

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032419\
 Data File : VX008404.D
 Acq On : 24 Mar 2019 19:57
 Operator : JC/SP
 Sample : K2059-06
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	16	20	22	rBV	405737	486544	10.03%	0.809%
2	1.404	37	41	46	rBV	369741	376332	7.76%	0.626%
3	1.788	99	104	117	rVB	2483527	3451708	71.14%	5.742%
4	2.001	134	139	147	rVB2	88733	148685	3.06%	0.247%
5	2.263	176	182	191	rVB	185323	296829	6.12%	0.494%
6	2.392	196	203	210	rBV	150369	299549	6.17%	0.498%
7	2.843	261	277	280	rBV	341434	730712	15.06%	1.216%
8	2.891	280	285	290	rVV	632165	1161285	23.93%	1.932%
9	3.172	321	331	346	rVB	798316	1843579	37.99%	3.067%
10	3.818	426	437	445	rBV2	82175	208656	4.30%	0.347%
11	3.928	445	455	464	rBV	100831	270556	5.58%	0.450%
12	4.196	493	499	506	rVV2	69844	208412	4.30%	0.347%
13	4.306	510	517	524	rVV	69536	222016	4.58%	0.369%
14	4.403	524	533	544	rVV	443265	1295368	26.70%	2.155%
15	4.531	544	554	570	rVB3	75778	245957	5.07%	0.409%
16	5.300	656	680	694	rVB7	65206	414742	8.55%	0.690%
17	5.501	699	713	720	rBV	154105	467588	9.64%	0.778%
18	5.604	720	730	734	rVV4	178883	678479	13.98%	1.129%
19	5.659	735	739	745	rVV	255782	723669	14.91%	1.204%
20	5.726	745	750	768	rVV3	227244	742814	15.31%	1.236%
21	5.927	770	783	796	rVV	344597	1036935	21.37%	1.725%
22	6.062	796	805	811	rVV	172778	445554	9.18%	0.741%
23	6.141	811	818	830	rVV	309810	882916	18.20%	1.469%
24	6.263	830	838	847	rVV5	174626	727780	15.00%	1.211%
25	6.354	847	853	862	rVV2	242037	726940	14.98%	1.209%
26	6.458	862	870	882	rVB2	171987	482135	9.94%	0.802%
27	6.702	896	910	925	rVB3	38109	119348	2.46%	0.199%
28	6.860	925	936	943	rBV	408275	1011316	20.84%	1.682%
29	6.939	943	949	960	rVB3	143105	410075	8.45%	0.682%
30	7.061	960	969	977	rBV	61012	151520	3.12%	0.252%
31	7.256	993	1001	1009	rBV	236466	507897	10.47%	0.845%
32	7.445	1022	1032	1046	rVB3	271517	808657	16.67%	1.345%
33	7.641	1058	1064	1074	rVB	54856	123867	2.55%	0.206%
34	7.732	1074	1079	1092	rVB2	72074	158814	3.27%	0.264%

