

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
 Data File : VX027412.D
 Acq On : 11 Mar 2022 19:15
 Operator : JC/MD
 Sample : N1895-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-6

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\82X030822W.M
 Title : SW846 8260

Signal : TIC: VX027412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	42	rBV2	50217	195280	10.77%	1.164%
2	1.746	104	108	118	rVB	31447	48648	2.68%	0.290%
3	2.538	229	238	250	rBV	16805	33108	1.83%	0.197%
4	2.788	270	279	283	rBV3	14213	35705	1.97%	0.213%
5	3.105	323	331	341	rVB3	27690	66029	3.64%	0.394%
6	4.215	504	513	522	rBV3	6676	21113	1.16%	0.126%
7	5.391	693	706	721	rBV	213333	625400	34.48%	3.728%
8	5.556	721	733	758	rVB	369838	1100535	60.68%	6.560%
9	5.958	789	799	812	rBV	200788	536839	29.60%	3.200%
10	6.166	823	833	839	rBV6	9229	28730	1.58%	0.171%
11	6.257	839	848	858	rVV3	40538	125952	6.94%	0.751%
12	6.763	921	931	944	rBV	537860	1312559	72.37%	7.823%
13	7.361	1020	1029	1041	rVB5	8414	22153	1.22%	0.132%
14	7.988	1122	1132	1144	rVB	32277	67698	3.73%	0.404%
15	8.110	1144	1152	1161	rBV	47924	100994	5.57%	0.602%
16	8.653	1227	1241	1250	rBV	1142402	1813664	100.00%	10.810%
17	9.165	1320	1325	1329	rBV	14555	22030	1.21%	0.131%
