	NF	NF	7.40E+06	NF	NF	NF	1.00E+06	6.40E+06	5.70E+06	1.20E+07

17W	9.60E+05	1.20E+06	5.20E+05	NF	NF	2.20E+06	8.60E+05	NF	1.00E+06	6.90E+05	2.20E+06	NF	2.20E+07
17P	3.40E+06	8.60E+05	7.40E+05	NF	3.70E+06	5.70E+05	7.30E+05	3.70E+05	NF	6.80E+06	7.50E+06	1.70E+07	9.20E+06
18W	NF	1.40E+06	5.20E+05	NF	NF	9.00E+05	5.90E+05	NF	1.00E+06	8.00E+05	1.00E+06	2.80E+06	1.40E+07
19W	3.90E+06	1.50E+06	5.10E+05	NF	NF	8.90E+05	NF	NF	1.20E+06	6.30E+05	2.80E+06	1.00E+07	5.50E+06
19P	1.60E+06	9.50E+05	6.20E+05	7.90E+05	2.20E+06	4.50E+06	7.40E+05	3.40E+05	NF	3.80E+06	2.80E+06	1.30E+07	NF
20W	NF	1.70E+06	5.40E+05	8.90E+05	1.70E+06	1.60E+06	NF	NF	1.90E+06	6.50E+05	NF	4.40E+06	1.10E+07
21W	2.80E+06	1.70E+06	5.00E+05	NF	NF	1.20E+06	NF	NF	2.40E+06	NF	9.90E+05	NF	1.00E+07
22W	NF	1.90E+06	NF	NF	NF	1.20E+06	6.70E+05	6.50E+05	2.30E+06	NF	1.10E+06	NF	1.50E+07
22SP	2.20E+06	1.70E+06	4.90E+05	NF	NF	1.50E+06	NF	NF	4.50E+06	NF	8.70E+05	4.30E+06	4.40E+06
23W	1.60E+06	2.20E+06	NF	NF	NF	3.10E+06	1.60E+06	1.10E+06	4.20E+06	3.00E+05	NF	1.50E+07	NF
24W	2.90E+06	2.30E+06	4.20E+05	NF	NF	NF	8.80E+05	NF	3.20E+06	NF	NF	1.00E+06	NF
24C	1.10E+06	1.50E+06	5.00E+05	NF	NF	5.10E+06	1.00E+07	1.80E+06	9.40E+05	1.50E+06	1.90E+06	4.10E+06	2.70E+07
25W	2.30E+06	NF	3.20E+05	NF	NF	7.20E+05	NF	NF	1.30E+06	3.70E+05	1.10E+06	1.50E+07	4.10E+06
26W	1.40E+06	4.00E+05	NF	NF	NF	NF	6.60E+05	5.80E+05	2.50E+06	NF	NF	1.20E+07	5.00E+06
27W	NF	3.60E+05	5.80E+05	NF	NF	1.90E+06	NF	NF	1.30E+06	4.70E+05	NF	3.40E+06	6.80E+06
27P	4.00E+06	NF	5.00E+05	6.50E+05	5.70E+06	3.10E+06	6.70E+06	1.40E+06	NF	4.50E+06	3.80E+06	1.40E+07	3.00E+06
28W	8.70E+06	3.80E+05	4.30E+05	NF	NF	1.20E+06	1.20E+06	9.40E+05	4.40E+06	4.80E+05	NF	6.60E+06	1.20E+06
28C	1.20E+06	4.40E+05	5.70E+05	NF	1.20E+06	2.40E+06	2.00E+06	7.40E+05	1.40E+06	7.50E+05	1.40E+06	6.30E+07	NF
30W	9.40E+05	7.50E+05	NF	NF	NF	2.50E+06	NF	NF	2.20E+06	NF	NF	1.50E+07	5.80E+06
31W	1.50E+06	7.40E+05	2.90E+05	NF	NF	8.70E+05	NF	NF	1.90E+06	NF	NF	3.20E+06	4.40E+06
31C	2.30E+06	1.30E+06	3.80E+05	NF	NF	1.30E+06	NF	NF	1.40E+06	4.00E+05	1.20E+06	2.90E+06	7.50E+06
32W	1.50E+06	3.50E+05	1.40E+06	NF	NF	2.00E+06	4.00E+05	NF	1.20E+07	1.70E+06	6.70E+06	6.70E+06	1.00E+07
32C	2.20E+06	3.70E+05	7.90E+05	NF	NF	1.00E+06	NF	NF	8.70E+06	1.20E+06	6.00E+06	5.80E+06	6.00E+06
33W	1.60E+06	NF	1.10E+06	NF	NF	5.70E+06	NF	NF	3.90E+06	1.50E+06	1.10E+07	2.70E+06	3.40E+07
33P1	1.70E+06	4.00E+05	NF	NF	NF	8.80E+05	NF	NF	5.30E+06	1.30E+06	5.80E+06	3.50E+07	NF
33P2	1.30E+06	4.20E+05	9.60E+05	NF	NF	1.70E+06	NF	NF	4.80E+06	8.90E+05	4.50E+06	1.40E+06	9.00E+06
34W	2.60E+06	4.50E+05	1.20E+06	NF	NF	8.10E+05	NF	NF	8.00E+06	9.20E+05	2.40E+06	2.90E+06	9.90E+06
34L	1.40E+07	3.10E+05	1.10E+06	1.60E+06	6.70E+06	1.50E+06	4.40E+06	2.40E+06	1.10E+06	6.10E+06	1.30E+07	6.00E+06	1.40E+07
35SP	7.80E+06	NF	8.20E+05	NF	NF	1.20E+06	NF	NF	1.60E+06	1.20E+06	1.40E+07	5.60E+07	NF
36W	2.60E+06	4.30E+05	8.30E+05	NF	NF	2.10E+06	9.20E+05	7.90E+05	5.10E+07	1.10E+06	6.80E+06	1.70E+06	5.40E+06
37SP	NF	5.60E+05	NF	NF	NF	7.60E+05	NF	NF	5.80E+06	1.10E+06	2.30E+06	NF	7.30E+06

