

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
 Data File : VX033040.D
 Acq On : 24 Nov 2022 05:41
 Operator : JC/MD
 Sample : N5741-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-32

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033040.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	42	rBV	263720	388685	66.69%	6.787%
2	1.752	105	109	115	rVB2	8041	11145	1.91%	0.195%
3	2.782	269	278	282	rBV2	3720	7617	1.31%	0.133%
4	3.111	324	332	340	rVB2	8808	19540	3.35%	0.341%
5	3.757	427	438	447	rBV3	3383	11196	1.92%	0.195%
6	4.300	519	527	537	rVB3	6065	17203	2.95%	0.300%
7	5.385	694	705	716	rBV2	65621	191162	32.80%	3.338%
8	5.556	722	733	755	rVB	139587	411082	70.53%	7.178%
9	5.958	787	799	809	rBV	71278	190176	32.63%	3.321%
10	6.037	810	812	820	rVB2	3391	6757	1.16%	0.118%
11	6.245	835	846	857	rVB2	6391	21703	3.72%	0.379%
12	6.763	921	931	942	rBV	210052	505292	86.69%	8.823%
13	7.373	1022	1031	1041	rVB7	4348	12497	2.14%	0.218%
14	7.982	1124	1131	1139	rVB	6709	13463	2.31%	0.235%
15	8.110	1145	1152	1156	rBV	10978	23517	4.03%	0.411%
16	8.141	1156	1157	1162	rVB	5710	6204	1.06%	0.108%
