AQRP Monthly Technical Report

PROJECT TITLE	Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ	**PROJECT #**	14-029
PROJECT PARTICIPANTS	Rebecca J. Sheesley Sascha Usenko	**DATE SUBMITTED**	11/8/2014
REPORTING PERIOD	**From:** October 1, 2014 **To:** October 31, 2014	**REPORT #**	3

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task

In October 2014, we focused on the method validation for the new, combined high pressure liquid extraction (HPLE) and gas chromatography mass spectrometry (GCMS) method for organic tracers and contaminants (see Table 1). Method validation included analysis of National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) for Urban Dust and House Dust (1649b and 2585, respectively). In addition, method detection limit studies were completed (n=7) for organic contaminants and is in progress for organic tracers. Manuscript is in preparation for submitting to *Journal of Chromatography A* in December 2014. Table 1 is not ready for distribution/public dissemination at this point.

In addition, we have fully cataloged and established a protocol for filter sharing and documenting the analysis of each filter collected during DISCOVER-AQ in Houston 2013.

Participated in analysis preparation with DISCOVER-AQ aerosol focus group collaborators (grants 14-024 and 14-009).

Discussion and preparation of filter samples for ion chromatography analysis (14-024).

Preliminary Analysis

Table 1: Breakdown of Target Analyte Analysis by which GC-MS is used. [a]These compounds co-elute and are subsequently quantitated together. [b]These were analyzed on GC-EI-MS. [c]A fourth ion (third qualifier) was used for the identification of these coeluting compounds. [d]This compound was analyzed for in SRM 1649b. [e]This compound was analyzed for in SRM 2585. [f]Reported concentrations were combined and error was propagated accordingly. [g]These compounds were quantified separate from other PAHs (with alkanes, hopanes, and steranes). [h]Informational values are not given with associated error. Yellow indicates preliminary data.

