LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX102220\
Data File : VX019058.D
Acq On : 23 Oct 2020 03:56
Operator : JC/SP
Sample : L4417-21
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.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	1.392	43	50	55	rBV	656888	716235	1.12%	0.197%
2	1.776	108	113	128	rVB	8345938	10954610	17.11%	3.015%
3	1.989	143	148	161	rVV3	2585334	4844761	7.57%	1.334%
4	2.105	161	167	173	rVV	1712997	2456228	3.84%	0.676%
5	2.197	177	182	186	rVV	985535	1496549	2.34%	0.412%
6	2.251	186	191	204	rVV	5182340	8134698	12.71%	2.239%
7	2.379	204	212	228	rVB	1086242	2193259	3.43%	0.604%
8	2.794	266	280	283	rBV	1752370	3656130	5.71%	1.006%
9	2.873	289	293	296	rBV	794793	1241986	1.94%	0.342%
10	2.916	296	300	327	rVB2	1479315	3622705	5.66%	0.997%
11	3.154	327	339	362	rVB2	1394804	3398861	5.31%	0.936%
12	3.501	387	396	408	rVB	367981	831074	1.30%	0.229%
13	3.794	437	444	453	rVB	1148280	2719294	4.25%	0.749%
14	3.904	453	462	468	rBV	578063	1512512	2.36%	0.416%
15	4.172	496	506	516	rBV	663204	1729116	2.70%	0.476%
16	4.379	530	540	551	rVB	1755369	5072761	7.92%	1.396%
17	4.501	551	560	574	rVB	255715	779344	1.22%	0.215%
18	5.275	663	687	704	rVB	992019	3285046	5.13%	0.904%
19	5.464	704	718	724	rBV	232401	702809	1.10%	0.193%
20	5.556	724	733	741	rBV3	698649	2299882	3.59%	0.633%
21	5.696	751	756	776	rVB3	303263	1121701	1.75%	0.309%
22	5.903	778	790	802	rBV3	305635	929662	1.45%	0.256%
23	6.117	816	825	837	rVB	2376159	6102381	9.53%	1.680%
24	6.281	837	852	855	rBV2	661030	2269244	3.54%	0.625%
25	6.434	869	877	887	rVB2	251844	688286	1.08%	0.189%
26	6.830	934	942	948	rBV	505025	1293737	2.02%	0.356%
27	6.915	950	956	965	rVB5	398447	1198210	1.87%	0.330%
28	7.232	1001	1008	1026	rVB	472529	1080168	1.69%	0.297%
29	7.440	1026	1042	1052	rBV3	692267	1845433	2.88%	0.508%
30	7.933	1112	1123	1131	rBV3	258943	901361	1.41%	0.248%
31	8.037	1131	1140	1151	rVB	355677	780393	1.22%	0.215%
32	8.159	1151	1160	1162	rBV	637008	1148212	1.79%	0.316%
33	8.189	1162	1165	1170	rVB	651032	1104258	1.73%	0.304%
34	8.549	1217	1224	1235	rVB	672381	1176197	1.84%	0.324%

LSC Area Percent Report

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Instrument : MSVOA_X
ClientSampleId : MW-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Title : SW846 8260

