

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
 Data File : VX042060.D
 Acq On : 26 Jun 2024 17:58
 Operator : JC/MD
 Sample : P3073-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW14-20240625

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\82X061824W.M
 Title : SW846 8260

Signal : TIC: VX042060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.647	1235	1240	1249	rVB	392430	623693	1.32%	0.401%
2	10.055	1466	1471	1476	rBV	427240	579202	1.23%	0.373%
3	10.963	1614	1620	1629	rBV	1411138	1809821	3.83%	1.165%
4	11.079	1634	1639	1645	rBV	406877	541326	1.15%	0.348%
5	11.305	1671	1676	1682	rBV	1237471	1484215	3.14%	0.955%
6	11.402	1684	1692	1696	rVV	806833	1054898	2.23%	0.679%
7	11.451	1696	1700	1708	rVB	413378	505792	1.07%	0.325%
8	11.610	1721	1726	1735	rVB	2900391	3589396	7.60%	2.310%
9	11.756	1740	1750	1755	rBV	9603898	12122001	25.65%	7.801%
10	12.018	1788	1793	1799	rVB2	787102	1185282	2.51%	0.763%
11	12.085	1799	1804	1809	rBV	3546354	4441751	9.40%	2.858%
12	12.244	1824	1830	1837	rBV	8274368	10466292	22.15%	6.735%
13	12.317	1837	1842	1847	rVV2	997371	1401017	2.96%	0.902%
14	12.530	1872	1877	1879	rBV	678880	883565	1.87%	0.569%
15	12.555	1879	1881	1885	rVB	779995	837169	1.77%	0.539%
16	12.615	1885	1891	1894	rBV	1603197	2060416	4.36%	1.326%
17	12.701	1900	1905	1911	rBV	3674988	4971529	10.52%	3.199%
18	12.847	1925	1929	1934	rVB	401340	514434	1.09%	0.331%
19	12.920	1934	1941	1944	rBV	651490	816430	1.73%	0.525%
20	12.963	1944	1948	1953	rVB	1313435	1659807	3.51%	1.068%
21	13.170	1977	1982	1987	rVB	2313390	2685202	5.68%	1.728%
22	13.286	1993	2001	2006	rBV2	2593385	3597273	7.61%	2.315%
23	13.341	2006	2010	2018	rVB	2243472	2689142	5.69%	1.731%
24	13.426	2018	2024	2030	rVB	8442065	10609649	22.45%	6.828%
25	13.499	2030	2036	2040	rBV	1114380	1458298	3.09%	0.938%
26	13.548	2040	2044	2047	rVV	462447	581800	1.23%	0.374%
27	13.670	2058	2064	2069	rVB2	383901	619916	1.31%	0.399%
28	13.786	2073	2083	2088	rBV	29756767	47257726	100.00%	30.411%
29	14.219	2149	2154	2158	rBV2	697639	1157741	2.45%	0.745%
30	14.255	2158	2160	2165	rVV2	326398	591773	1.25%	0.381%
31	14.316	2165	2170	2177	rVB	936793	1687734	3.57%	1.086%
32	14.524	2200	2204	2211	rVB	430928	642769	1.36%	0.414%
33	14.639	2218	2223	2233	rVB	8922554	10971259	23.22%	7.060%
34	14.780	2240	2246	2256	rBV	9636610	12448478	26.34%	8.011%
35	15.206	2308	2316	2321	rBV	422497	612005	1.30%	0.394%
36	15.377	2338	2344	2347	rBV	505586	730701	1.55%	0.470%

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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\82X061824W.M
Title : SW846 8260

37	15.475	2355	2360	2371	rBV	519126	846102	1.79%	0.544%
38	15.615	2376	2383	2386	rVV	1017455	1651965	3.50%	1.063%
39	15.652	2386	2389	2395	rVB	336501	493021	1.04%	0.317%
40	15.834	2409	2419	2432	rBV	275548	799766	1.69%	0.515%
41	16.328	2491	2500	2511	rBV	886165	1714683	3.63%	1.103%