18	10.055	1465	1471	1481	rBV	1184069	1555157	85.75%	9.269%
19	10.195	1490	1494	1502	rVB	27775	39151	2.16%	0.233%
20	10.305	1502	1512	1517	rVB	54481	79127	4.36%	0.472%
21	10.647	1563	1568	1575	rVB	20620	26929	1.48%	0.161%
22	11.085	1634	1640	1652	rBV	944458	1212714	66.87%	7.228%
23	11.616	1722	1727	1731	rBV	50871	67822	3.74%	0.404%
24	11.756	1746	1750	1756	rVB	24052	28695	1.58%	0.171%
25	12.024	1789	1794	1802	rBV	1238596	1498278	82.61%	8.930%
26	12.244	1823	1830	1837	rBV2	1387852	1750216	96.50%	10.432%
27	12.317	1837	1842	1848	rVB	101452	122594	6.76%	0.731%
28	12.408	1852	1857	1863	rVB2	50629	67626	3.73%	0.403%
29	12.475	1863	1868	1872	rVB2	31074	44090	2.43%	0.263%
30	12.530	1872	1877	1885	rVB	32346	40375	2.23%	0.241%
31	12.616	1885	1891	1894	rBV	568806	677533	37.36%	4.038%
32	12.646	1894	1896	1900	rVV	105422	112335	6.19%	0.670%
33	12.701	1900	1905	1912	rVB	327952	420974	23.21%	2.509%
34	12.841	1922	1928	1933	rVB	13019	18340	1.01%	0.109%
35	12.920	1933	1941	1946	rBV	301684	389661	21.48%	2.323%
36	12.963	1946	1948	1954	rVB	29119	36047	1.99%	0.215%

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37	13.024	1954	1958	1965	rVB3	37009	56438	3.11%	0.336%
38	13.116	1965	1973	1974	rBV3	15765	22623	1.25%	0.135%