*Samples were coded by water source and site number. W= Well; SP= Spring; P= Pond; C=Creek; L=Lake

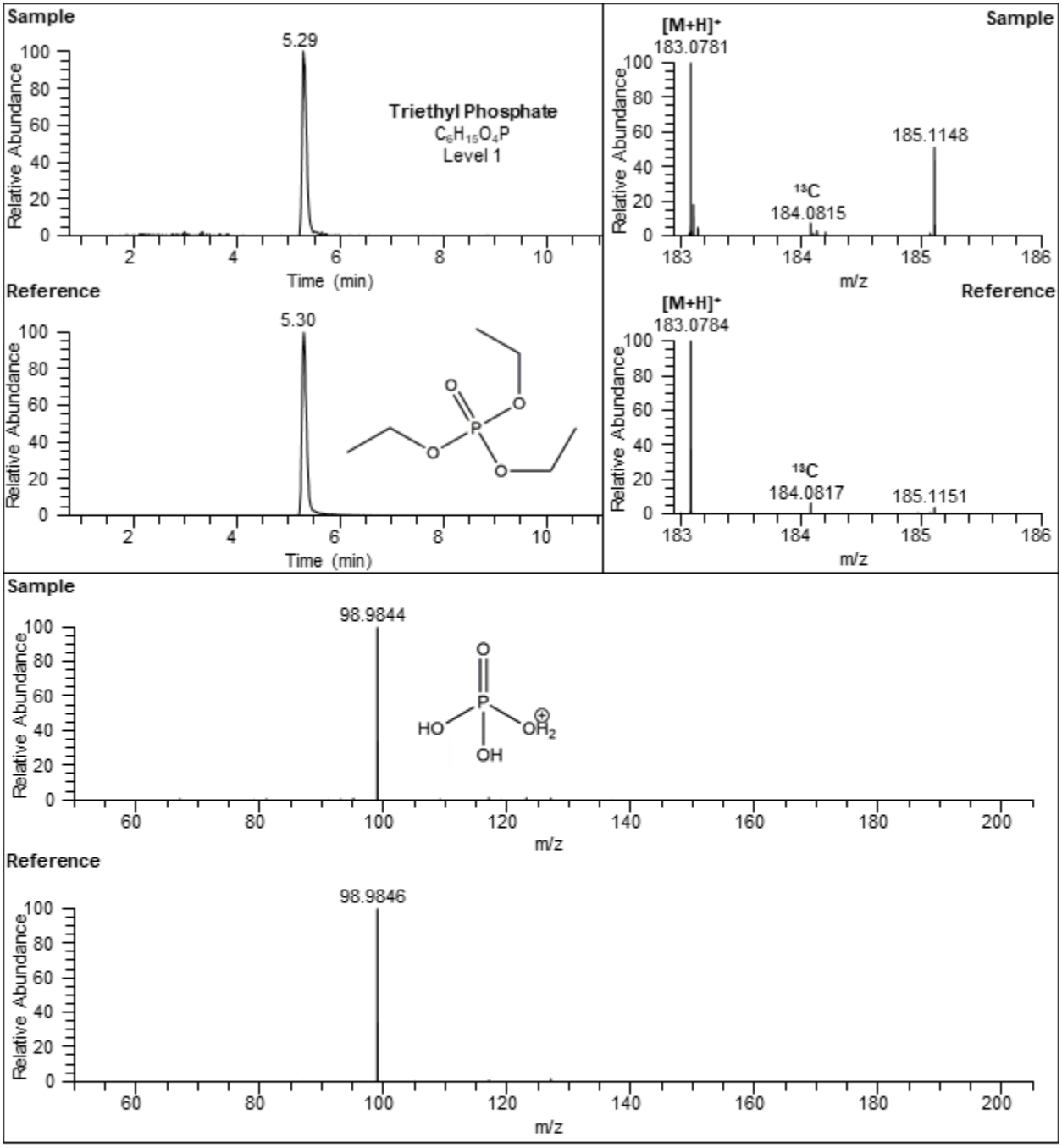

Figure ESI1. Confirmation of triethyl phosphate shown in sample 6P. RT of 5.3 min and the exact mass of the protonated adduct (m/z 183.0782, Δm = -2.46 ppm) were obtained. The suspected molecular formula is $C_6H_{15}O_4P$ so ^{13}C intensity of 6% of the parent compound is reasonable for molecular formula assigned, but the formula is generic. MS/MS fragments were obtained and compared to those in mzCloud. The dominant fragment, 98.9844, was a match to that in mzCloud. An analytical standard was obtained and the RT and MS/MS fragments were a match. Current level of classification is Level 1. This m/z value was prioritized in "AR Antagonist."