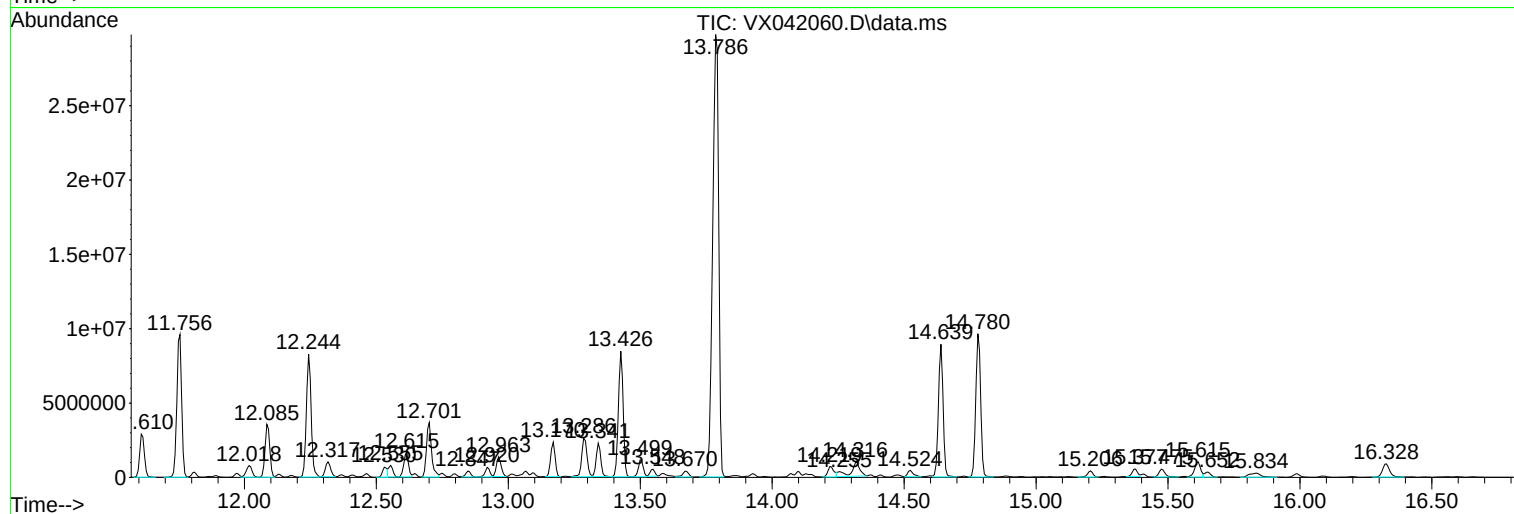
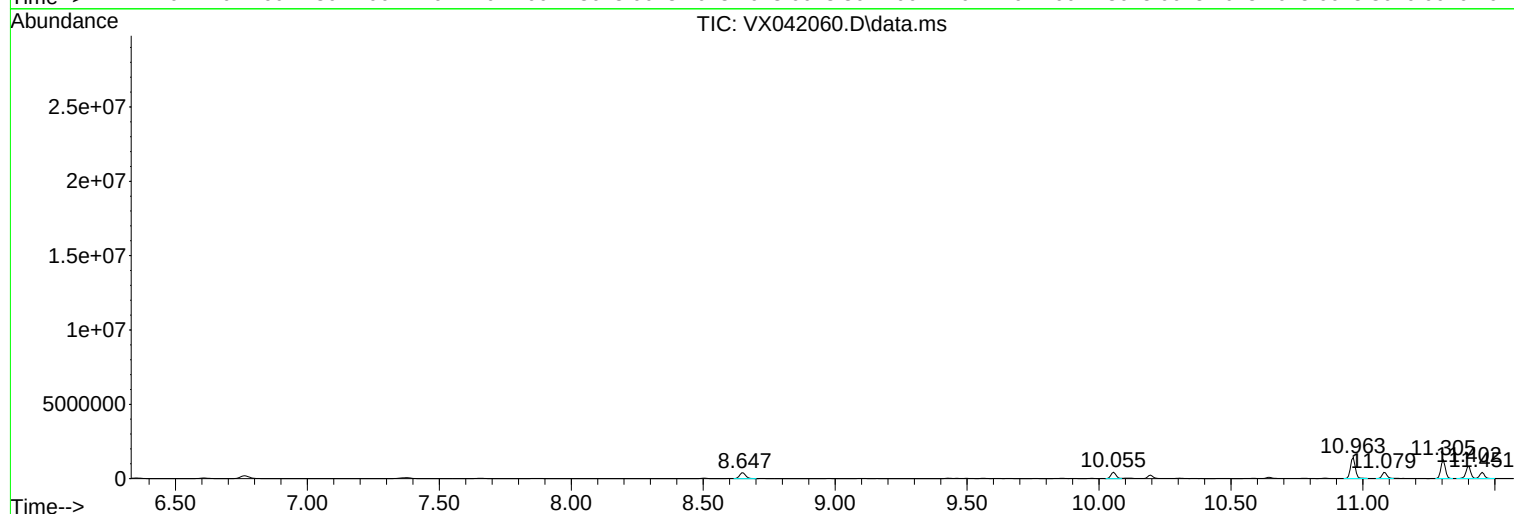
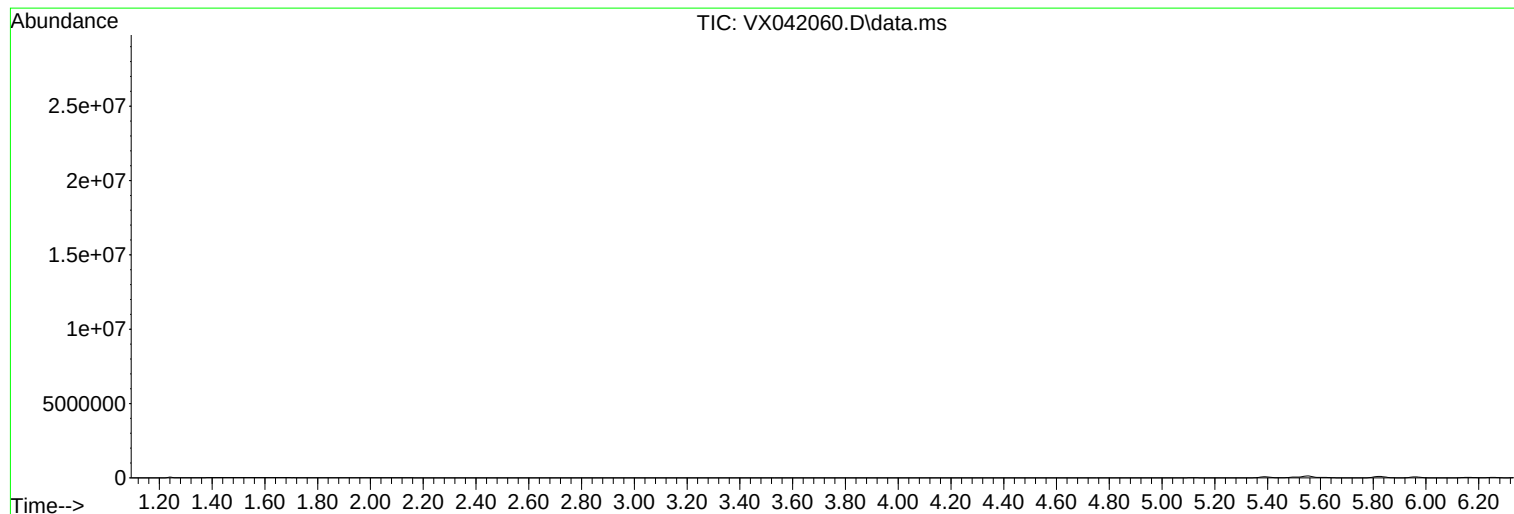
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