17	8.506	1212	1217	1225	rVB4	3707	6432	1.10%	0.112%
18	8.647	1234	1240	1248	rVV	336377	515718	88.48%	9.005%
19	8.720	1248	1252	1258	rVB	4059	6980	1.20%	0.122%
20	8.958	1287	1291	1297	rVB4	6553	11269	1.93%	0.197%
21	9.049	1301	1306	1311	rVB2	3737	5959	1.02%	0.104%
22	10.055	1465	1471	1481	rBV	435444	582846	100.00%	10.177%
23	10.195	1489	1494	1501	rBV	215095	280341	48.10%	4.895%
24	10.305	1505	1512	1518	rVB2	11636	16570	2.84%	0.289%
25	10.640	1563	1567	1574	rBV	6821	9181	1.58%	0.160%
26	10.963	1615	1620	1625	rBV	19973	24899	4.27%	0.435%
27	11.079	1634	1639	1650	rBV	278611	357472	61.33%	6.242%
28	11.305	1671	1676	1685	rBV	57694	69021	11.84%	1.205%
29	11.402	1689	1692	1697	rVB2	7336	9158	1.57%	0.160%
30	11.616	1721	1727	1735	rVB	57224	73051	12.53%	1.276%
31	11.750	1744	1749	1755	rBV	120129	151829	26.05%	2.651%
32	11.969	1781	1785	1788	rBV2	9674	11194	1.92%	0.195%
33	12.024	1788	1794	1801	rVV	440935	576950	98.99%	10.074%
34	12.085	1801	1804	1809	rVB	15060	19624	3.37%	0.343%
35	12.244	1824	1830	1838	rBV	286624	355658	61.02%	6.210%