GC-ECNI-MS										
Polybrominated Diphenyl Ethers (PBDEs)										
Compound	RT (min)	Ions (m/z)	Quantitation Standard	SRMs 1649b and 2585			Reproducibility study (%) n=7	MDL (ppb)	Linear Range (ppb)	R^2
				Detected	Reported	% Error				
PBDE 15	22.83	81,79	$^{13}C_{12}$-PBDE 77	---	---	---	77.3 ± 7.8	10.3	4.9 – 1500	0.997
PBDE 17[e]	27.50	79,161,81	$^{13}C_{12}$-PBDE 77	<MDL	11.5 ± 1.2	---	70.6 ± 4.5	8.72	4.9 – 1500	0.999
PBDE 28+33[e]	28.48	79,161,163	$^{13}C_{12}$-PBDE 77	23.1 ± 0.5	46.9 ± 4.4	51%	69.9 ± 3.4	8.43	4.9 – 1500	0.999
PBDE 75[e]	32.59	81,79,161	$^{13}C_{12}$-PBDE 77	<MDL	10.1 ± 2.0	---	77.8 ± 1.9	3.15	4.9 – 1500	0.999
PBDE 49[e]	33.04	81,79,161	$^{13}C_{12}$-PBDE 77	58.7 ± 2.4	53.5 ± 4.2	10%	71.6 ± 2.1	3.37	4.9 – 1500	0.994
PBDE 47[e]	33.92	79,161,163	$^{13}C_{12}$-PBDE 77	477 ± 17	497 ± 46	4%	79.1 ± 2.6	2.47	4.9 – 1500	0.999
PBDE 66[e]	34.77	79,81,161	$^{13}C_{12}$-PBDE 77	32.8 ± 1.6	29.5 ± 6.2	11%	84.6 ± 0.8	1.67	4.9 – 1500	0.999
$^{13}C_{12}$-PBDE 77	36.05	81,79,498	$^{13}C_{12}$-PCB 138	---	---	---	88.3 ± 5.7	---	---	---
PBDE 100[e]	37.76	79,161,163	$^{13}C_{12}$-PBDE 126	177 ± 14	145 ± 11	22%	89.8 ± 1.8	2.67	4.9 – 1500	0.999
PBDE 119[e]	38.27	79,81,161	$^{13}C_{12}$-PBDE 126	<MDL	<0.2[h]	---	95.4 ± 2.5	2.93	4.9 – 1500	0.998
PBDE 99[e]	39.00	79,161,562	$^{13}C_{12}$-PBDE 126	1130 ± 95	892 ± 53	27%	93.3 ± 2.3	1.87	4.9 – 1500	0.998
PBDE 85+155[c,e,f]	41.06	81,79,160	$^{13}C_{12}$-PBDE 126	35.6 ± 2.3	47.7 ± 1.6	25%	96.0 ± 2.7	2.68	4.9 – 1500	0.999
$^{13}C_{12}$-PBDE 126	41.50	79,81,576	$^{13}C_{12}$-PCB 138	---	---	---	88.9 ± 6.6	---	---	---
PBDE 154[e]	41.89	79,161,562	$^{13}C_{12}$-PBDE 126	125 ± 7	83.5 ± 2.0	50%	85.0 ± 4.3	7.58	4.9 – 1500	0.999
PBDE 153[a,e]	43.37	79,161,564	$^{13}C_{12}$-PBDE 126	141 ± 11	119 ± 1	18%	90.3 ± 3.0	3.26	4.9 – 1500	0.999
PBDE 183[e]	46.92	79,161,564	$^{13}C_{12}$-PBDE 126	61.5 ± 2.5	43.0 ± 3.5	43%	92.6 ± 2.2	2.27	4.9 – 1500	0.979
Polychlorinated Biphenyls (PCBs)										
PCB 101[d]	25.22	326,328,324	$^{13}C_{12}$-PCB 77	<MDL	55.1 ± 5.1	---	77.1 ± 4.1	6.69	4.9 – 1500	0.998
PCB 81[d]	26.61	292,290,294	$^{13}C_{12}$-PCB 77	<MDL	13.5 ± 0.7	---	89.7 ± 1.4	1.74	4.9 – 1500	0.999
PCB 110[d]	26.88	326,324,328	$^{13}C_{12}$-PCB 77	<MDL	32.9 ± 3.0	---	85.4 ± 1.6	4.57	4.9 – 1500	0.999
$^{13}C_{12}$-PCB 77	27.09	304,302,306	$^{13}C_{12}$-PCB 138	---	---	---	73.7 ± 8.6	---	---	---
PCB 77	27.09	292,290,294	$^{13}C_{12}$-PCB 77	---	---	---	92.5 ± 1.7	2.13	4.9 – 1500	0.998
PCB 123	28.03	326,324,328	$^{13}C_{12}$-PCB 77	---	---	---	89.5 ± 3.0	2.88	4.9 – 1500	0.999
PCB 118[d]	28.21	326,328,324	$^{13}C_{12}$-PCB 77	<MDL	23.8 ± 4.0	---	91.9 ± 4.1	3.24	4.9 – 1500	0.999
PCB 114	28.67	326,324,328	$^{13}C_{12}$-PCB 77	---	---	---	98.8 ± 3.2	2.00	4.9 – 1500	0.999
PCB 153[d]	29.22	360,362,358	$^{13}C_{12}$-PCB 126	67.0 ± 5.8	74.8 ± 1.0	10%	75.7 ± 2.4	3.50	4.9 – 1500	0.994
PCB 105[d]	29.41	326,324	$^{13}C_{12}$-PCB 126	<MDL	9.7 ± 1.0	---	71.9 ± 2.3	3.86	4.9 – 1500	0.995
$^{13}C_{12}$-PCB 138	30.4	372,374,370	-IS-	---	---	---	---	---	---	---
PCB 138[d]	30.43	360,362,358	$^{13}C_{12}$-PCB 126	54.0 ± 4.9	59.0 ± 14.0	8%	76.8 ± 1.8	2.70	4.9 – 1500	0.993