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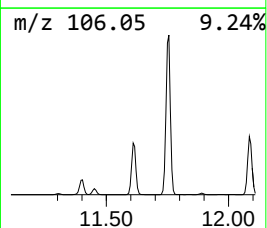
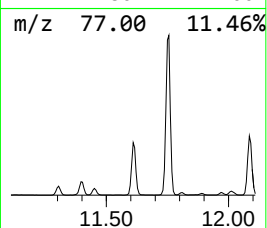
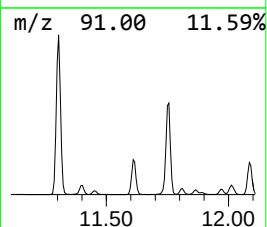
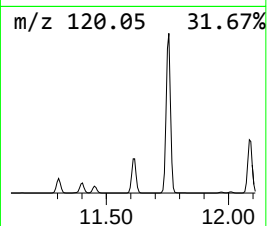
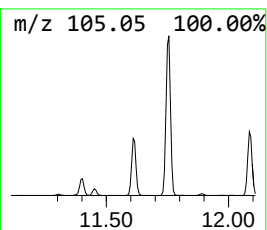
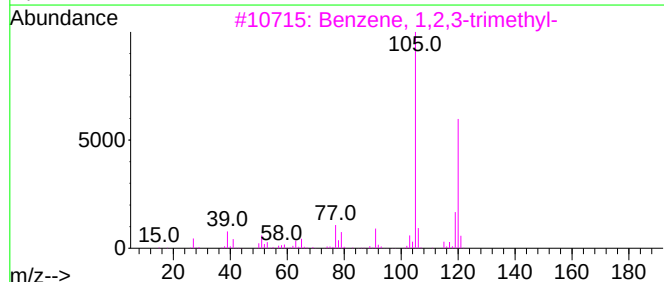
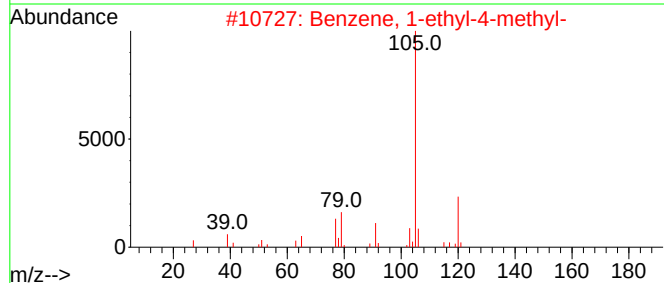
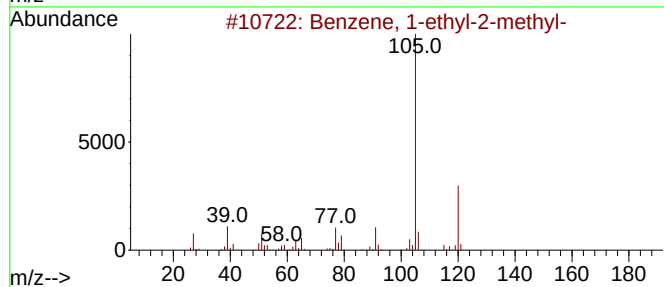
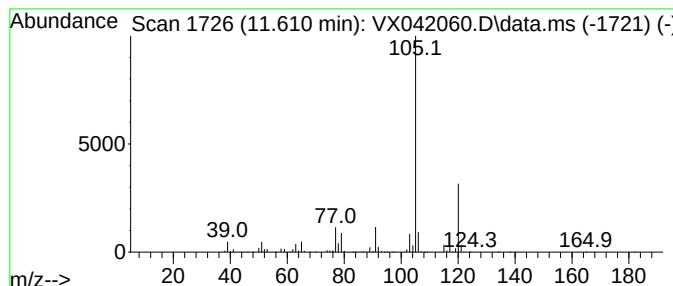
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	151.41 ug/l	3589400	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			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW14-20240625