36	12.311	1838	1841	1848	rVB3	14876	25144	4.31%	0.439%

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37	12.414	1853	1858	1862	rBV2	15129	21648	3.71%	0.378%
38	12.463	1862	1866	1872	rVB	19876	23855	4.09%	0.417%
39	12.530	1872	1877	1885	rBV	18247	27143	4.66%	0.474%
40	12.615	1885	1891	1893	rBV	18855	22898	3.93%	0.400%
41	12.646	1893	1896	1900	rVV	15186	18937	3.25%	0.331%
42	12.701	1900	1905	1913	rVB2	47020	69767	11.97%	1.218%
43	12.920	1935	1941	1944	rBV	33225	40345	6.92%	0.704%
44	12.963	1944	1948	1955	rVB	65259	76691	13.16%	1.339%
45	13.170	1978	1982	1987	rVB	36938	44426	7.62%	0.776%
46	13.292	1997	2002	2007	rVB2	68385	90425	15.51%	1.579%
47	13.341	2007	2010	2013	rBV4	5857	7243	1.24%	0.126%
48	13.426	2019	2024	2029	rVB	23875	32986	5.66%	0.576%
49	13.542	2039	2043	2046	rVV	9053	13055	2.24%	0.228%
50	13.585	2046	2050	2056	rVV3	9759	20400	3.50%	0.356%
51	13.664	2060	2063	2069	rVB2	8180	13867	2.38%	0.242%
52	13.774	2075	2081	2090	rBV	94106	122895	21.09%	2.146%
53	13.865	2090	2096	2101	rVV2	8406	14347	2.46%	0.251%
54	13.926	2101	2106	2110	rVV3	6393	9048	1.55%	0.158%