39	13.170	1979	1982	1985	rBV	38429	38456	2.12%	0.229%
40	13.262	1990	1997	1998	rBV2	27756	33872	1.87%	0.202%
41	13.292	1998	2002	2008	rVV	587685	761859	42.01%	4.541%
42	13.341	2008	2010	2013	rVV2	62876	81793	4.51%	0.488%
43	13.372	2013	2015	2020	rVV	30998	37366	2.06%	0.223%
44	13.426	2020	2024	2031	rVB	84112	112143	6.18%	0.668%
45	13.542	2039	2043	2046	rVV	65091	90919	5.01%	0.542%
46	13.585	2046	2050	2054	rVV3	99988	144858	7.99%	0.863%
47	13.646	2054	2060	2061	rVV3	49371	82542	4.55%	0.492%
48	13.664	2061	2063	2072	rVB2	104782	151460	8.35%	0.903%
49	13.780	2072	2082	2091	rBV	35093	63542	3.50%	0.379%
50	13.926	2099	2106	2110	rBV2	44136	60827	3.35%	0.363%
51	13.975	2110	2114	2117	rBV	39434	48354	2.67%	0.288%
52	14.079	2126	2131	2137	rBV	72378	91784	5.06%	0.547%
53	14.213	2149	2153	2159	rBV	62846	91751	5.06%	0.547%
54	14.323	2167	2171	2176	rBV	33593	44459	2.45%	0.265%
55	14.378	2176	2180	2184	rVB	47580	61974	3.42%	0.369%
56	14.481	2192	2197	2202	rBV3	16126	25591	1.41%	0.153%
57	14.603	2211	2217	2223	rBV2	22906	38903	2.14%	0.232%
58	14.780	2241	2246	2256	rBV	217756	291629	16.08%	1.738%

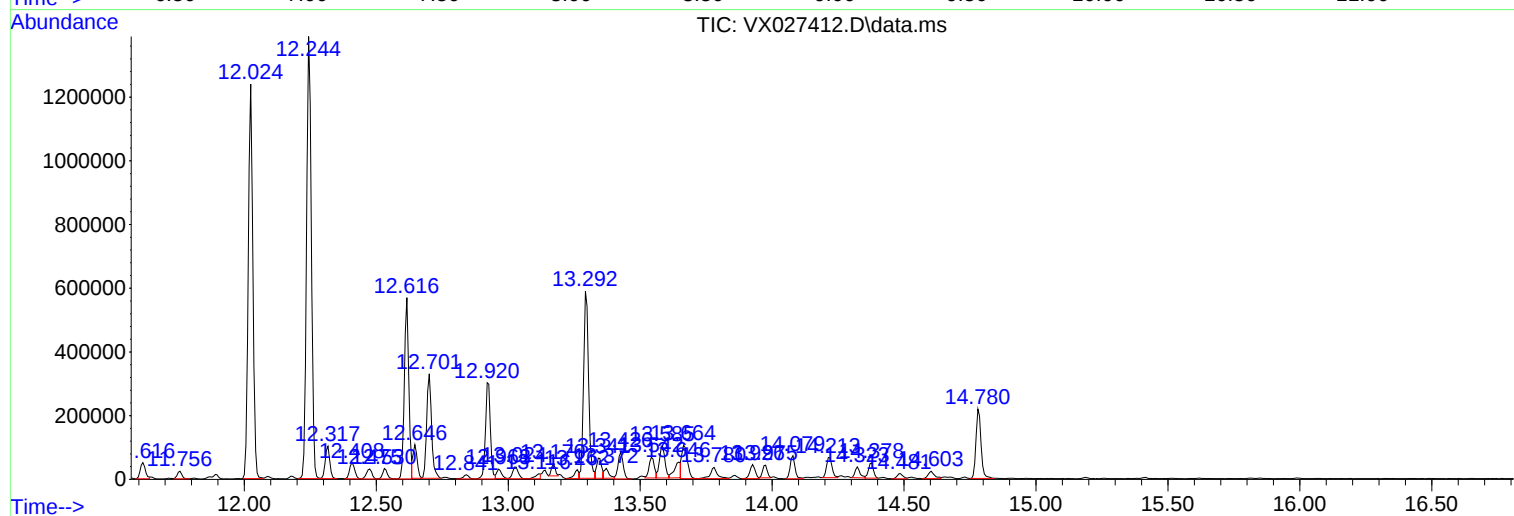
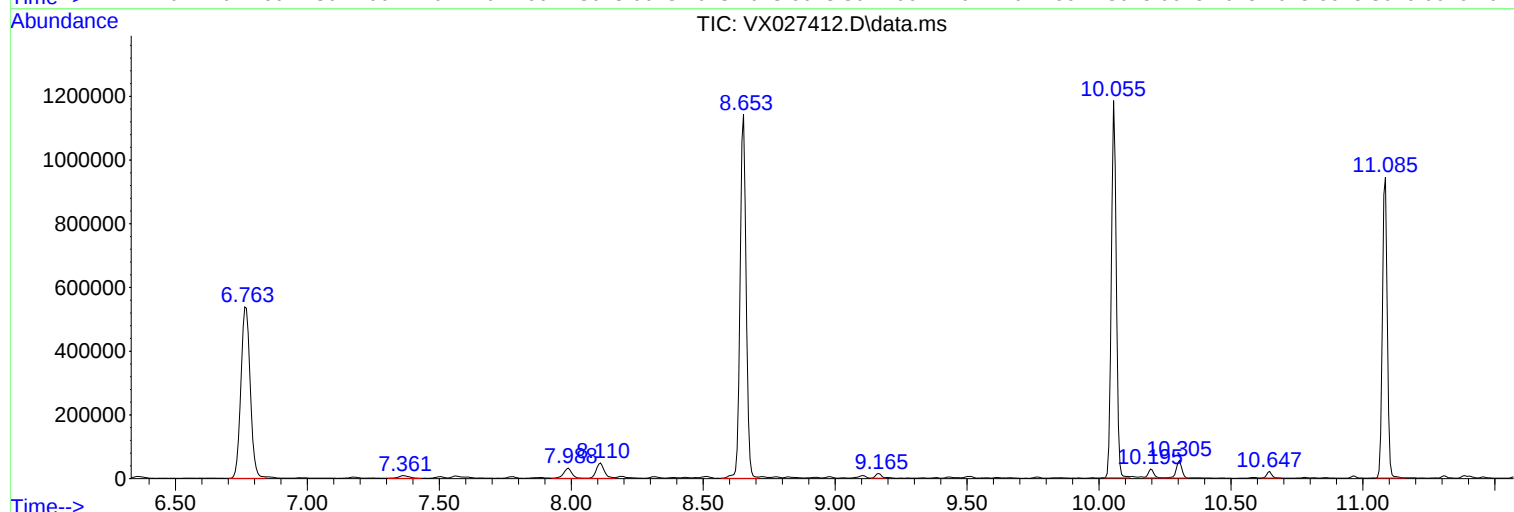
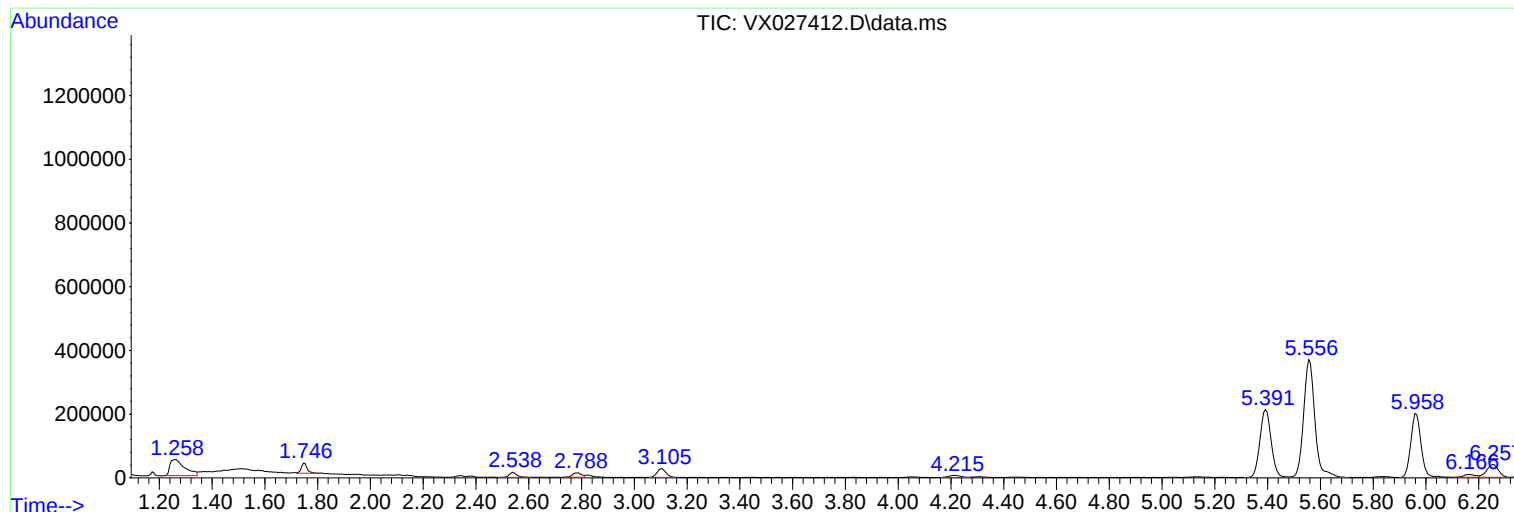