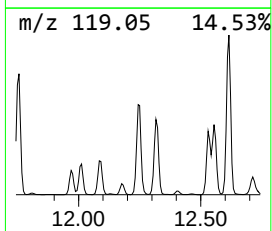
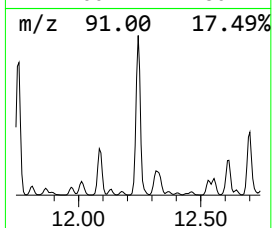
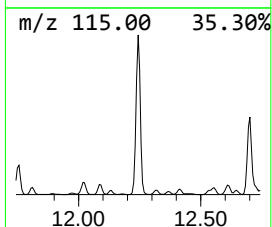
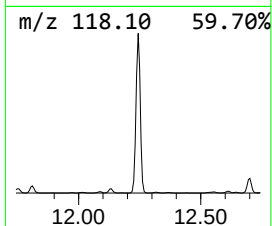
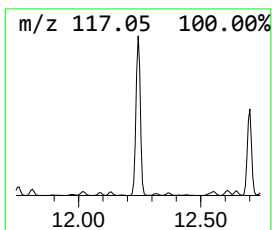
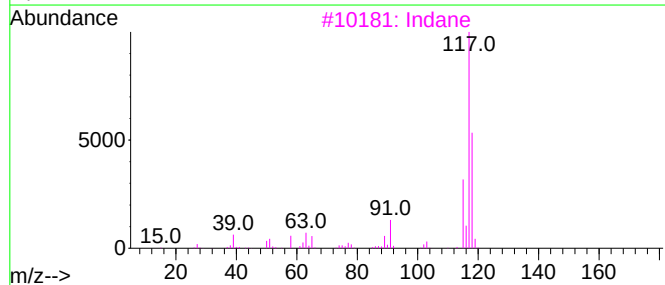
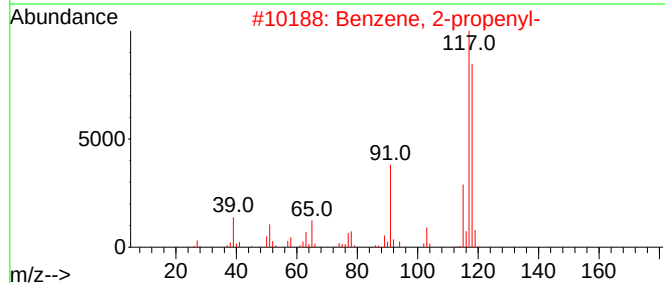
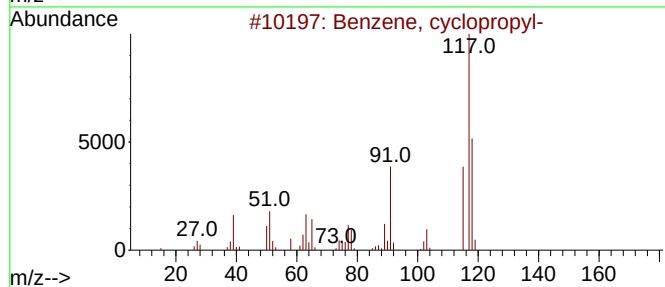
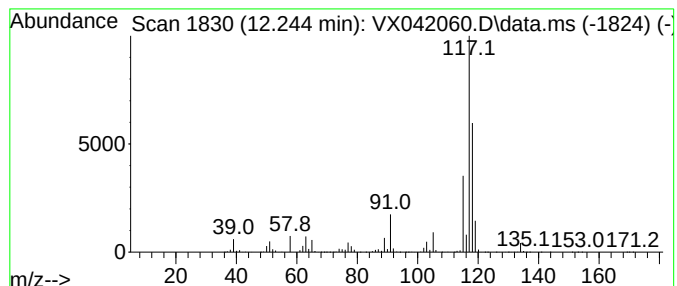
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	441.51 ug/l	10466300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3			Indane	118	C9H10	000496-11-7	76
4			Δtacyclene	118	C9H10	007785-10-6	50
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	49