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35	7.848	1092	1098	1105	rVB3	58726	122780	2.53%	0.204%
36	7.958	1105	1116	1124	rBV5	92238	343648	7.08%	0.572%
37	8.055	1124	1132	1144	rVB	110658	287441	5.92%	0.478%
38	8.177	1144	1152	1154	rBV2	206816	395398	8.15%	0.658%
39	8.214	1154	1158	1163	rVV	434632	771118	15.89%	1.283%
40	8.256	1163	1165	1175	rVB4	67695	117716	2.43%	0.196%
41	8.378	1176	1185	1190	rBV5	86137	163784	3.38%	0.272%
42	8.500	1200	1205	1209	rBV2	87885	135969	2.80%	0.226%
43	8.567	1211	1216	1226	rVB3	245597	473027	9.75%	0.787%
44	8.671	1226	1233	1235	rBV2	122815	215548	4.44%	0.359%
45	8.714	1235	1240	1247	rVB	877468	1412828	29.12%	2.350%
46	8.787	1247	1252	1257	rBV3	103374	188012	3.87%	0.313%
47	8.884	1264	1268	1270	rBV2	84143	138974	2.86%	0.231%
48	8.988	1280	1285	1289	rVV	140339	215257	4.44%	0.358%
49	9.037	1289	1293	1298	rVB3	74443	128435	2.65%	0.214%
50	9.165	1306	1314	1319	rVV	131590	245901	5.07%	0.409%
51	9.220	1319	1323	1335	rVB	351418	595545	12.27%	0.991%
52	9.518	1369	1372	1375	rVV2	83132	129741	2.67%	0.216%
53	9.567	1375	1380	1385	rVV2	120329	261040	5.38%	0.434%
54	9.658	1392	1395	1401	rVV2	136692	210582	4.34%	0.350%
55	9.823	1415	1422	1428	rBV2	117788	205457	4.23%	0.342%
56	10.110	1465	1469	1474	rVV	763170	999972	20.61%	1.664%
57	10.158	1474	1477	1479	rVV2	93438	120191	2.48%	0.200%
58	10.195	1479	1483	1488	rVV4	97412	228972	4.72%	0.381%
59	10.250	1488	1492	1497	rVB	385156	474669	9.78%	0.790%
60	10.360	1506	1510	1515	rVB	267294	375452	7.74%	0.625%
61	10.640	1548	1556	1562	rBV2	87114	179876	3.71%	0.299%
62	11.018	1612	1618	1624	rBV	1642731	2016932	41.57%	3.355%
63	11.134	1633	1637	1642	rBV	622005	778675	16.05%	1.295%
64	11.329	1663	1669	1670	rBV2	115948	160643	3.31%	0.267%
65	11.359	1670	1674	1682	rVV	1041572	1294226	26.67%	2.153%
66	11.451	1682	1689	1693	rVV2	63020	115139	2.37%	0.192%
67	11.664	1717	1724	1733	rBV	515811	687270	14.16%	1.143%
68	11.768	1734	1741	1744	rBV	75414	120975	2.49%	0.201%
69	11.920	1760	1766	1767	rBV	120103	143379	2.95%	0.239%
70	11.945	1767	1770	1775	rVB	213002	268159	5.53%	0.446%
71	12.079	1786	1792	1798	rBV	763309	979755	20.19%	1.630%

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72	12.140	1798	1802	1813	rBV2	167676	283091	5.83%	0.471%
73	12.298	1822	1828	1835	rBV	3964263	4852328	100.00%	8.072%
74	12.365	1835	1839	1849	rVB2	440965	675878	13.93%	1.124%
75	12.457	1849	1854	1860	rBV	336788	414295	8.54%	0.689%
76	12.518	1860	1864	1870	rVB	194269	233272	4.81%	0.388%
77	12.670	1883	1889	1892	rBV	2937740	3649362	75.21%	6.071%
78	12.701	1892	1894	1898	rVB	338301	349005	7.19%	0.581%
79	12.755	1898	1903	1910	rBV2	1460885	2120736	43.71%	3.528%
80	12.896	1921	1926	1932	rVB2	90854	135216	2.79%	0.225%
81	12.975	1932	1939	1944	rBV	1940132	2342147	48.27%	3.896%
82	13.079	1951	1956	1965	rBV3	203347	346702	7.15%	0.577%
83	13.170	1965	1971	1973	rBV2	210340	314961	6.49%	0.524%
84	13.225	1976	1980	1987	rVB	803558	999593	20.60%	1.663%
85	13.292	1987	1991	1992	rBV	139785	153225	3.16%	0.255%
86	13.310	1992	1994	1996	rVV	147533	183180	3.78%	0.305%
87	13.347	1996	2000	2006	rVV2	1250534	1894919	39.05%	3.152%
88	13.426	2010	2013	2018	rVB	168515	240729	4.96%	0.400%
89	13.481	2018	2022	2029	rVB2	110856	147920	3.05%	0.246%
90	13.560	2029	2035	2038	rBV2	97129	153376	3.16%	0.255%
91	13.597	2038	2041	2044	rVV	297845	416371	8.58%	0.693%
92	13.633	2044	2047	2052	rVB3	386081	504688	10.40%	0.840%
93	13.719	2058	2061	2067	rVB2	332573	584571	12.05%	0.972%
94	13.835	2076	2080	2089	rVB2	84997	167929	3.46%	0.279%
95	13.981	2097	2104	2109	rBV2	129698	200855	4.14%	0.334%
96	14.133	2124	2129	2134	rBV	210248	263761	5.44%	0.439%
97	14.274	2147	2152	2157	rBV	155887	246535	5.08%	0.410%
98	14.377	2165	2169	2174	rBV	128853	154072	3.18%	0.256%
99	14.432	2174	2178	2183	rVB2	122558	169368	3.49%	0.282%
100	14.834	2239	2244	2254	rBV	250880	343325	7.08%	0.571%