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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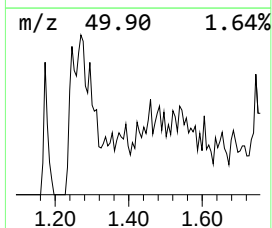
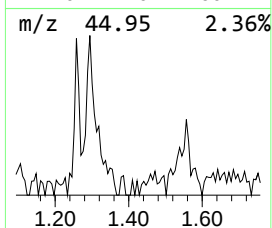
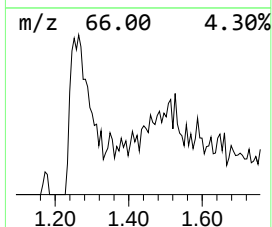
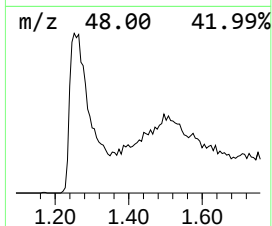
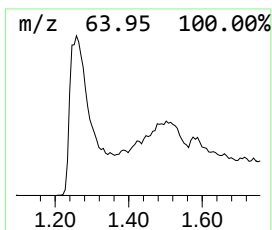
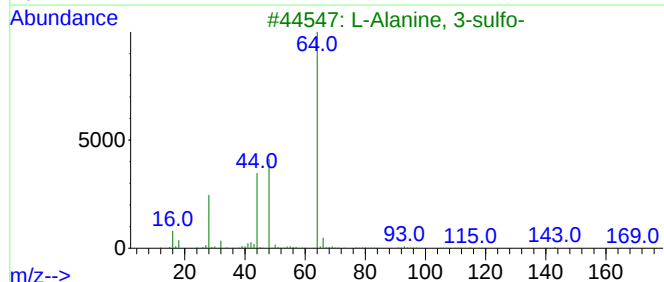
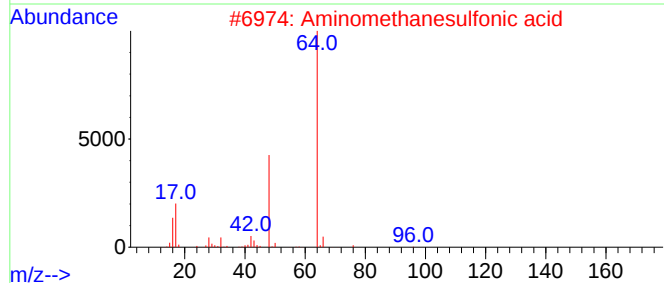
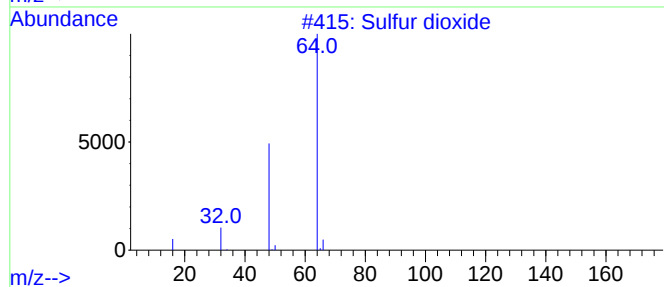
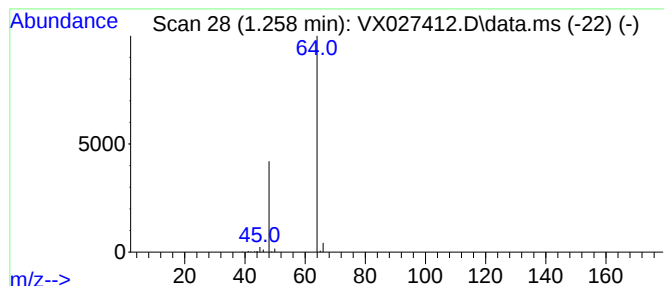
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	8.87 ug/l	195280	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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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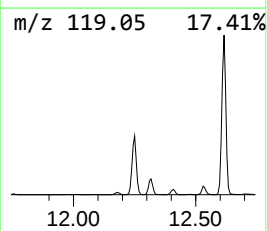
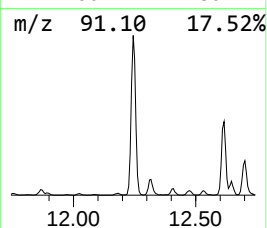
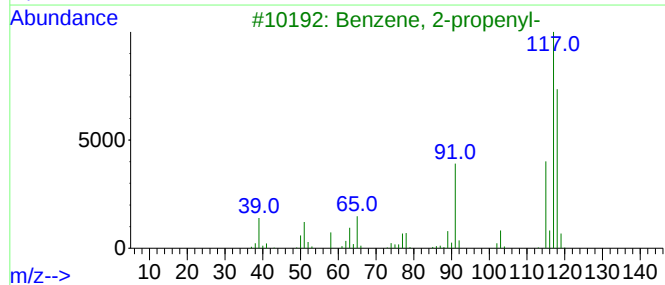
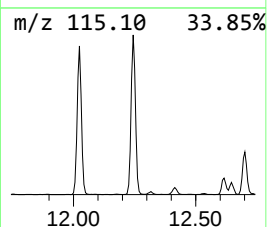
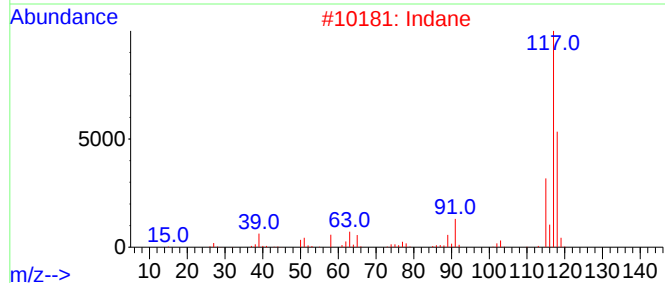
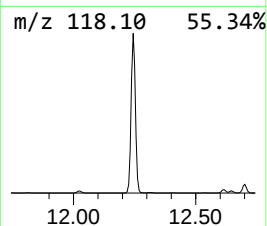
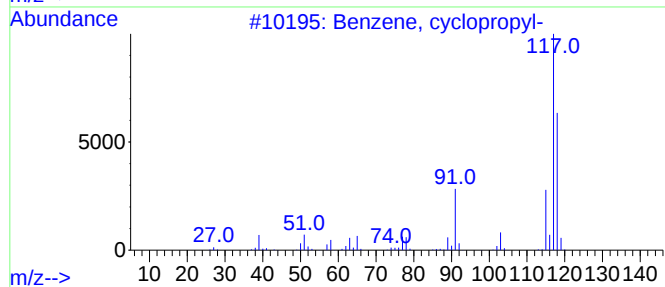
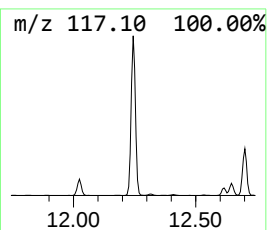
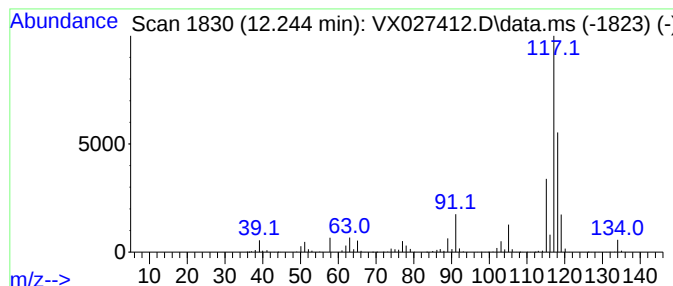
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	58.41 ug/l	1750220	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			Indane	118	C9H10	000496-11-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5			Deltacyclene	118	C9H10	007785-10-6	58