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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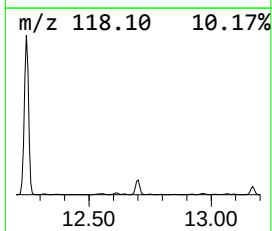
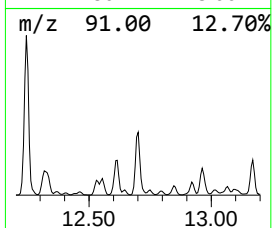
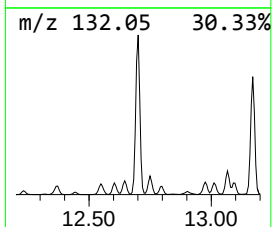
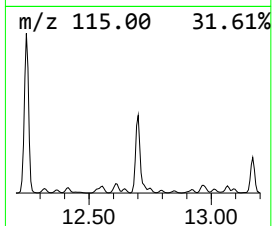
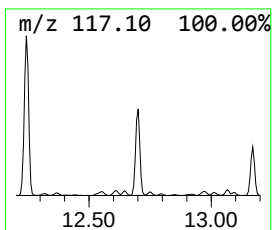
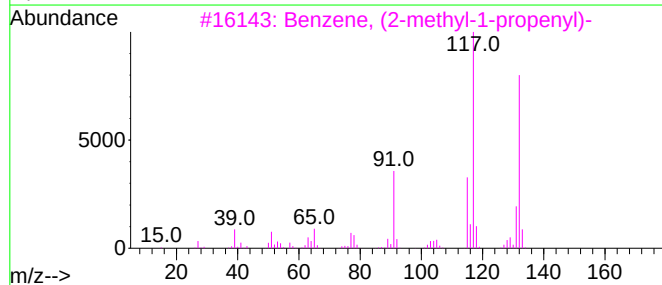
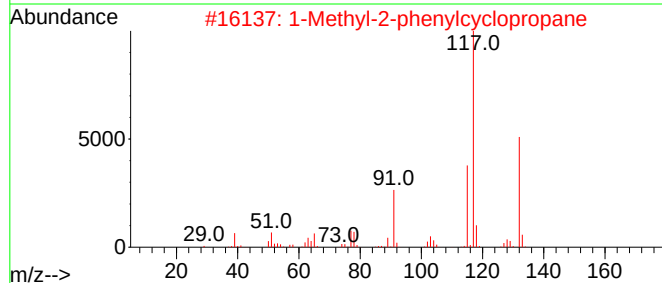
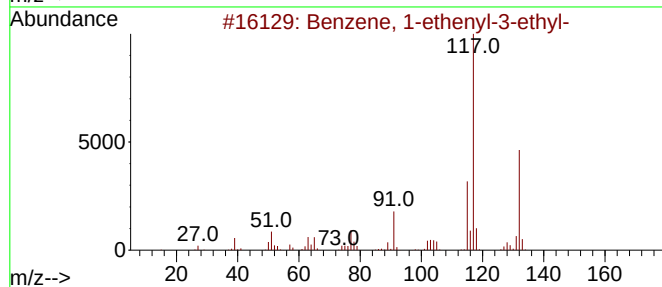
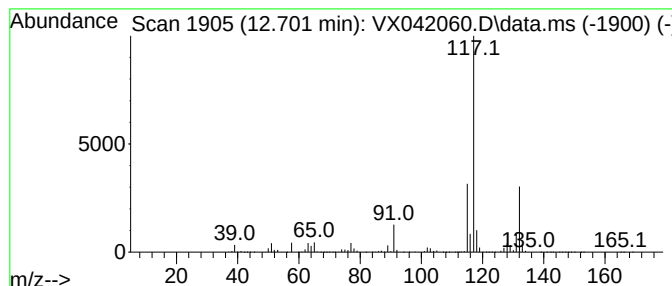
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	209.72 ug/l	4971530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4			Indan, 1-methyl-	132	C10H12	000767-58-8	90
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87