55	14.079	2124	2131	2136	rBV	6256	8837	1.52%	0.154%
56	14.213	2148	2153	2159	rBV3	8305	13541	2.32%	0.236%
57	14.323	2167	2171	2175	rBV2	4278	6031	1.03%	0.105%
58	14.371	2175	2179	2183	rVB2	5432	6739	1.16%	0.118%
59	14.481	2193	2197	2203	rBV3	4419	6503	1.12%	0.114%
60	14.609	2211	2218	2221	rBV3	2918	6329	1.09%	0.111%
61	14.780	2240	2246	2251	rBV	35134	45092	7.74%	0.787%
62	15.481	2355	2361	2365	rBV2	5229	8420	1.44%	0.147%
63	15.615	2377	2383	2387	rBV	5912	9215	1.58%	0.161%

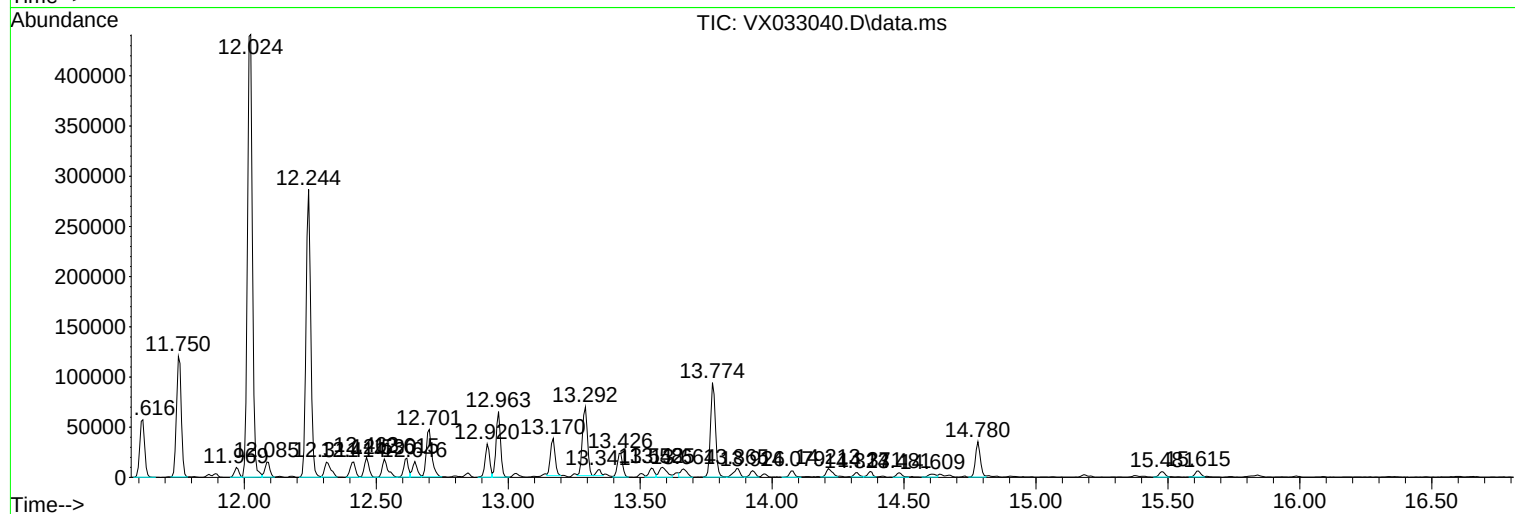
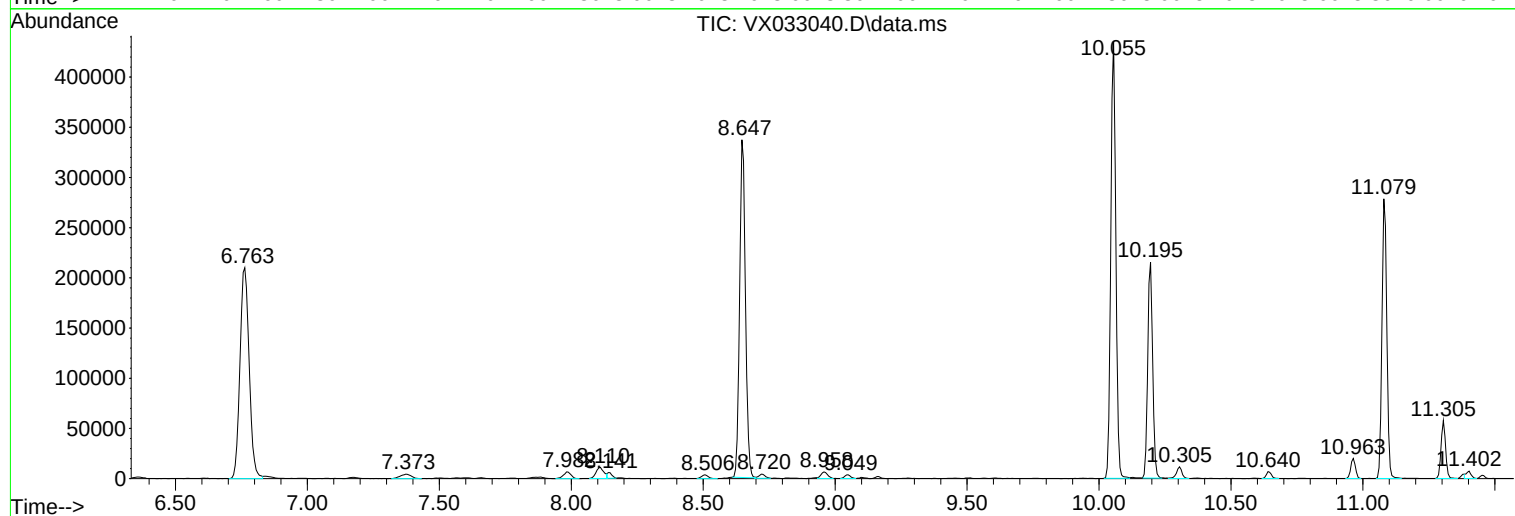
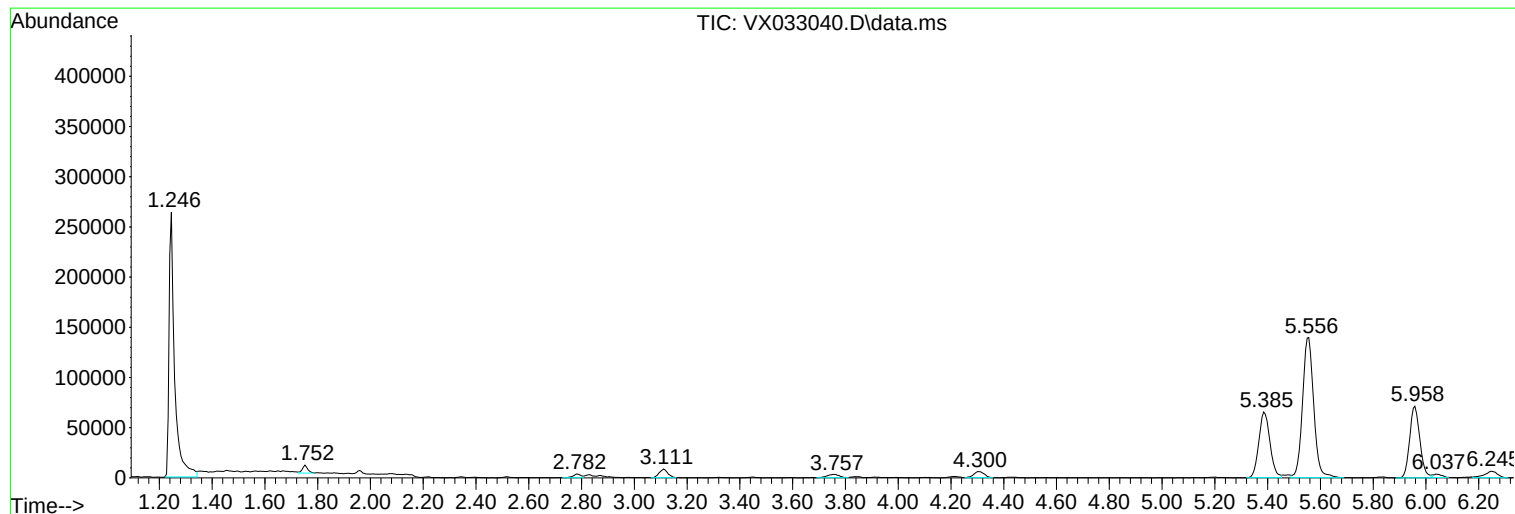
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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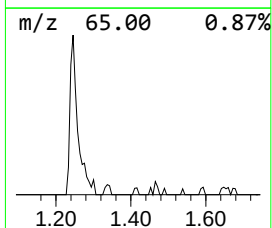
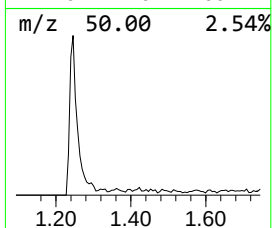
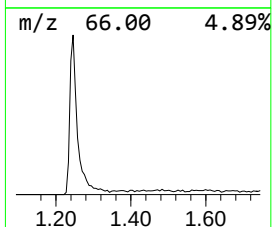
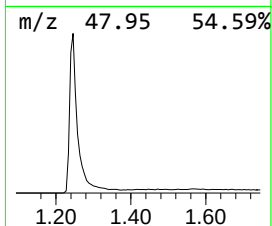
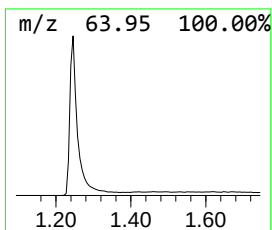
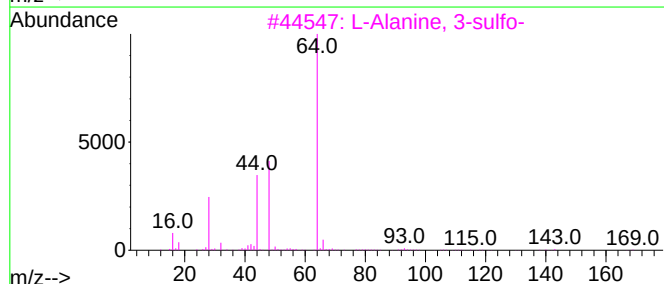
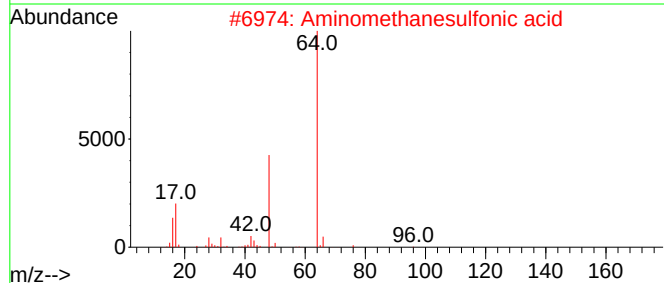
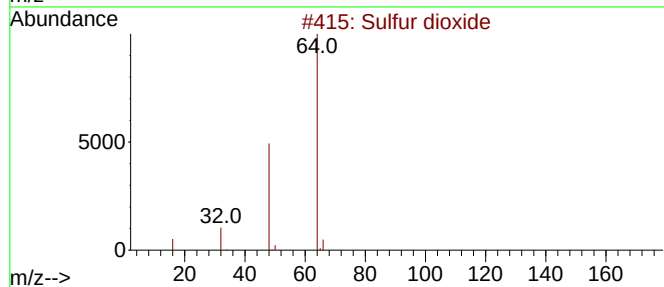
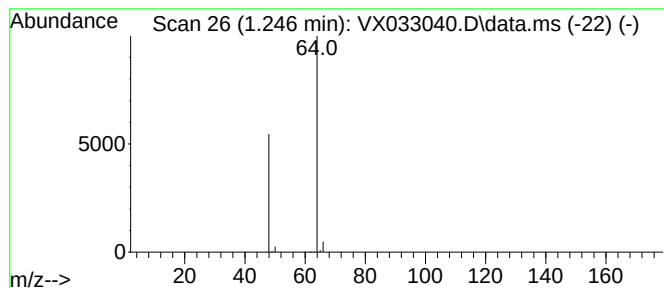