35	8.695	1235	1248	1253	rBV2	1276709	2331720	3.64%	0.642%
36	8.775	1253	1261	1272	rVB	25804343	41830237	65.35%	11.514%
37	10.098	1473	1478	1482	rVB	1048526	1368518	2.14%	0.377%
38	10.244	1495	1502	1507	rBV	43537201	64014182	100.00%	17.621%
39	10.348	1512	1519	1524	rBV	21802910	29395457	45.92%	8.091%
40	10.683	1568	1574	1583	rVB	5222786	6460986	10.09%	1.778%
41	11.006	1619	1627	1632	rBV	13507926	17467016	27.29%	4.808%
42	11.122	1641	1646	1651	rBV	989430	1277860	2.00%	0.352%
43	11.347	1677	1683	1689	rVB	14199996	17873015	27.92%	4.920%
44	11.421	1689	1695	1696	rVV	3599419	4311378	6.74%	1.187%
45	11.439	1696	1698	1702	rVV	3328713	3602896	5.63%	0.992%
46	11.488	1702	1706	1714	rVB	3239932	4086113	6.38%	1.125%
47	11.652	1727	1733	1743	rVB	3652006	4379607	6.84%	1.206%
48	11.792	1751	1756	1761	rVB	11583667	13827525	21.60%	3.806%
49	12.061	1795	1800	1805	rVB	1370589	1695414	2.65%	0.467%
50	12.128	1805	1811	1815	rBV	3296161	4054555	6.33%	1.116%
51	12.286	1831	1837	1844	rBV	15586868	19856982	31.02%	5.466%
52	12.353	1844	1848	1858	rVB2	1175883	2003980	3.13%	0.552%
53	12.451	1858	1864	1868	rBV2	646255	904273	1.41%	0.249%
54	12.500	1868	1872	1878	rVB	999290	1205621	1.88%	0.332%
55	12.652	1891	1897	1900	rBV	4187600	4815592	7.52%	1.326%
56	12.737	1907	1911	1919	rVB2	1626199	2275473	3.55%	0.626%
57	12.963	1940	1948	1951	rBV	2616451	3259977	5.09%	0.897%
58	13.000	1951	1954	1959	rVB	668626	780203	1.22%	0.215%
59	13.207	1984	1988	1994	rVB	1881993	2210976	3.45%	0.609%
60	13.329	2003	2008	2013	rVB2	3935485	5396742	8.43%	1.486%
61	13.463	2025	2030	2036	rVB	695585	869894	1.36%	0.239%
62	13.816	2082	2088	2097	rBV	11272113	13638268	21.31%	3.754%
63	14.676	2224	2229	2240	rVB	2342481	2908014	4.54%	0.800%
64	14.822	2247	2253	2261	rBV	1462039	1901192	2.97%	0.523%

Sum of corrected areas: 363290769

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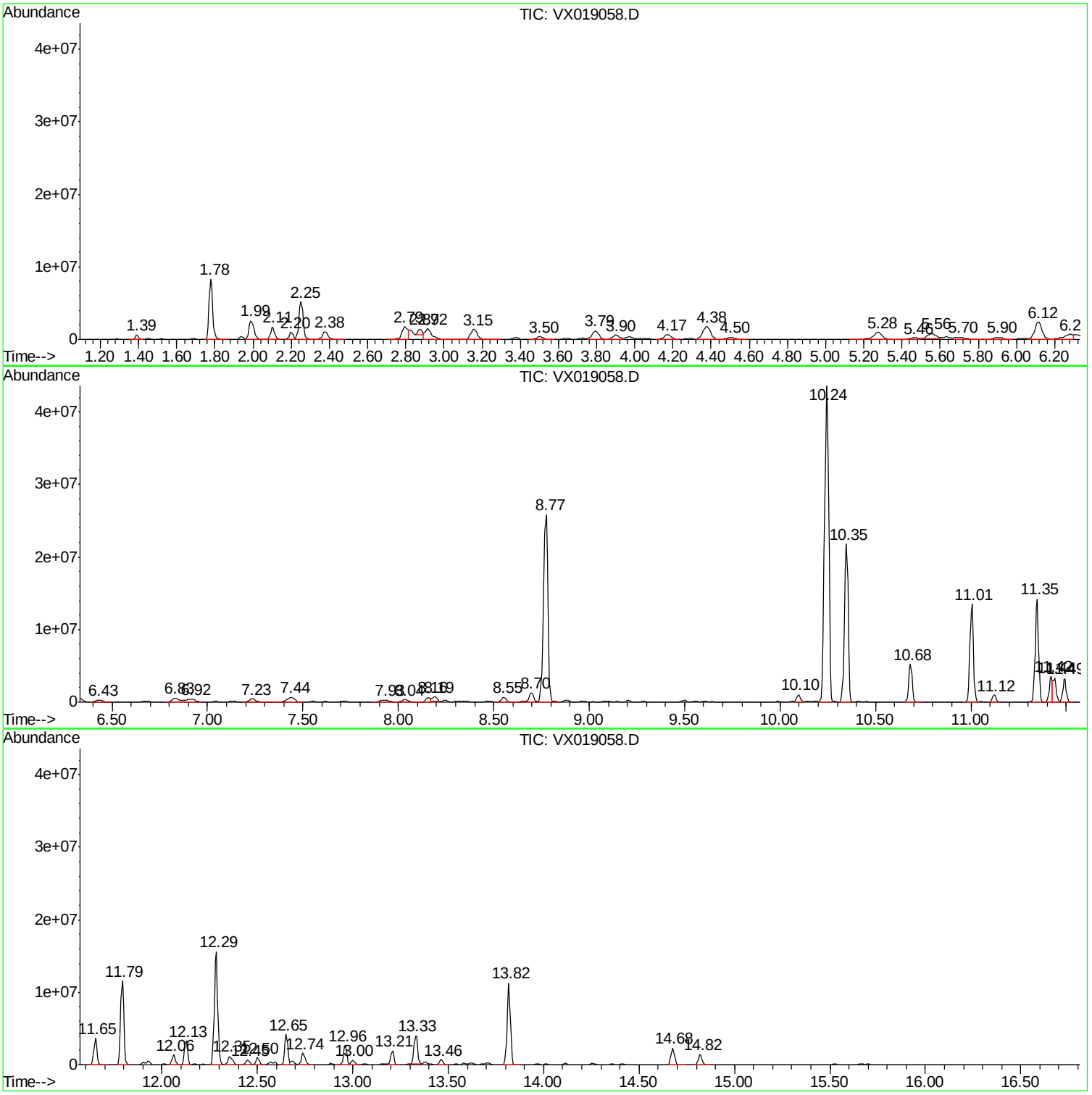
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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