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Instrument :
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ClientSampleId :
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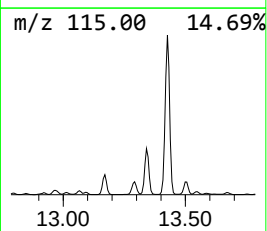
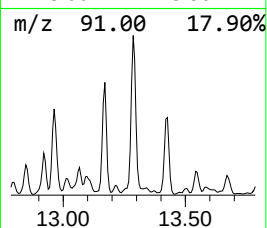
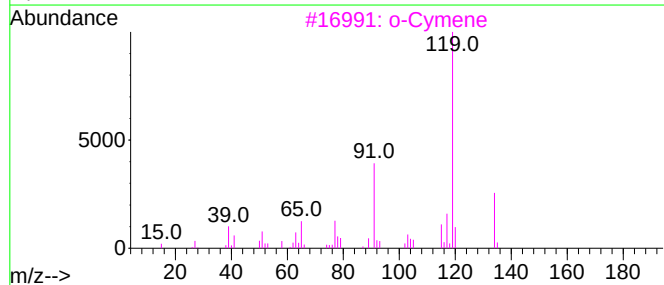
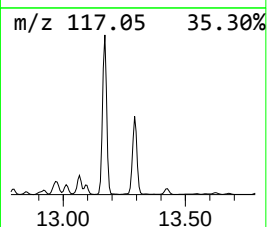
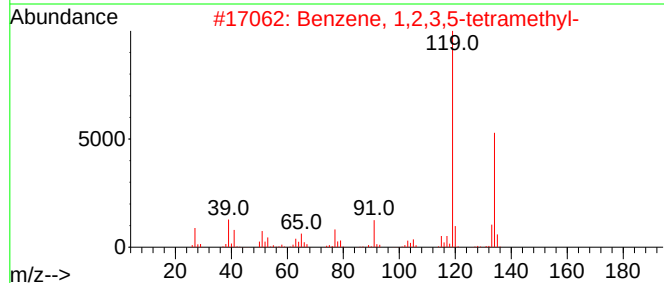
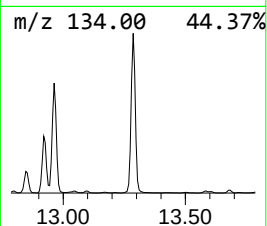
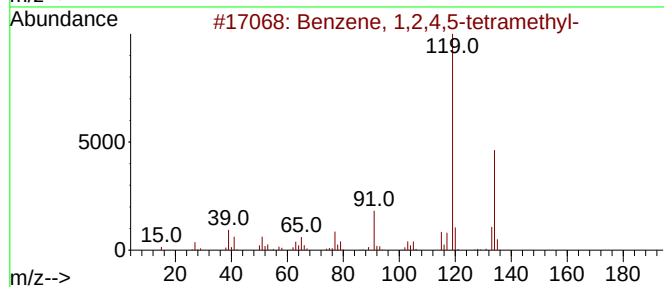
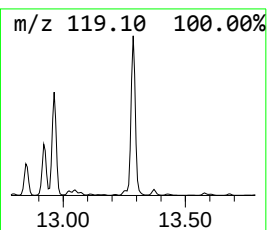
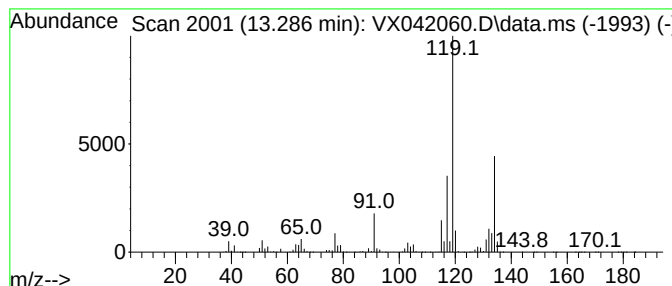
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	151.75 ug/l	3597270	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	93
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
3			o-Cymene	134	C10H14	000527-84-4	81
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	81



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ClientSampleId :
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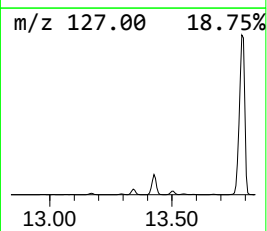
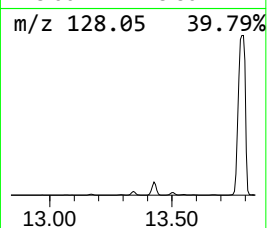
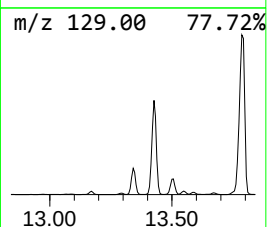
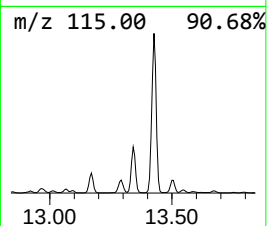
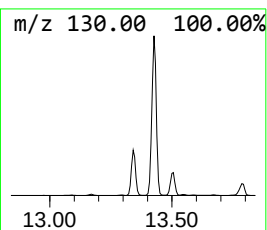
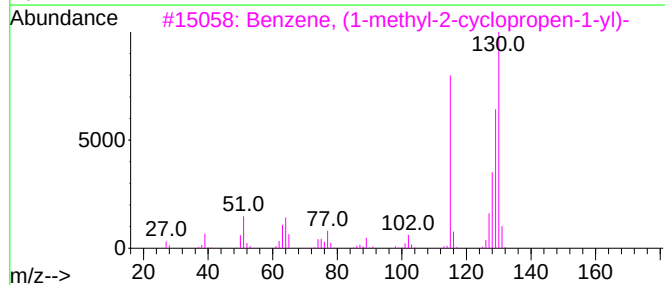
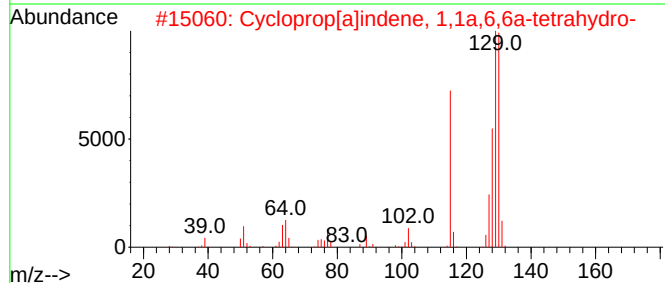
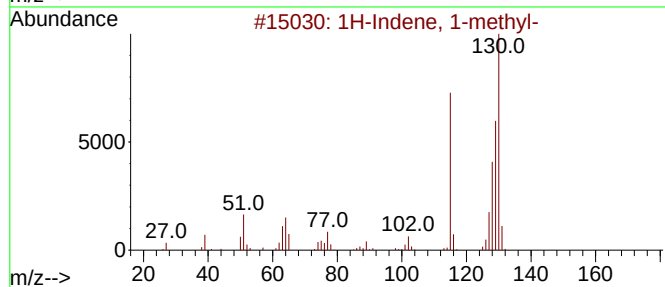
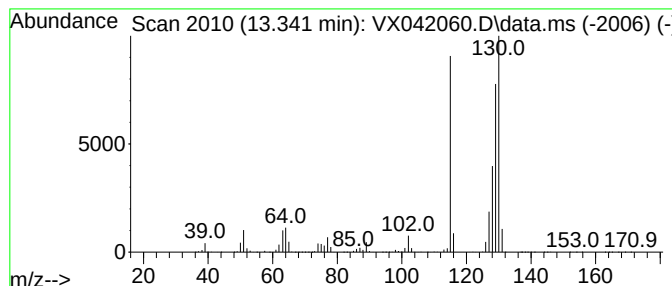
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	113.44 ug/l	2689140	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
2			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95
3			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94
4			2-Methylindene	130	C10H10	002177-47-1	93
5			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	92