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	47.28 ug/l	388685	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



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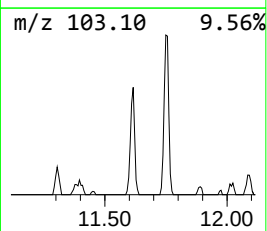
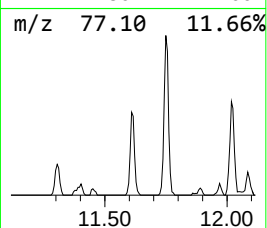
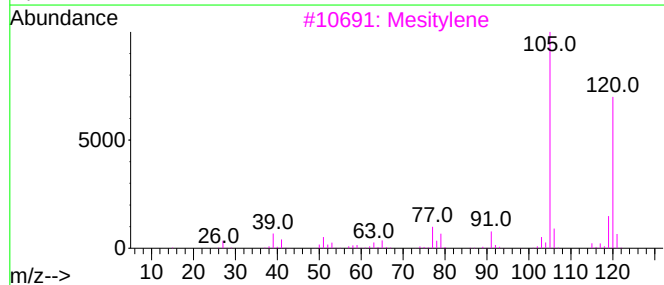
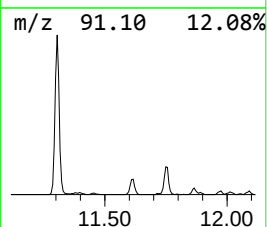
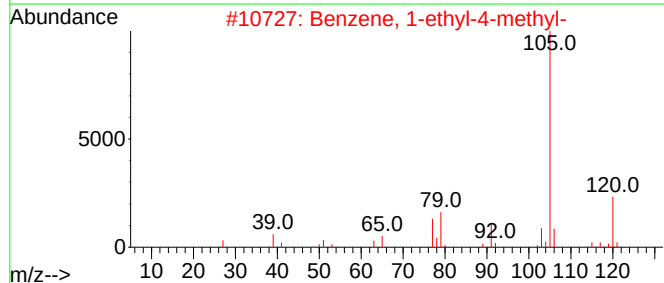
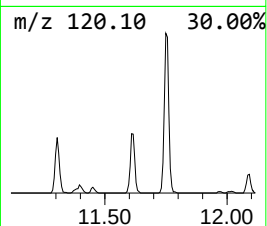
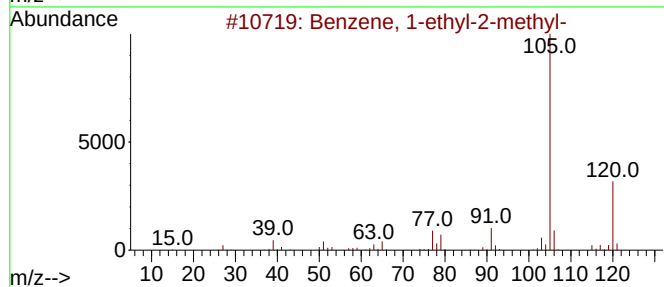
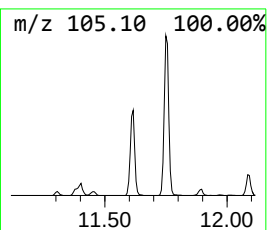
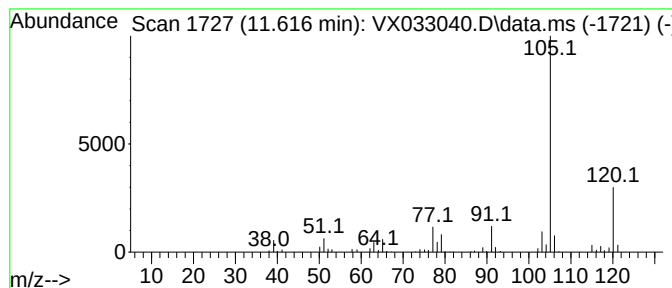
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	6.33 ug/l	73051	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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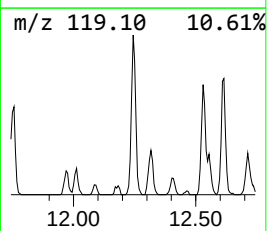
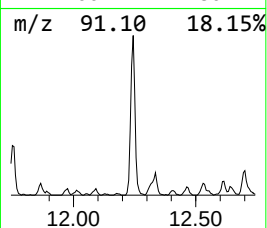
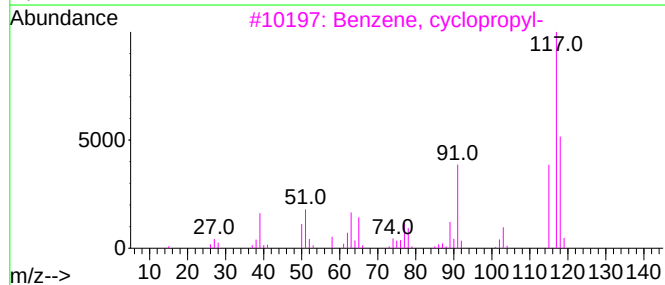
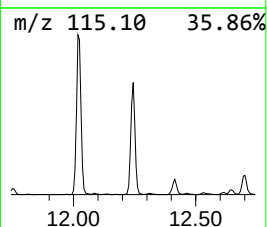
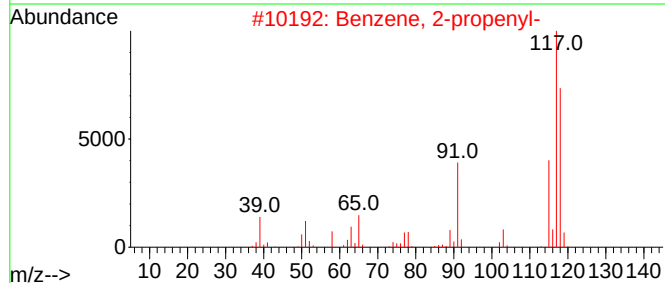
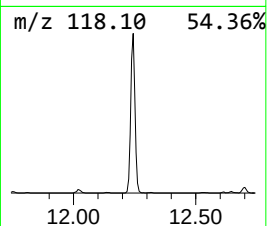
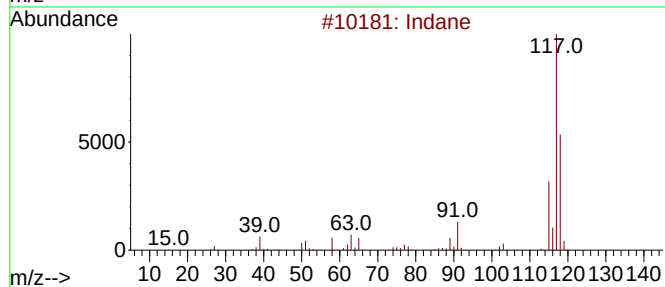
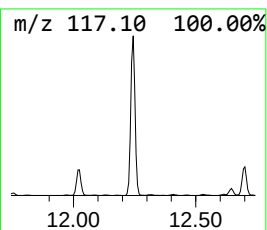
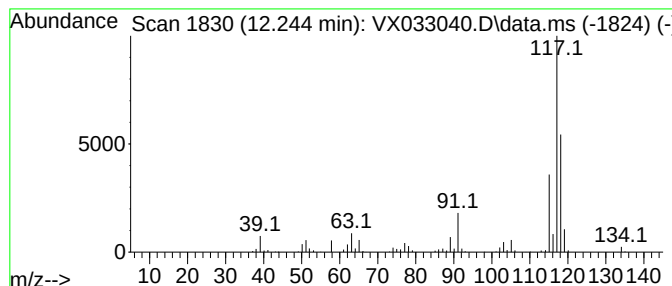