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TIC Integration Parameters: LSCINT.P

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	488.30 ug/l	10954600	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	47
3	Pentane	72	C5H12	000109-66-0	38
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33

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Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	215.96 ug/l	4844760	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	78
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Isobutylene epoxide	72	C4H8O	000558-30-5	43
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	40
5	Butane, 2-methyl-	72	C5H12	000078-78-4	36

****

Peak Number 3 2-Butene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	362.61 ug/l	8134700	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	2-Methyl-1-butene	70	C5H10	000563-46-2	90
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	80

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Peak Number 4 Cyclopentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Acq On : 23 Oct 2020 03:56
Operator : JC/SP
Sample : L4417-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	162.97 ug/l	3656130	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	1,4-Pentadiene	68	C5H8	000591-93-5	62
3	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	56
4	1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	53
5	Cyclopropane, ethylidene-	68	C5H8	018631-83-9	53

****

Peak Number 5 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	161.48 ug/l	3622710	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	Methyl propargyl ether	70	C4H6O	000627-41-8	45
4	2-Pentene, (E)-	70	C5H10	000646-04-8	43
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	43

****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	226.12 ug/l	5072760	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	83
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	56
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	52

****

Peak Number 7 Cyclopentene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.28	146.43 ug/l	3285050	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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

1	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3 87
2	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0 87
3	Cyclohexene	82	C6H10	000110-83-8 87
4	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4 86
5	Isopropenylcyclopropane	82	C6H10	004663-22-3 86

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Peak Number 8 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	585.61 ug/l	19857000	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53

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Peak Number 9 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	142.02 ug/l	4815590	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	o-Cymene	134	C10H14	000527-84-4	97
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95

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Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	159.16 ug/l	5396740	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Indan, 1-methyl-	132	C10H12	000767-58-8	70
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70

Library Search Compound Report

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Quant Title : SW846 8260

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

4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70

Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	1.78	488.3	ug/l	10954600	1	5.63	1121700	50.0
Pentane	1.99	216.0	ug/l	4844760	1	5.63	1121700	50.0
2-Butene, 2-methyl-	2.25	362.6	ug/l	8134700	1	5.63	1121700	50.0
Cyclopentene	2.79	163.0	ug/l	3656130	1	5.63	1121700	50.0
1-Pentene	2.92	161.5	ug/l	3622710	1	5.63	1121700	50.0
Cyclopentane, met...	4.38	226.1	ug/l	5072760	1	5.63	1121700	50.0
Cyclopentene, 3-m...	5.28	146.4	ug/l	3285050	1	5.63	1121700	50.0
Benzene, cyclopro...	12.29	585.6	ug/l	19857000	4	12.06	1695410	50.0
Benzene, 1-ethyl-...	12.65	142.0	ug/l	4815590	4	12.06	1695410	50.0
Benzene, 2-etheny...	13.33	159.2	ug/l	5396740	4	12.06	1695410	50.0