$^{13}C_{12}$-PCB 126	31.00	338,340,336	$^{13}C_{12}$-PCB 138	---	---	---	81.2 ± 6.5	---	---	---
PCB 126	31.00	326,328,324	$^{13}C_{12}$-PCB 126	---	---	---	89.5 ± 1.6	2.17	4.9 – 1500	0.998
PCB 187[d]	31.12	394,396,398	$^{13}C_{12}$-PCB 126	36.5 ± 1.7	38.5 ± 2.9	5%	88.0 ± 1.9	2.27	4.9 – 1500	0.997
PCB 167	31.85	360,362,358	$^{13}C_{12}$-PCB 126	---	---	---	93.4 ± 1.2	2.45	4.9 – 1500	0.997
PCB 156[d]	32.85	360,362,358	$^{13}C_{12}$-PCB 169	<MDL	7.2 ± 2.0	---	88.0 ± 1.9	3.15	4.9 – 1500	0.999
PCB 157[d]	33.06	360,362,326	$^{13}C_{12}$-PCB 169	<MDL	1.59 ± 0.07	---	81.7 ± 3.1	3.37	4.9 – 1500	0.999
PCB 180[d]	33.58	394,396,360	$^{13}C_{12}$-PCB 169	111 ± 8	72.4 ± 1.0	53%	87.9 ± 1.6	2.67	4.9 – 1500	0.998
$^{13}C_{12}$-PCB 169	34.63	376,338,336	$^{13}C_{12}$-PCB 138	---	---	---	84.4 ± 6.2	---	---	---
PCB 169	34.65	360,362,359	$^{13}C_{12}$-PCB 169	---	---	---	91.0 ± 1.2	1.80	4.9 – 1500	0.998
PCB 189[d]	36.22	394,396,398	$^{13}C_{12}$-PCB 169	<MDL	1.6 ± 0.1	---	94.6 ± 2.4	2.05	4.9 – 1500	0.999
Historic and Current Use Pesticides										
PeCB[d]	10.09	250,248,252	$^{13}C_6$-HCB	<MDL	61 ± 19	---	89.5 ± 2.4	11.9	4.9 – 750	0.972
d_{14}-Trifluralin	13.64	349,348,350	$^{13}C_{12}$-PCB 138	---	---	---	52.0 ± 12.0	---	---	---
Trifluralin	13.86	335,336	d_{14}-Trifluralin	4.1 ± 2.2	---	---	89.9 ± 0.6	0.93	4.9 – 750	0.945
α-HCH[d]	14.62	71,73,70	$^{13}C_6$-δ-HCH	<MDL	13.4 ± 2.1	---	89.1 ± 6.0	22.4	4.6 – 1400	0.999
$^{13}C_6$-HCB	14.79	290,292,288	$^{13}C_{12}$-PCB 138	---	---	---	48.7 ± 10.2	---	---	---
HCB[d]	14.79	284,286,282	$^{13}C_6$-HCB	<MDL	2.91 ± 0.67	---	93.0 ± 1.0	2.86	4.9 – 750	0.983
PCA	15.09	280,278,282	$^{13}C_6$-HCB	---	---	---	95.2 ± 1.3	3.48	4.9 – 750	0.963
PCNB	16.06	249,247,251	d_{14}-Trifluralin	---	---	---	103 ± 3	1.85	4.9 – 750	0.968
β+γ-HCH[d]	16.29	71,73,70	$^{13}C_6$-δ-HCH	<MDL	3.1 ± 0.9	---	89.5 ± 5.4	15.3	4.6 – 1400	0.999