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	30.82 ug/l	355658	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Deltacyclene	118	C9H10	007785-10-6	68
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



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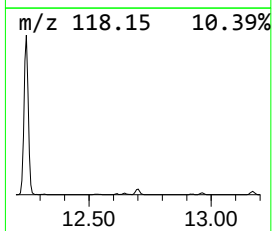
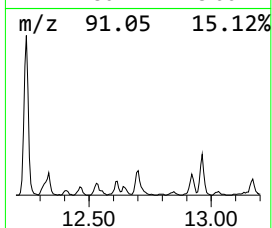
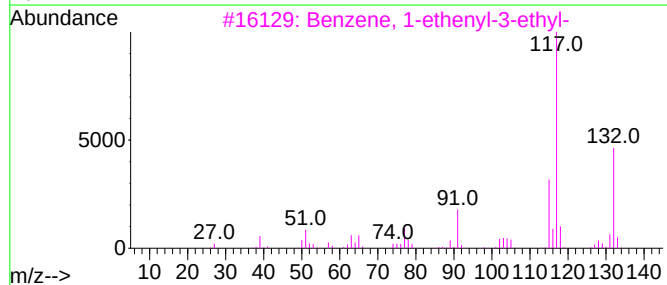
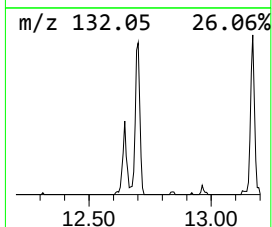
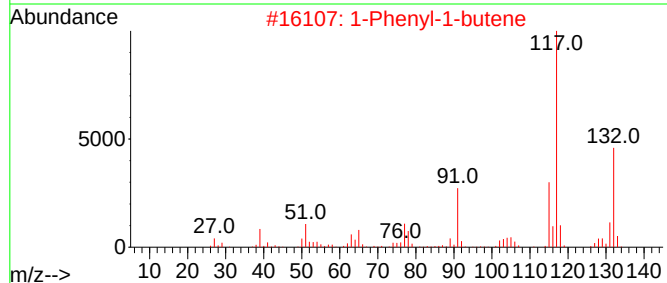
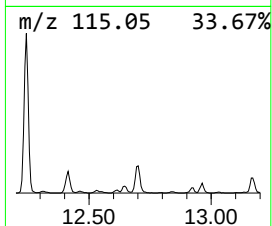
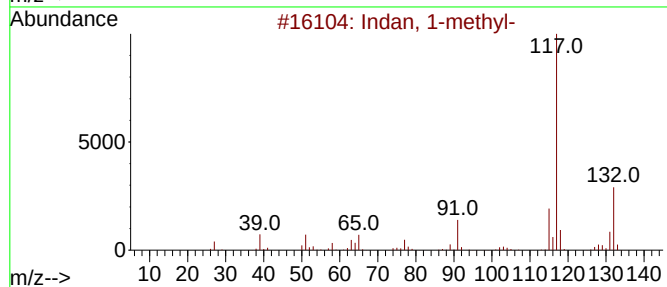
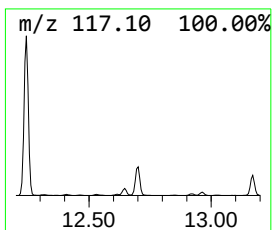
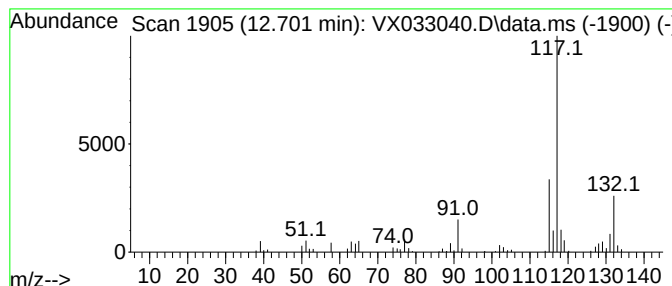
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	6.05 ug/l	69767	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indan, 1-methyl-	132	C10H12	000767-58-8	87
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81



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MW-32

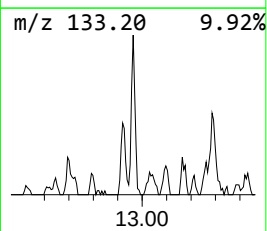
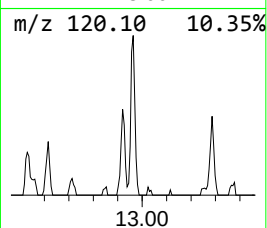
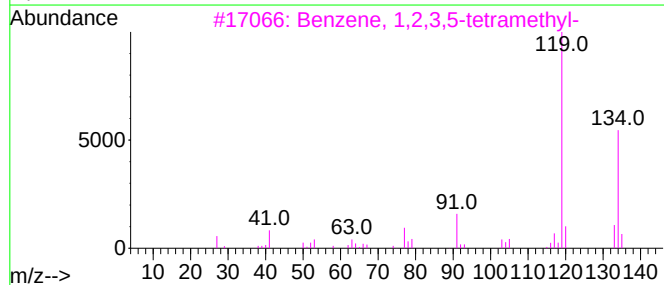
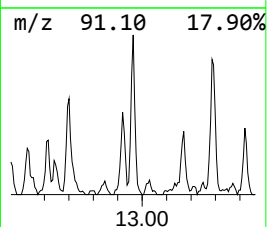