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042060.D
Acq On : 26 Jun 2024 17:58
Operator : JC/MD
Sample : P3073-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW14-20240625

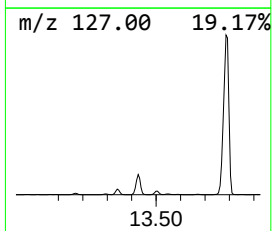
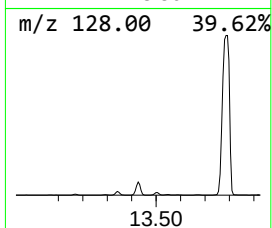
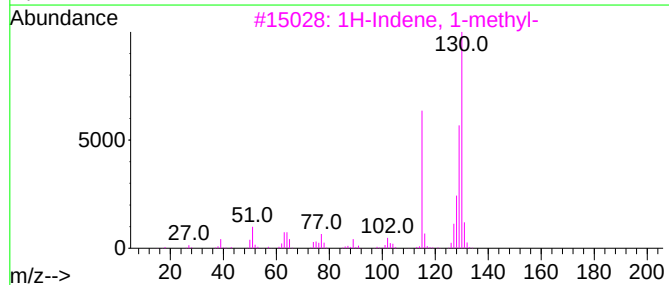
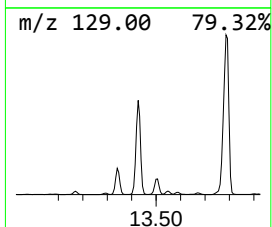
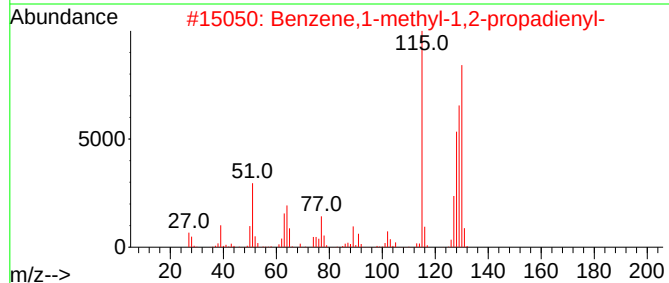
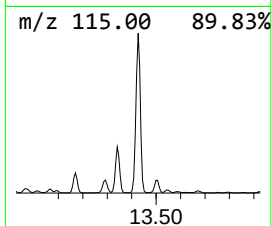
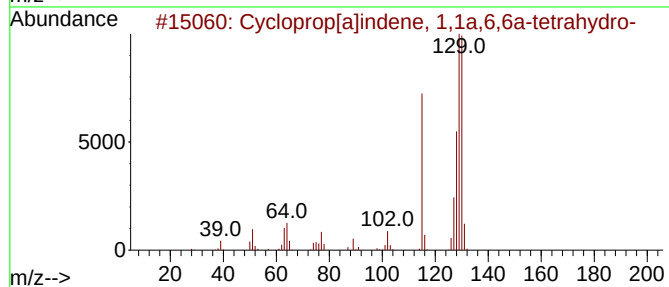
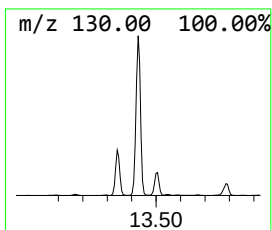
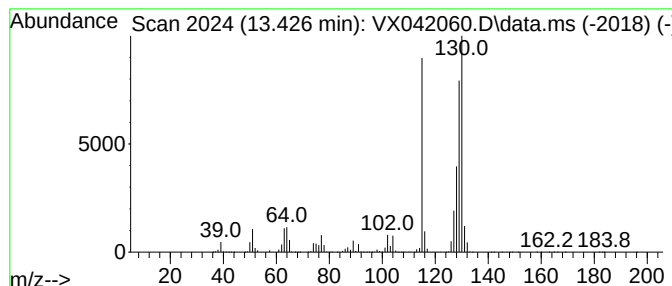
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Quant Title : SW846 8260

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

Peak Number 7 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	447.56 ug/l	10609600	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95
2		Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
3		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4		Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94
5		2-Methylindene	130	C10H10	002177-47-1	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042060.D
Acq On : 26 Jun 2024 17:58
Operator : JC/MD
Sample : P3073-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