Chlorothalonil	17.55	266,264,245	$^{13}C_6$-δ-HCH	---	---	---	95.4 ± 8.4	2.72	4.9 – 750	0.945
δ-HCH	17.89	255,257,253	$^{13}C_6$-δ-HCH	---	---	---	87.8 ± 3.3	4.56	4.6 – 1400	0.999
$^{13}C_6$-δ-HCH	17.89	263,261	$^{13}C_{12}$-PCB 138	---	---	---	56.1 ± 9.0	---	---	---
Heptachlor	19.82	266,270,264	$^{13}C_6$-δ-HCH	---	---	---	84.3 ± 6.9	18.7	4.6 – 1400	0.998
Aldrin	21.55	237,239,330	$^{13}C_6$-δ-HCH	---	---	---	86.8 ± 8.7	19.4	4.6 – 720	0.996
Dacthal	21.88	332,330,334	$^{13}C_6$-δ-HCH	12.5 ± 2.2	---	---	98.1 ± 4.0	10.0	4.9 – 750	0.965
Heptachlor Epoxide	23.54	237,318,282	d_4-Endosulfan I	---	---	---	73.7 ± 2.7	3.14	4.6 – 1400	0.990
Trans-chlordane[d]	24.73	410,408,412	d_4-Endosulfan I	42.9 ± 1.2	50.7 ± 5.1	15%	83.0 ± 4.1	4.42	4.6 – 1400	0.990
d_4-Endosulfan I	25.20	410,376,244	$^{13}C_{12}$-PCB 138	---	---	---	68.3 ± 13.0	---	---	---
Endosulfan I	25.30	404,372,370	d_4-Endosulfan I	---	---	---	94.9 ± 4.6	2.27	4.6 – 1400	0.992
Cis-chlordane[d]	25.47	444,446,442	d_4-Endosulfan I	N.D.	45.5 ± 8.1	---	88.4 ± 2.9	4.04	4.6 – 1400	0.998
Trans-nonachlor[d]	25.50	444,442,446	d_4-Endosulfan I	22.5 ± 0.4	33.0 ± 3.5	32%	96.4 ± 3.5	3.66	4.9 – 1500	0.997
Dieldrin[e]	26.61	237,239,235	d_4-Endosulfan I	---	---	---	81.1 ± 4.0	1.60	4.6 – 1400	0.991
Endrin	27.60	380,237,346	d_4-Endosulfan II	---	---	---	98.0 ± 7.7	10.8	4.6 – 1400	0.999
d_4-Endosulfan II	28.12	410,409,276	$^{13}C_{12}$-PCB 138	---	---	---	79.8 ± 8.2	---	---	---
Endosulfan II	28.21	406,372,336	d_4-Endosulfan II	---	---	---	71.3 ± 1.7	3.14	4.6 – 1400	0.996
Cis-nonachlor[d]	28.45	444,446,334	d_4-Endosulfan II	<MDL	12.7 ± 0.4	---	79.5 ± 1.6	2.90	4.2 – 650	0.968
Endrin Aldehyde	28.93	380,382,272	d_4-Endosulfan II	---	---	---	84.3 ± 3.3	4.70	4.6 – 1400	0.999
Endosulfan Sulfate	30.07	386,388,422	d_4-Endosulfan II	---	---	---	90.0 ± 5.6	6.68	4.6 – 1400	0.998