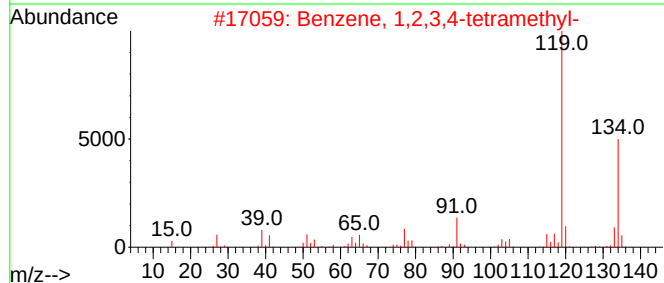
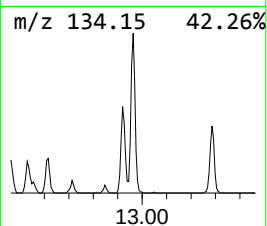
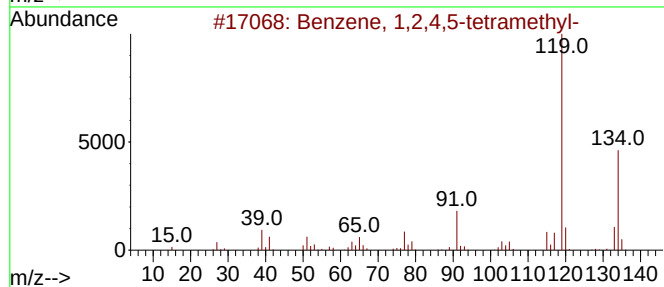
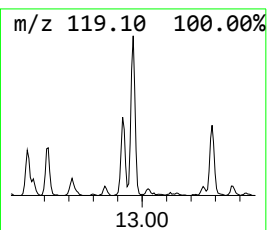
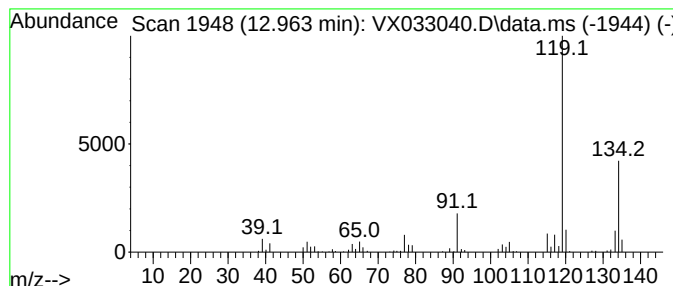
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	6.65 ug/l	76691	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033040.D
Acq On : 24 Nov 2022 05:41
Operator : JC/MD
Sample : N5741-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

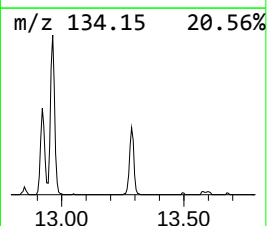
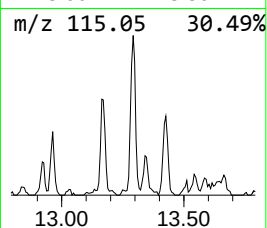
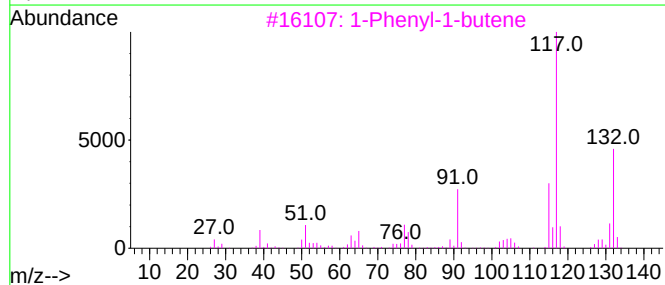
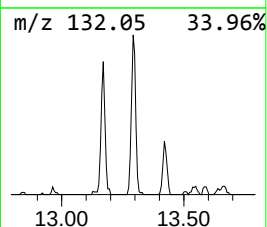
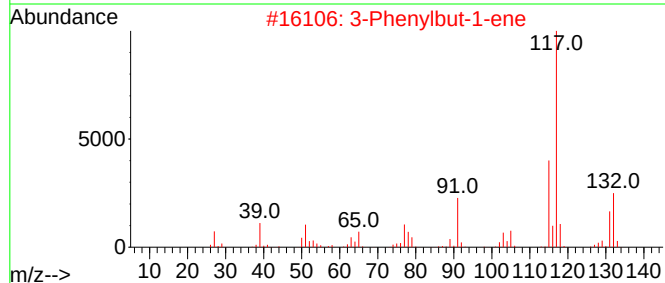
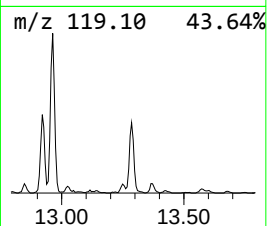
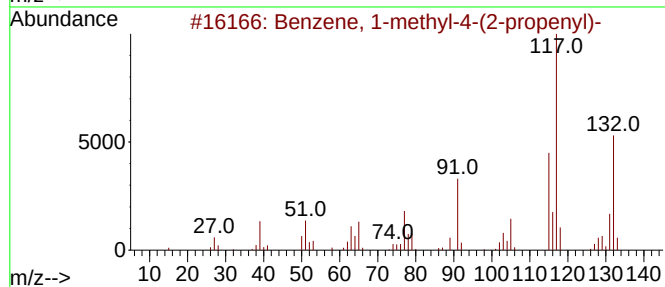
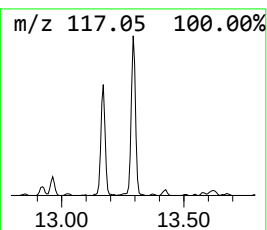
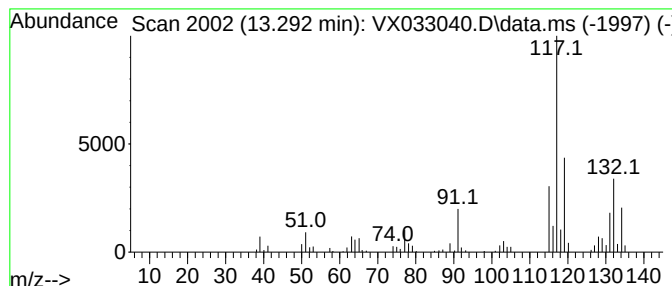
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-methyl-4-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.84 ug/l	90425	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033040.D
Acq On : 24 Nov 2022 05:41
Operator : JC/MD
Sample : N5741-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