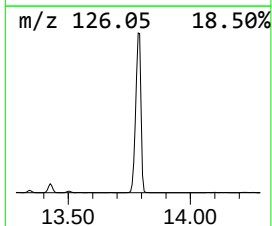
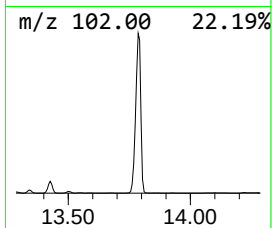
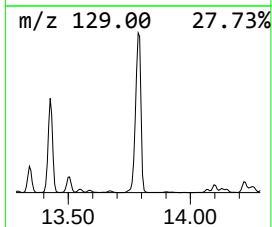
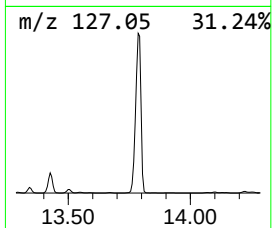
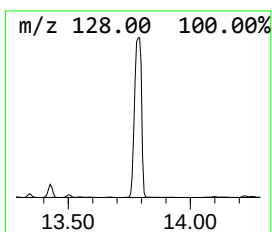
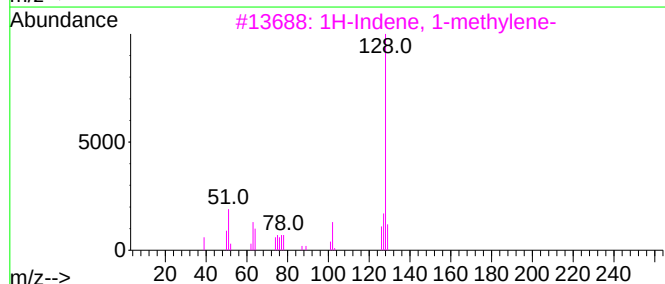
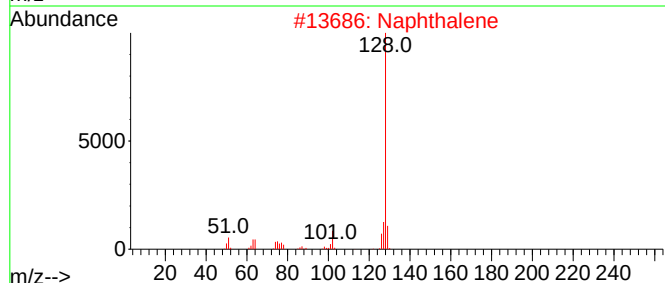
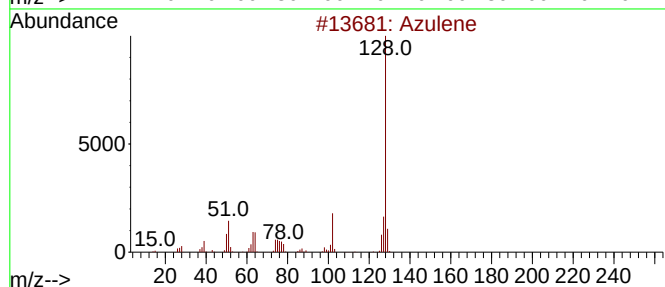
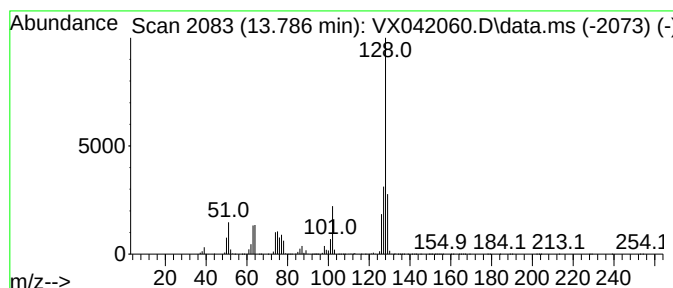
Instrument :
MSVOA_X
ClientSampleId :
MW14-20240625

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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

Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.786	1993.52 ug/l	47257700	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene	128	C10H8	000275-51-4	87
2	Naphthalene	128	C10H8	000091-20-3	87
3	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	83
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	76
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062624\
Data File : VX042060.D
Acq On : 26 Jun 2024 17:58
Operator : JC/MD
Sample : P3073-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW14-20240625

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.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
Benzene, 1-ethy...	11.610	151.4	ug/l	3589400	4	12.024	1185280	50.0
Benzene, cyclop...	12.244	441.5	ug/l	10466300	4	12.024	1185280	50.0
Benzene, 1-ethe...	12.701	209.7	ug/l	4971530	4	12.024	1185280	50.0
Benzene, 1,2,4,...	13.286	151.8	ug/l	3597270	4	12.024	1185280	50.0
1H-Indene, 1-me...	13.341	113.4	ug/l	2689140	4	12.024	1185280	50.0
Cycloprop[a]ind...	13.426	447.6	ug/l	10609600	4	12.024	1185280	50.0
Azulene	13.786	1993.5	ug/l	47257700	4	12.024	1185280	50.0