Endrin Ketone	32.24	308,310,306	d_4-Endosulfan II	---	---	---	89.6 ± 4.2	3.36	4.6 – 1400	0.997
Bifenthrin	32.92	360,362,326	$^{13}C_{12}$-PCB 169	---	---	---	80.2 ± 2.6	1.39	4.9 – 1500	0.991
Mirex[d]	35.13	439,404,441	$^{13}C_{12}$-PCB 169	<MDL	1.30 ± 0.06	---	103 ± 3	14.8	5.1 – 780	0.947
λ-cyhalothrin	35.46	241,205,243	$^{13}C_{12}$-PCB 169	---	---	---	80.4 ± 1.5	2.68	4.9 – 1500	0.987
Deltamethrin[a]	43.37	79,81,297	$^{13}C_{12}$-PBDE 77	---	---	---	90.3 ± 3.0	3.26	4.9 – 1500	0.999
Cis-permethrin[b]	37.47	183,184,163	$^{13}C_6$-trans-permethrin	---	---	---	82.7 ± 11.2	11.3	34 – 2700	0.987
Trans-permethrin[b]	37.70	183,163	$^{13}C_6$-trans-permethrin	---	---	---	90.1 ± 2.4	7.83	8.7 – 2700	0.980
$^{13}C_6$-trans-permethrin[b]	37.70	189	d_{12}-BeP	---	---	---	85.0 ± 12.2	---	---	---
GC-EI-MS										
Organophosphate Flame Retardants (OPFRs)										
TBP	19.80	99,211,155	d_{15}-TPP	---	---	---	88.7 ± 5.7	18.6	25 – 2800	0.999
d_{12}-TCEP	21.71	261,263,148	d_{12}-BeP	---	---	---	51.0 ± 10.2	---	---	---
TCEP	21.90	249,143,99	d_{12}-TCEP	---	---	---	103 ± 4	23.8	25 – 2800	0.999
TCPP	22.55	125,99,157	d_{12}-TCEP	---	---	---	87.5 ± 3.3	11.6	25 – 2800	0.999
TDCPP	30.83	191,99,379	d_{12}-TCEP	---	---	---	116 ± 15	21.3	25 – 2800	0.998
d_{15}-TPP	31.61	341,340,243	d_{12}-BeP	---	---	---	50.0 ± 5.2	---	---	---
TPP	31.73	326,215,169	d_{15}-TPP	---	---	---	121 ± 5	16.7	25 – 2800	0.999
TBEP	31.92	326, 83	d_{15}-TPP	---	---	---	91.0 ± 2.8	26.5	25 – 2800	0.999
TEHP	32.69	99,113	d_{15}-TPP	---	---	---	93.5 ± 14.3	6.36	25 – 2800	0.999
TOTP	34.21	368,277,165	d_{15}-TPP	---	---	---	90.6 ± 4.3	20.1	25 – 2800	0.990
TPTP	36.08	368,261,107	d_{15}-TPP	---	---	---	120. ± 5	8.2	25 – 2800	0.999
T2IPPP	36.55	452,118,251	d_{15}-TPP	---	---	---	89.8 ± 3.8	13.8	25 – 2800	0.999
T35DMPP	37.61	410,194	d_{15}-TPP	---	---	---	112 ± 5	11.8	25 – 2800	0.999
Polycyclic Aromatic Hydrocarbons (PAHs)										
d_{10}-Flu	19.76	175,174,177	d_{12}-BeP	---	---	---	61.6 ± 11.5	---	---	---
Flu[d]	19.85	165,166	d_{10}-Flu	<MDL	222 ± 16	---	104 ± 4	10.4	8.6 – 2600	0.999
d_{10}-PA	23.82	188,160	d_{12}-BeP	---	---	---	68.5 ± 13.8	---	---	---
PA+Ant[d]	23.91	178,152,176	d_{10}-PA	2283 ± 208	4344 ± 47[f]	47%	99.6 ± 3.6	5.87	8.6 – 2600	0.997
Ant[d]		178,176,152	d_{10}-PA				92.8 ± 3.9			
d_{10}-FL	28.66	212,208	d_{12}-BeP	---	---	---	76.5 ± 12.7	---	---	---
FL[d]	28.72	202,200,101	d_{10}-FL	4308 ± 652	6140 ± 120	30%	105 ± 5	5.17	8.6 – 2600	0.999
d_{10}-Pyr	29.52	212,211,106	d_{12}-BeP	---	---	---	79.6 ± 12.1	---	---	---
Pyr[d]	29.57	202,201,101	d_{10}-Pyr	7404 ± 945	4784 ± 29	55%	101 ± 6	4.11	8.6 – 2600	0.999
d_{12}-BaA+d_{12}-CHR	34.65	240,237	d_{12}-BeP	---	---	---	92.9 ± 9.8	---	---	---
BaA+CHR[d]	34.77	228,226,114	d_{12}-BaA	7476 ± 940	5100 ± 65[f]	47%	87.6 ± 8.6	3.58	8.6 – 2600	0.999
d_{12}-CHR		240,241,237	d_{12}-BeP	---	---	---	99.2 ± 11.2	---	---	---
CHR[d]		228,227	d_{12}-CHR			---	107 ± 5			
d_{12}-BaP	38.68	264,261,132	d_{12}-BeP	---	---	---	91.1 ± 7.8	---	---	---
BaP[d]	38.74	252,253,126	d_{12}-BaP	4130 ± 420	2470 ± 170	67%	87.9 ± 5.5	3.73	8.6 – 2600	0.996