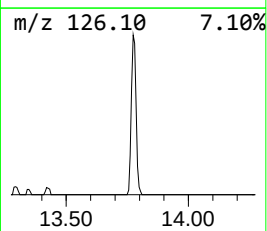
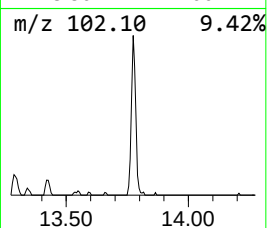
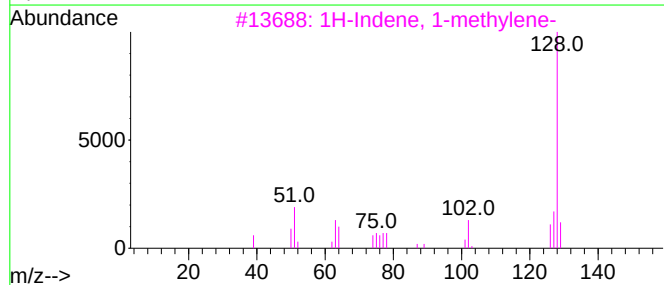
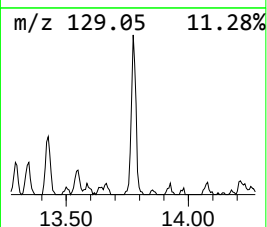
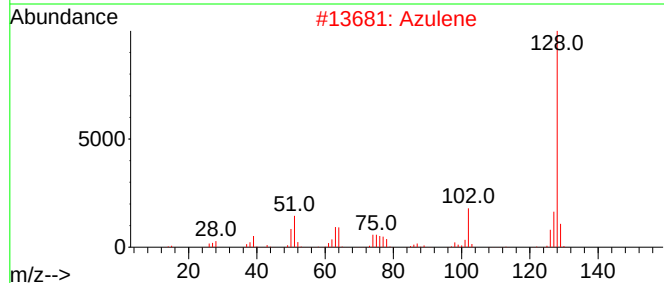
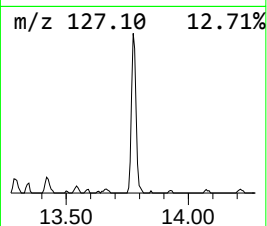
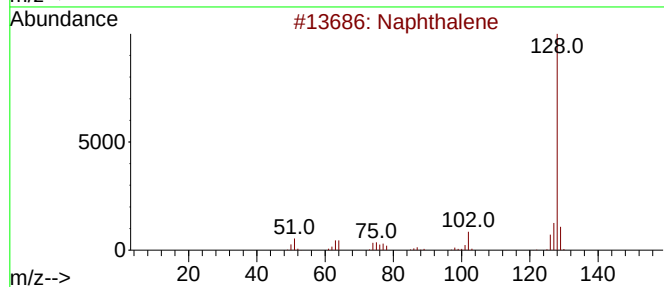
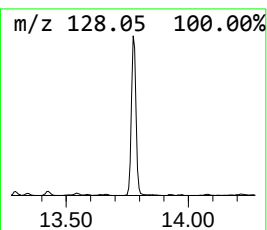
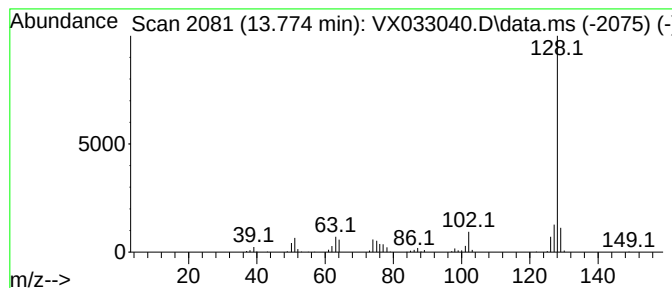
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	10.65 ug/l	122895	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	72
4			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033040.D
Acq On : 24 Nov 2022 05:41
Operator : JC/MD
Sample : N5741-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	47.3	ug/l	388685	1	5.556	411082	50.0
Benzene, 1-ethy...	11.616	6.3	ug/l	73051	4	12.024	576950	50.0
Indane	12.244	30.8	ug/l	355658	4	12.024	576950	50.0
Indan, 1-methyl-	12.701	6.0	ug/l	69767	4	12.024	576950	50.0
Benzene, 1,2,4,...	12.963	6.7	ug/l	76691	4	12.024	576950	50.0
Benzene, 1-meth...	13.292	7.8	ug/l	90425	4	12.024	576950	50.0
Azulene	13.774	10.7	ug/l	122895	4	12.024	576950	50.0