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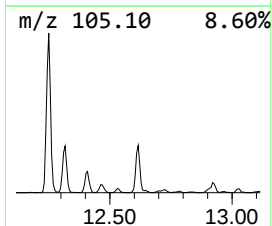
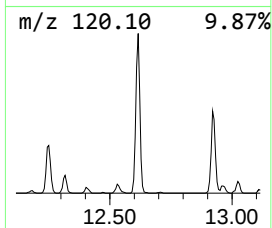
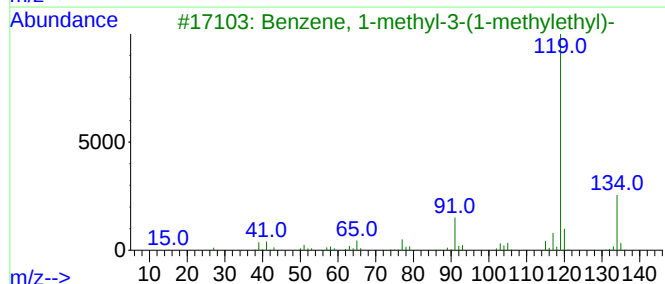
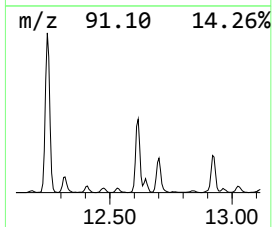
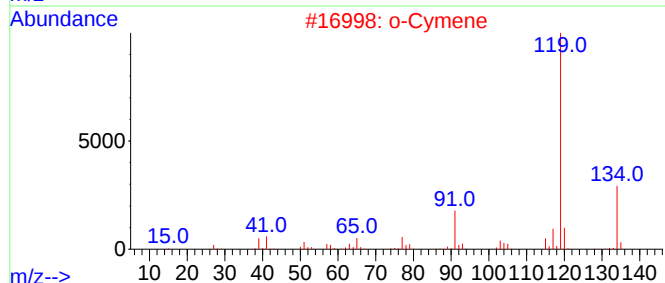
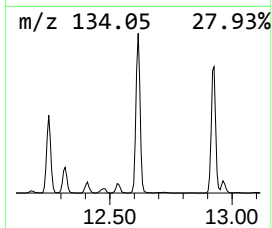
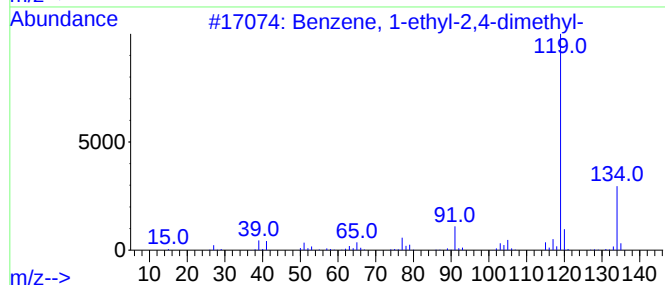
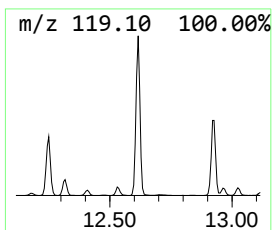
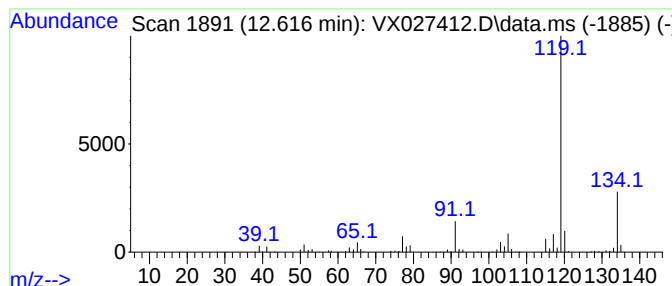
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	22.61 ug/l	677533	1,4-Dichlorobenzene-d4	12.024

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-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



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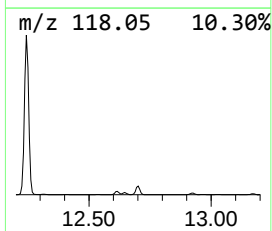
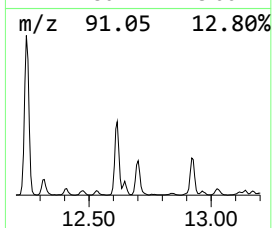
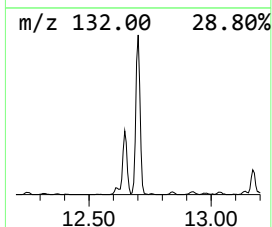
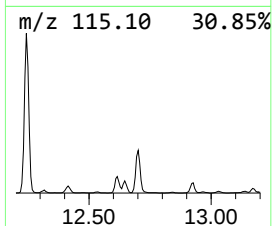
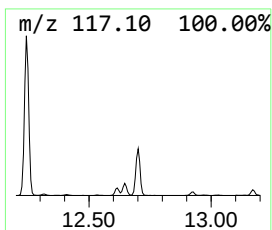
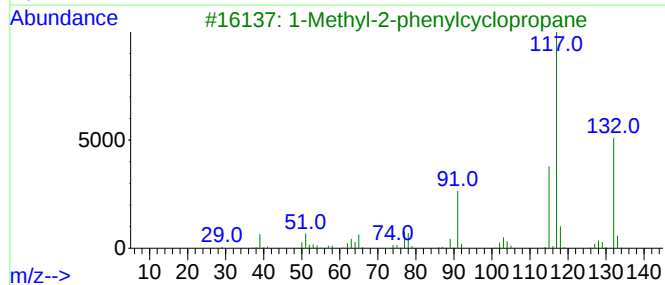
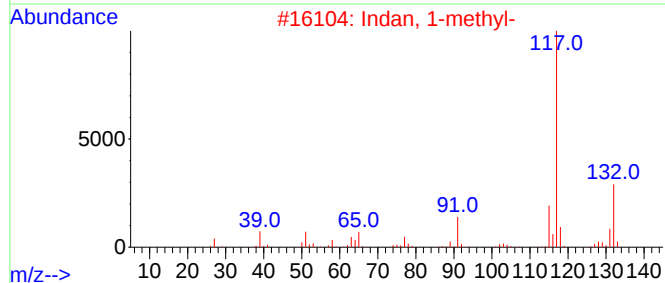
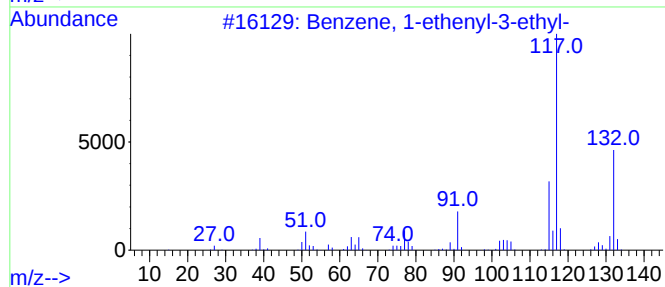
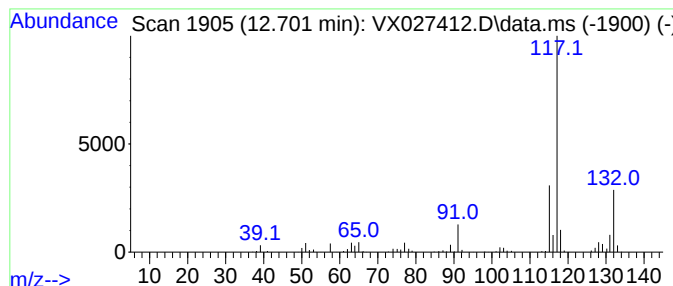