d_{12}-BkF	38.80	265,132	d_{12}-BeP	---	---	---	91.9 ± 11.2	---	---	---
BkF[d]	38.86	252,253,126	d_{12}-BkF	1783 ± 472	1748 ± 83	2%	103 ± 11	10.8	8.6 – 2600	0.997
d_{12}-BeP	39.63	264,265,261	-IS-	---	---	---	---	---	---	---
d_{12}-BbF	39.84	264,132	d_{12}-BeP	---	---	---	78.4 ± 10.1	---	---	---
BbF[d]	39.90	252,251,126	d_{12}-BbF	1397 ± 331	5990 ± 200	77%	87.2 ± 3.2	5.79	8.6 – 2600	0.998
d_{12}-IND	43.91	288,289,144	d_{12}-BeP	---	---	---	83.3 ± 7.3	---	---	---
IND[d]	43.97	276,138,137	d_{12}-IND	1613 ± 215	2960 ± 170	46%	82.3 ± 3.5	5.19	8.6 – 2600	0.998
d_{14}-DBA	44.01	292,293,144	d_{12}-BeP	---	---	---	74.0 ± 7.2	---	---	---
DBA[d]	44.14	278,274,139	d_{14}-DBA	303 ± 56	290 ± 4	5%	91.0 ± 7.5	5.12	8.6 – 2600	0.998
d_{12}-BghiP	44.75	288,285	d_{12}-BeP	---	---	---	90.0 ± 11.9	---	---	---
BghiP[d]	44.81	276,274,138	d_{12}-BghiP	3208 ± 352	3937 ± 52	19%	91.3 ± 7.8	7.35	8.6 – 2600	0.999
2-MN[g]	13.30	142,115	d10-AcNap	---	---	---		69.9	250 – 5000	0.999
1-MN[g]	13.66	142,115	d10-AcNap	---	---	---		53.5	250 – 5000	0.999
2,6-DMN[g]	15.83	156,141	d10-AcNap	---	---	---		30.0	250 – 5000	0.999
d10-Acp[g]	17.44	164,162	-IS-	---	---	---		---	---	---
9-MAnt[g]	26.87	192	d10-Pyr	---	---	---		23.7	250 – 5000	0.997
d10-Pyr[g]	29.48	212	-IS-	---	---	---		---	---	---
RET[d,g]	30.90	219,234	d10-Pyr	1993 ± 444	251 ± 38	12%		15.3	125 – 2500	0.997
BghiF[g]	33.74	226	d12-BaA	---	---	---		42.2	50 – 1000	0.999
d12-BaA[g]	34.52	240	-IS-	---	---	---		---	---	---
CYC[d,g]	34.52	226	d12-BaA	331 ± 141	235 ± 60	41%		24.7	50 – 1000	0.992
BeP[g]	39.72	252		---	---	---		50.8	50 – 1000	0.999
PER[d,g]	40.21	252	d12-BaA	276 ± 46	606 ± 13	54%		15.3	50 – 1000	0.999
PIC[d,g]	44.10	278	d12-COR	221 ± 49	390 ± 28	43%		16.8	50 – 1000	0.999
d12-COR	50.11	312	-IS-	---	---	---		---	---	---
COR[d,g]	50.23	300,302	d12-COR	3678 ± 155	2830 ± 460	30%		16.8	50 – 1000	0.998
DBaeP[d,g]	50.34	300,302	d12-COR	800 ± 329	538 ± 24	3%		0	25 – 500	0.999
				Alkanes						
Undecane	6.29	57,71,85	d32-Pentadecane	---	---	---		492	625 – 12500	0.785
Dodecane	8.45	57,71,85	d32-Pentadecane	---	---	---		163	625 – 12500	0.797
Tridecane	10.78	57,71,85	d32-Pentadecane	---	---	---		406	625 – 12500	0.814
Tetradecane	15.48	57,71,85	d32-Pentadecane	---	---	---		561	625 – 12500	0.814
d32-Pentadecane	17.18	66,82,98	-IS-	---	---	---		---	---	---
Pentadecane	17.68	57,71,85	d32-Pentadecane	---	---	---		399	625 – 12500	0.822
Hexadecane	19.77	57,71,85	d32-Pentadecane	---	---	---		310	625 – 12500	0.829
Heptadecane	21.76	57,71,85	d42-Eicosane	---	---	---		73.5	625 – 12500	0.994
Pristane	21.81	57,71,85	d42-Eicosane	---	---	---		879	625 – 12500	0.997
Octadecane	23.65	57,71,85	d42-Eicosane	---	---	---		35.6	625 – 12500	0.987
Phytane	23.74	57,71,85	d42-Eicosane	---	---	---		47.5	625 – 12500	0.995
Nonadecane	25.46	57,71,85	d42-Eicosane	---	---	---		368	625 – 12500	0.999
d42-Eicosane	26.62	66,82,98	-IS-	---	---	---		---	---	---
Eicosane[d]	27.17	57,71,85	d42-Eicosane	1200 ± 890	1900[h]	37%		94.0	625 – 12500	0.999
Heneicosane	28.79	57,71,85	d42-Eicosane	---	---	---		130	625 – 12500	0.998