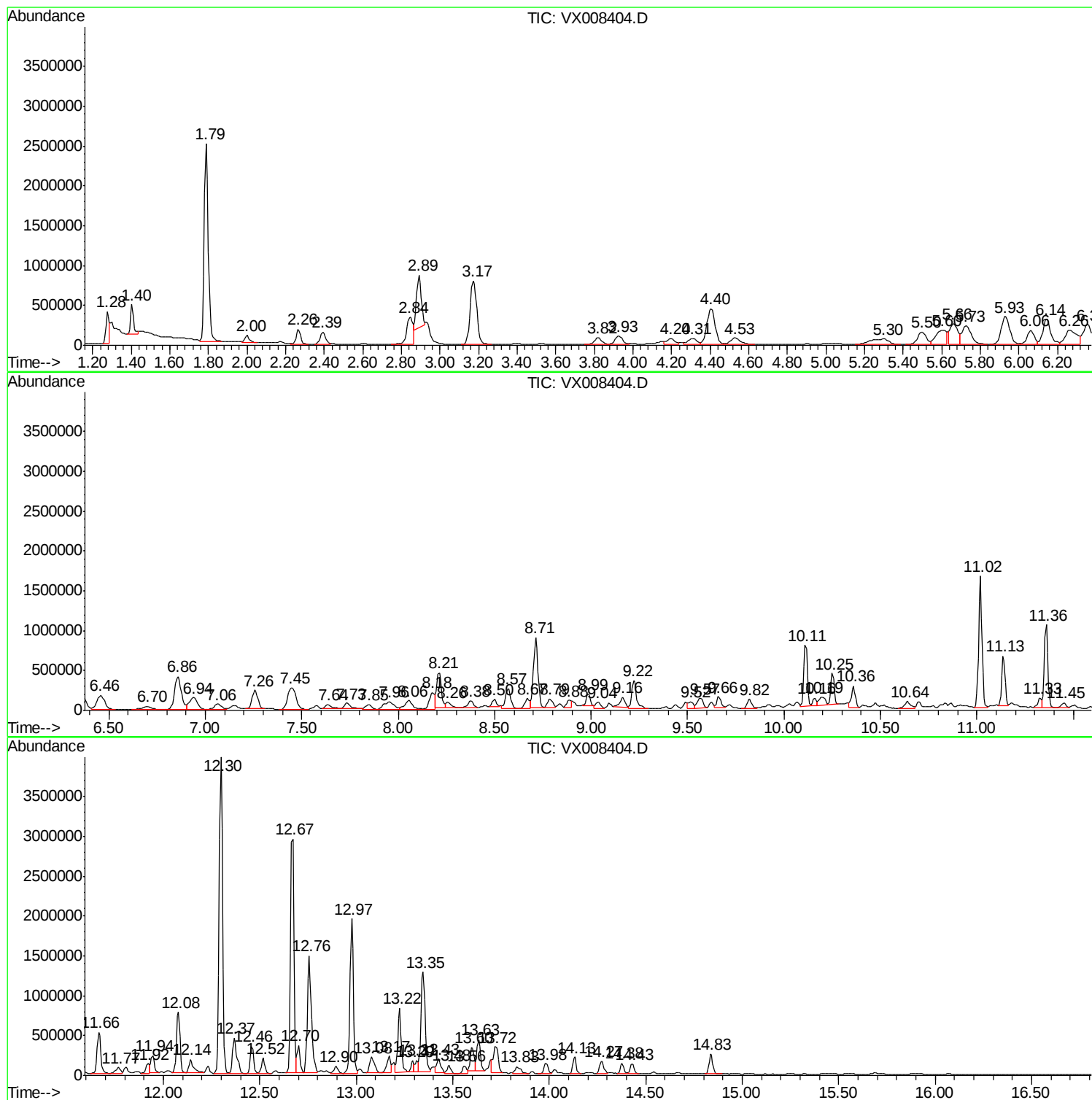
Sum of corrected areas: 60111130

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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 Peak Number 1 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	238.49 ug/l	3451710	Pentafluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	94
2			Pentane	72	C5H12	000109-66-0	33
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	9
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	9