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	14.05 ug/l	420974	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			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



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MW-6

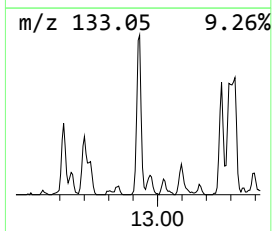
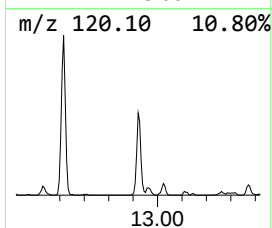
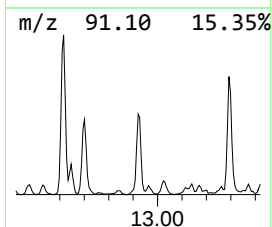
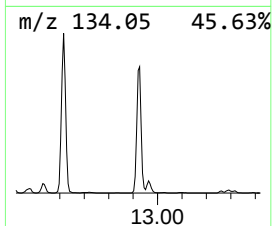
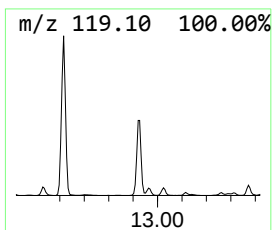
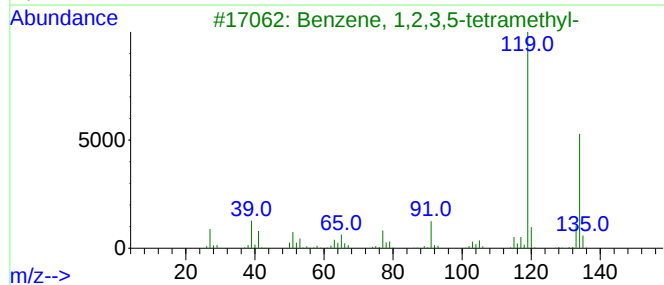
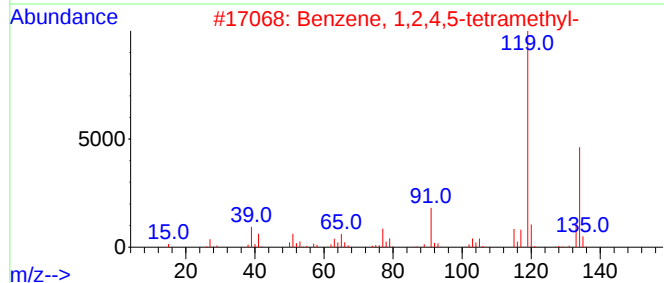
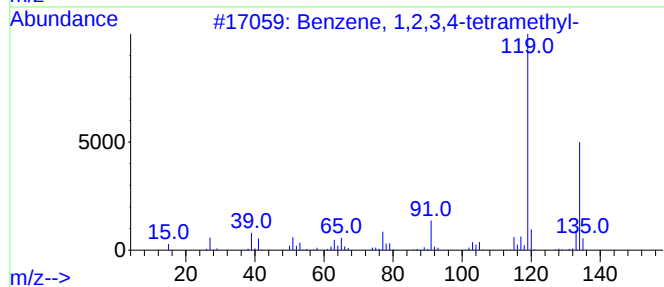
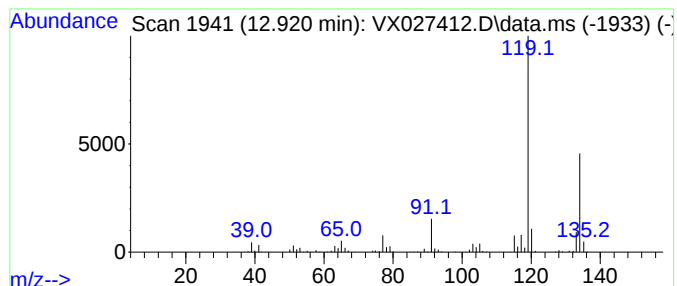
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	13.00 ug/l	389661	1,4-Dichlorobenzene-d4	12.024

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	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027412.D
Acq On : 11 Mar 2022 19:15
Operator : JC/MD
Sample : N1895-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

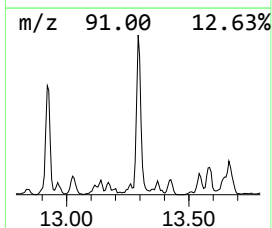
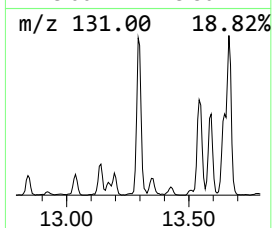
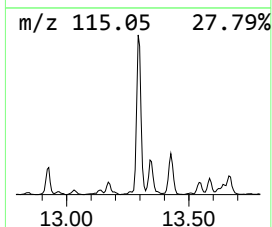
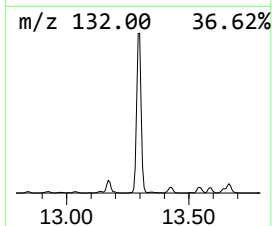
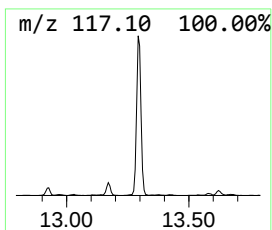
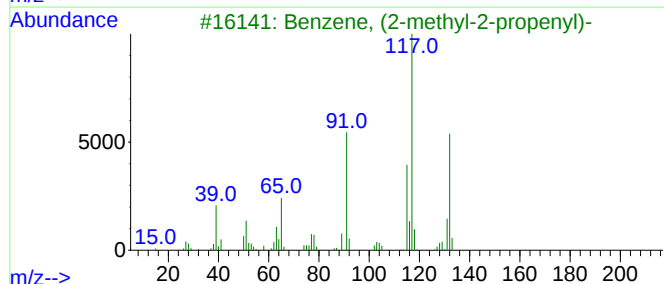
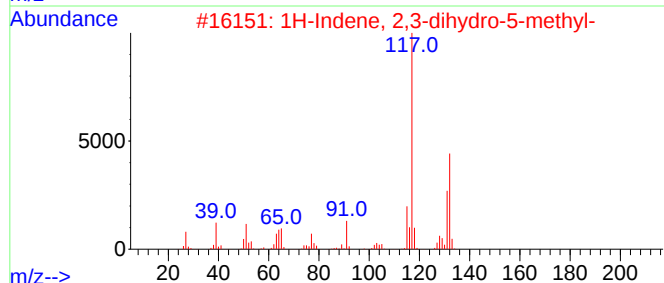
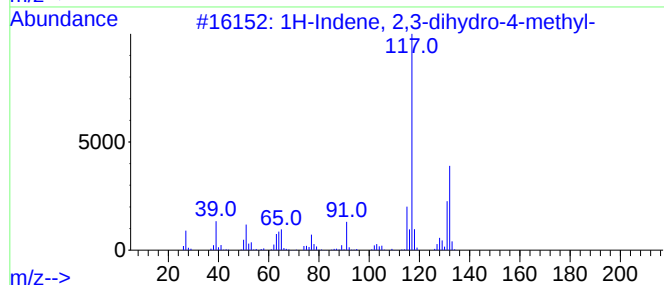
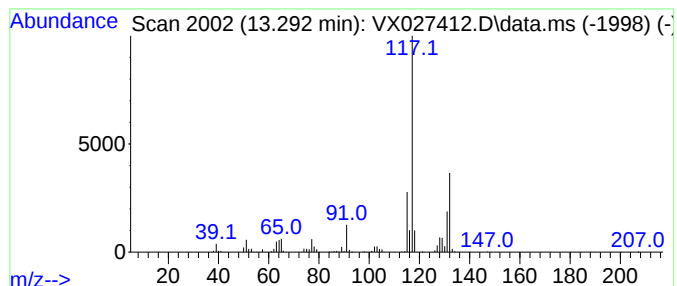