Docosane[d]	30.37	57,71,85	d50-Tetracosane	2900 ± 130	5200[h]	44%	64.6	625 – 12500	0.999
Tricosane[d]	31.85	57,71,85	d50-Tetracosane	6800 ± 370	16000[h]	58%	102	625 – 12500	0.999
d50-Tetracosane	32.73	66,82,98	-IS-	---	---	---	---	---	---
Tetracosane[d]	33.32	57,71,85	d50-Tetracosane	9500 ± 470	27000[h]	65%	67.5	625 – 12500	0.999
Pentacosane[d]	34.68	57,71,85	d50-Tetracosane	68000 ± 2100	65000[h]	5%	139	625 – 12500	0.999
Hexacosane[d]	36.01	57,71,85	d50-Tetracosane	67000 ± 2600	66000[h]	2%	139	625 – 12500	0.999
Heptacosane[d]	37.30	57,71,85	d58-Triacontane	65000 ± 5200	62000[h]	5%	342	625 – 12500	0.995
Octacosane[d]	38.53	57,71,85	d58-Triacontane	39000 ± 630	42000[h]	7%	509	625 – 12500	0.997
Nonacosane[d]	39.72	57,71,85	d58-Triacontane	76000 ± 2400	58000[h]	31%	491	625 – 12500	0.999
d58-Triacontane	40.24	66,82,98	-IS-	---	---	---	---	---	---
Triacontane[d]	40.85	57,71,85	d58-Triacontane	24000 ± 1800	25000[h]	4%	200	625 – 12500	0.998
Hentriacontane[d]	42.04	57,71,85	d66-Dotriacontane	46000 ± 3100	41000[h]	12%	119	625 – 12500	0.999
d66-Dotriacontane	42.59	66,82,98	-IS-	---	---	---	---	---	---
Dotriacontane[d]	43.39	57,71,85	d66-Dotriacontane	15000 ± 630	14000[h]	7%	217	625 – 12500	0.994
Triatriacontane	44.75	57,71,85	d66-Dotriacontane	---	---	---	549	625 – 12500	0.984
Tetratriacontane	45.88	57,71,85	d74-Hexatriacontane	---	---	---	211	625 – 12500	0.998
Pentatriacontane	47.10	57,71,85	d74-Hexatriacontane	---	---	---	87.7	625 – 12500	0.996
d74-Hexatriacontane	47.53	66,82,98	-IS-	---	---	---	---	---	---
Hexatriacontane	48.47	57,71,85	d74-Hexatriacontane	---	---	---	158	625 – 12500	0.994
Heptatriacontane	50.03	57,71,85	d74-Hexatriacontane	---	---	---	210	625 – 12500	0.992
Octatriacontane	51.83	57,71,85	d74-Hexatriacontane	---	---	---	303	625 – 12500	0.990
Nonatriacontane	53.95	57,71,85	d74-Hexatriacontane	---	---	---	392	625 – 12500	0.989
Hopanes and Steranes									
αββ-20R-C_{27}-Cholestane	38.86	218,217	d4-Cholestane	---	---	---	11.9	25 – 500	0.999
ααα-20S-C_{27}-Cholestane	38.99	218,217	d4-Cholestane	---	---	---	16.8	25 – 500	0.996
d4-Cholestane	39.29	221	-IS-	---	---	---	---	---	---
αββ-20R-Ergostane	40.18	218,217	d4-Cholestane	---	---	---	15.3	25 – 500	0.999
17α(H)-22,29,30-Trisnorhopane[d]	40.39	191	d4-Cholestane	2900 ± 330	2800[h]	4%	54.0	25 – 500	0.999
αββ-20R-Sitosane	41.13	218,217	d4-Cholestane	---	---	---	16.8	25 – 500	0.981
17α(H)-21β(H)-30-Norhopane	41.91	191	d4-Cholestane	---	---	---	16.8	12.5 – 250	0.999
17α(H)-21β(H)-Hopane	43.04	191	d4-Cholestane	---	---	---	11.9	25 – 500	0.999
17α(H)-21β(H)-22S-Homohopane[d]	44.43	191	d4-Cholestane	11000 ± 1300	5400[h]	104%	15.3	12.5 – 250	0.999