 Peak Number 2 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	80.24 ug/l	1161290	Pentafluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-			86	C6H14	000107-83-5	91
2	Pentane			72	C5H12	000109-66-0	49
3	Butane, 2,3-dimethyl-			86	C6H14	000079-29-8	47
4	Hexane, 2,3-dimethyl-			114	C8H18	000584-94-1	38
5	Pentane, 3,3-dimethyl-			100	C7H16	000562-49-2	28

 Peak Number 3 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	127.38 ug/l	1843580	Pentafluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40

 Peak Number 4 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
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4.40	89.50 ug/l	1295370	Pentafluorobenzene	5.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentane, methyl-	84 C6H12	000096-37-7 91
2		Cyclopropane, propyl-	84 C6H12	002415-72-7 80
3		Cyclobutane, ethyl-	84 C6H12	004806-61-5 72
4		1H-Tetrazole, 5-methyl-	84 C2H4N4	004076-36-2 50
5		Cyclopentane, 1,1-dimethyl-	98 C7H14	001638-26-2 43

 Peak Number 5 Hexane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	71.64 ug/l	1036940	Pentafluorobenzene	5.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Hexane, 3-methyl-	100 C7H16	000589-34-4 91
2		Heptane	100 C7H16	000142-82-5 80
3		Heptane, 4-methyl-	114 C8H18	000589-53-7 59
4		Pentane, 3-ethyl-	100 C7H16	000617-78-7 58
5		Decane, 3,3,4-trimethyl-	184 C13H28	049622-18-6 53

 Peak Number 6 Benzene, 1-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	247.63 ug/l	4852330	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-propenyl-	118 C9H10	000637-50-3 90
2		Benzene, cyclopropyl-	118 C9H10	000873-49-4 60
3		Benzene, 2-propenyl-	118 C9H10	000300-57-2 60
4		Indane	118 C9H10	000496-11-7 60
5		Benzene, 1-ethenyl-3-methyl-	118 C9H10	000100-80-1 42

 Peak Number 7 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	186.24 ug/l	3649360	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual

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1 Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2 o-Cymene	134	C10H14	000527-84-4	95
3 Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4 Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5 Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94

 Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	108.23 ug/l	2120740	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3		Indan, 1-methyl-	132	C10H12	000767-58-8	87
4		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87
5		Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87

 Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	119.53 ug/l	2342150	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4		o-Cymene	134	C10H14	000527-84-4	95
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94

 Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	96.70 ug/l	1894920	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2		2,4-Dimethylstyrene	132	C10H12	002234-20-0	90
3		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	70

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4 Benzene, (1-methyl-1-propenyl)-,...	132 C10H12	000768-00-3	70
5 Benzene, 2-ethenyl-1,3-dimethyl-	132 C10H12	002039-90-9	70

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.79	238.5	ug/l	3451710	1	5.66	723669	50.0
Pentane, 2-methyl-	2.89	80.2	ug/l	1161290	1	5.66	723669	50.0
Pentane, 3-methyl-	3.17	127.4	ug/l	1843580	1	5.66	723669	50.0
Cyclopentane, met...	4.40	89.5	ug/l	1295370	1	5.66	723669	50.0
Hexane, 3-methyl-	5.93	71.6	ug/l	1036940	1	5.66	723669	50.0
Benzene, 1-propenyl-	12.30	247.6	ug/l	4852330	4	12.08	979755	50.0
Benzene, 4-ethyl-...	12.67	186.2	ug/l	3649360	4	12.08	979755	50.0
Benzene, 1-etheny...	12.76	108.2	ug/l	2120740	4	12.08	979755	50.0
Benzene, 1,2,3,4-...	12.98	119.5	ug/l	2342150	4	12.08	979755	50.0
Benzene, 2-etheny...	13.35	96.7	ug/l	1894920	4	12.08	979755	50.0