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	25.42 ug/l	761859	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3		Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
4		Indan, 1-methyl-	132	C10H12	000767-58-8	83
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027412.D
Acq On : 11 Mar 2022 19:15
Operator : JC/MD
Sample : N1895-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

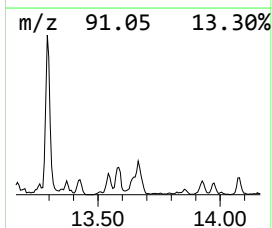
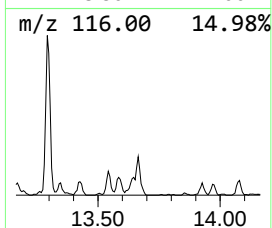
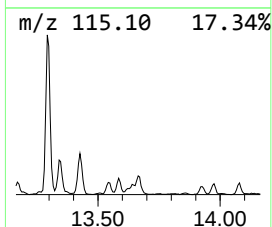
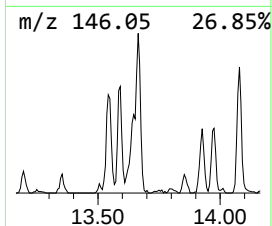
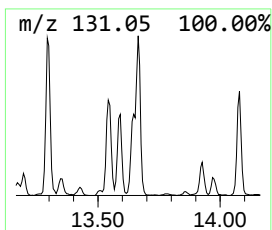
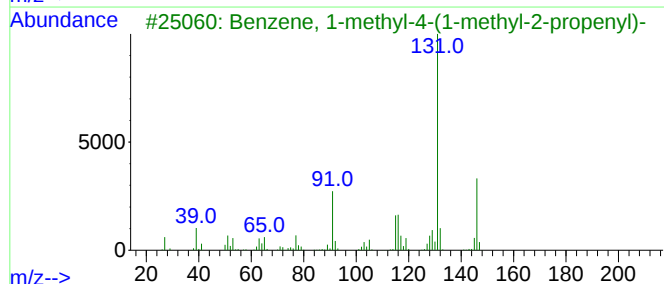
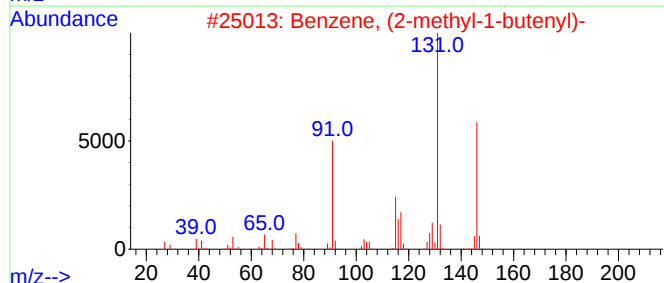
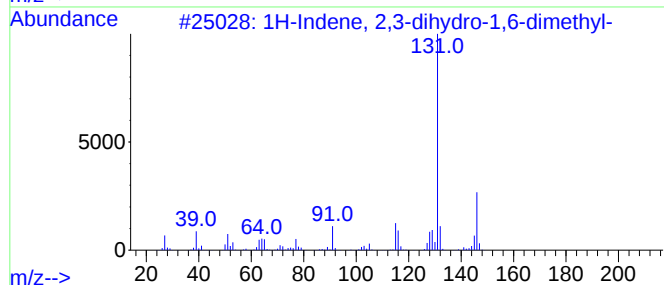
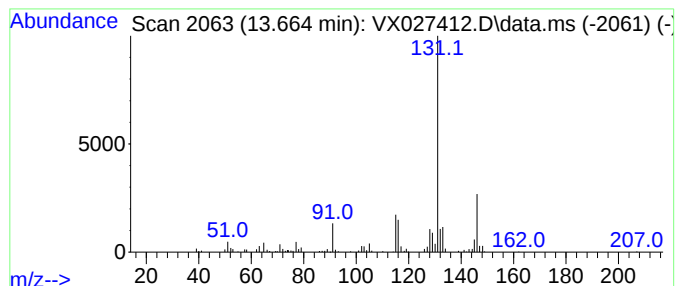
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	5.05 ug/l	151460	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	93
2			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	93
3			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	90
4			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	90
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027412.D
Acq On : 11 Mar 2022 19:15
Operator : JC/MD