Data Collected

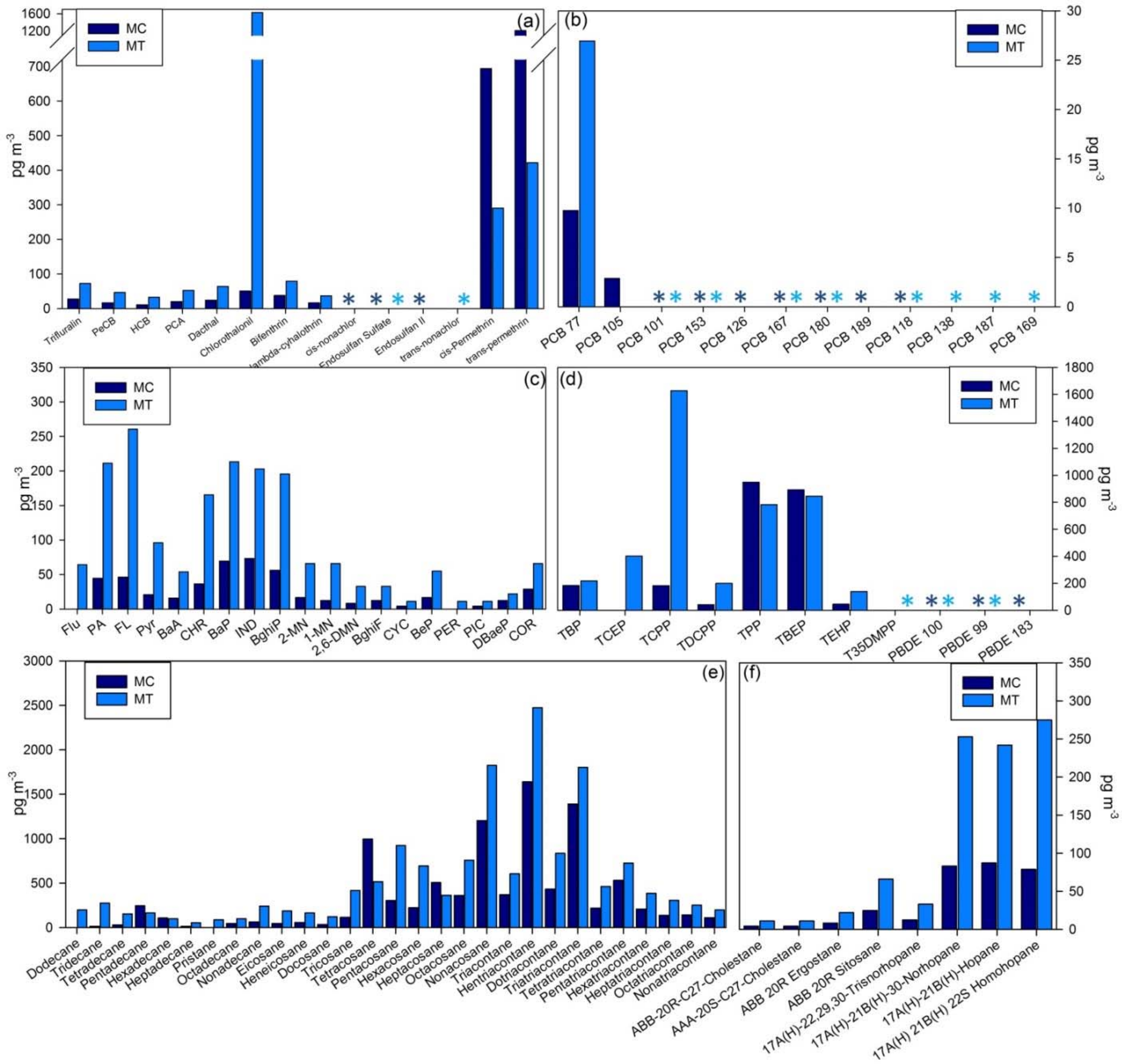

Fig 1. Compounds detected in the environmental samples included (a) CUPS/HUPS, (b) PCBs, (c) PAHs, (d) current and historic-use flame retardants (OPFRs and PBDEs), (e) alkanes, and (f) hopanes and steranes. Dark blue bars indicate the Manvel Croix (MC; suburban area south of Houston, TX) location, while the light blue indicates the Moody Tower (MT; downtown Houston, TX) location. * indicate that compounds were detected below MDLs and color indicates site. 75 of the 139 target analytes in Table 1 were detected.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

NA

Goals and Anticipated Issues for the Succeeding Reporting Period

We intend to finalize filter preparation and shipment for inorganic ion analysis for Conroe in collaboration with 14-024.

We intend to prepare posters on organic analysis, spatio-temporal bulk carbon trends for presentation at AGU in December 2014. These will be submitted to AQRP for pre-approval prior to presentation.
Manuscript preparation for combined organic tracer and contaminant paper will continue in November.

Detailed Analysis of the Progress of the Task Order to Date

- Shared WSOC data for Conroe.
- Completed WSOC analysis for Conroe, Moody Tower, Manvel Croix and La Porte.
- Purchased and prepared standards for organic tracer analysis
- Began preliminary sample analysis for organic tracers and contaminants at Moody Tower and Manvel Croix.
- Validated method for organic tracers and contaminants using NIST SRMs 1649b and 2585.

Submitted to AQRP by: Rebecca J. Sheesley
Principal Investigator: Rebecca J. Sheesley