Sample : N1895-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

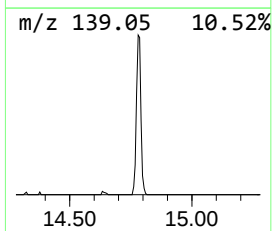
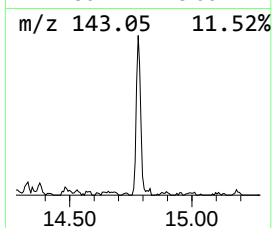
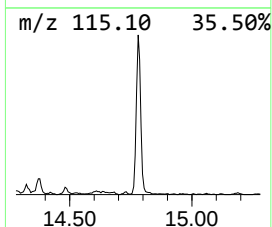
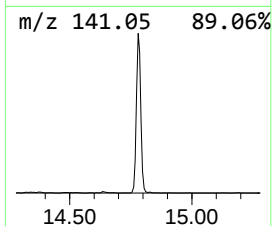
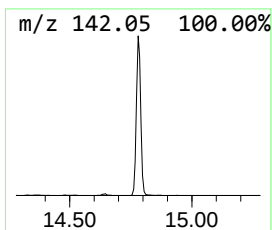
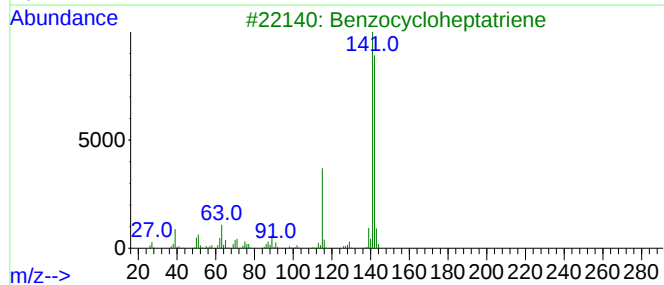
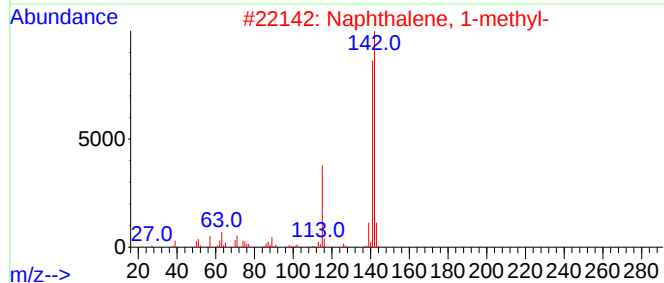
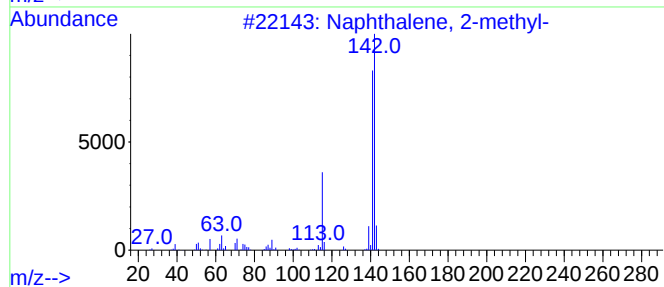
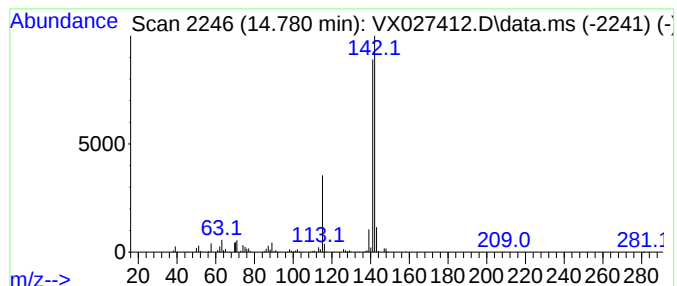
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	9.73 ug/l	291629	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031122\
Data File : VX027412.D
Acq On : 11 Mar 2022 19:15
Operator : JC/MD
Sample : N1895-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.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	1.258	8.9	ug/l	195280	1	5.556	1100540	50.0
Benzene, cyclop...	12.244	58.4	ug/l	1750220	4	12.024	1498280	50.0
Benzene, 1-ethy...	12.616	22.6	ug/l	677533	4	12.024	1498280	50.0
Benzene, 1-ethe...	12.701	14.1	ug/l	420974	4	12.024	1498280	50.0
Benzene, 1,2,3,...	12.921	13.0	ug/l	389661	4	12.024	1498280	50.0
1H-Indene, 2,3-...	13.292	25.4	ug/l	761859	4	12.024	1498280	50.0
1H-Indene, 2,3-...	13.664	5.0	ug/l	151460	4	12.024	1498280	50.0
Benzocyclohepta...	14.780	9.7	ug/l	291629	4	12.024	1498280	50.0