

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
 Data File : VX035447.D
 Acq On : 01 May 2023 17:51
 Operator : JC/MD
 Sample : 02522-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.550	720	732	750	rVB	251505	723348	1.65%	0.376%
2	6.763	921	931	941	rBV	380372	930368	2.12%	0.483%
3	7.379	1019	1032	1046	rBV	219288	494154	1.13%	0.257%
4	8.647	1235	1240	1248	rVB	815458	1271693	2.90%	0.660%
5	10.055	1466	1471	1475	rBV	791977	1071580	2.45%	0.556%
6	10.195	1488	1494	1503	rVB	8400923	10993791	25.11%	5.708%
7	10.305	1503	1512	1517	rVB	627820	928046	2.12%	0.482%
8	10.640	1562	1567	1583	rVB	733382	946259	2.16%	0.491%
9	10.964	1614	1620	1630	rBV	2529680	3327653	7.60%	1.728%
10	11.079	1634	1639	1644	rBV	713116	896714	2.05%	0.466%
11	11.305	1670	1676	1682	rBV	2504533	3001307	6.86%	1.558%
12	11.396	1682	1691	1696	rVV	1530185	2052332	4.69%	1.066%
13	11.451	1696	1700	1708	rVB	1921831	2288719	5.23%	1.188%
14	11.610	1721	1726	1736	rVB	4420544	5621398	12.84%	2.919%
15	11.756	1738	1750	1755	rBV	10632627	13829555	31.59%	7.180%
16	11.969	1779	1785	1789	rBV	668172	860208	1.96%	0.447%
17	12.018	1789	1793	1799	rVB2	1135856	1641198	3.75%	0.852%
18	12.085	1799	1804	1809	rBV	5225845	6542050	14.94%	3.396%
19	12.244	1824	1830	1837	rBV	13982102	18137659	41.43%	9.417%
20	12.317	1837	1842	1847	rVV2	1178149	1615063	3.69%	0.839%
21	12.530	1872	1877	1879	rBV	897550	1096328	2.50%	0.569%
22	12.555	1879	1881	1885	rVB	675310	706385	1.61%	0.367%
23	12.616	1885	1891	1894	rBV	1493897	1959683	4.48%	1.017%
24	12.701	1900	1905	1916	rBV	5526343	7238960	16.53%	3.758%
25	12.847	1925	1929	1934	rVB	577830	693315	1.58%	0.360%
26	12.921	1934	1941	1944	rBV	1041700	1247476	2.85%	0.648%
27	12.963	1944	1948	1954	rVB	2173327	2548720	5.82%	1.323%
28	13.170	1974	1982	1987	rBV	3965073	4730089	10.80%	2.456%
29	13.286	1993	2001	2007	rBV2	4414124	6240732	14.25%	3.240%
30	13.341	2007	2010	2018	rVV	1178562	1449630	3.31%	0.753%
31	13.427	2018	2024	2031	rVB	4038539	5161394	11.79%	2.680%
32	13.500	2031	2036	2040	rBV	426223	557418	1.27%	0.289%
33	13.548	2040	2044	2047	rVV	506700	706377	1.61%	0.367%
34	13.585	2047	2050	2057	rVV2	222283	448889	1.03%	0.233%
35	13.670	2060	2064	2069	rVB2	360666	542775	1.24%	0.282%
36	13.786	2074	2083	2088	rBV	29561022	43782093	100.00%	22.731%

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Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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

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37	14.225	2149	2155	2159	rBV2	314709	593031	1.35%	0.308%
38	14.323	2166	2171	2176	rVB	374082	574114	1.31%	0.298%
39	14.640	2218	2223	2233	rVB	7932262	9890539	22.59%	5.135%
40	14.786	2241	2247	2256	rBV	12681070	16869384	38.53%	8.758%
41	15.207	2308	2316	2321	rBV	1333467	1745734	3.99%	0.906%
42	15.377	2334	2344	2347	rBV	363178	600677	1.37%	0.312%
43	15.475	2354	2360	2373	rVV	635460	1082047	2.47%	0.562%
44	15.615	2373	2383	2387	rVV	1218137	1992365	4.55%	1.034%
45	15.835	2409	2419	2431	rVB	321390	932209	2.13%	0.484%
46	15.987	2438	2444	2454	rVB	267356	440421	1.01%	0.229%
47	16.328	2492	2500	2510	rBV	871280	1608135	3.67%	0.835%

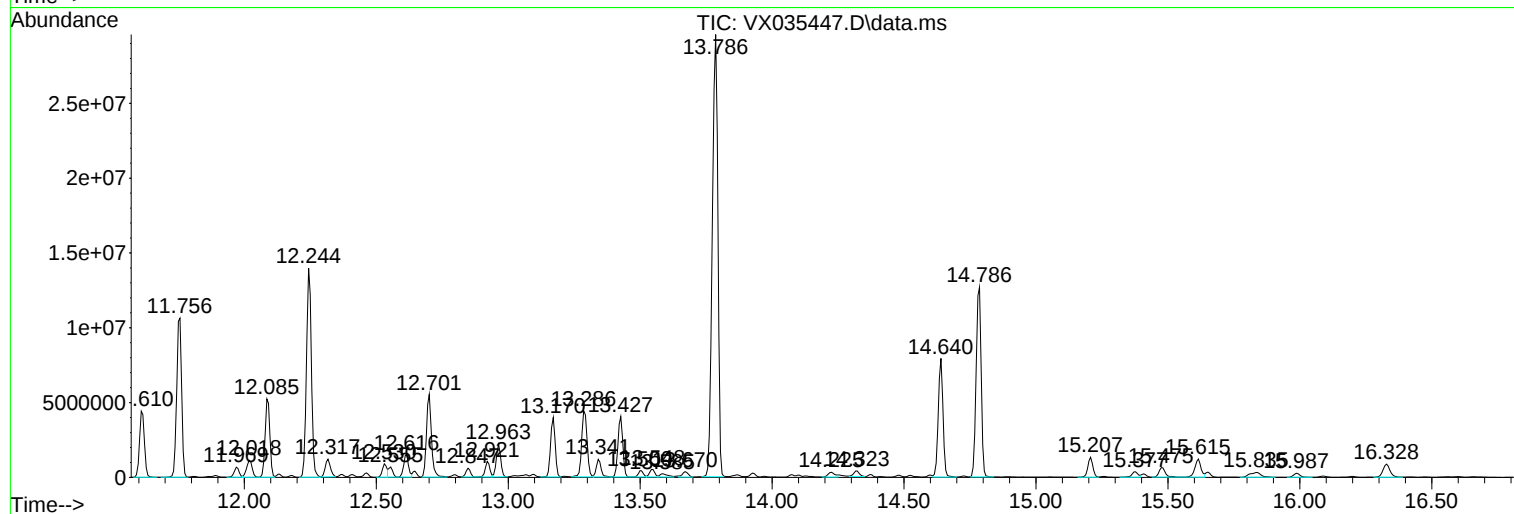
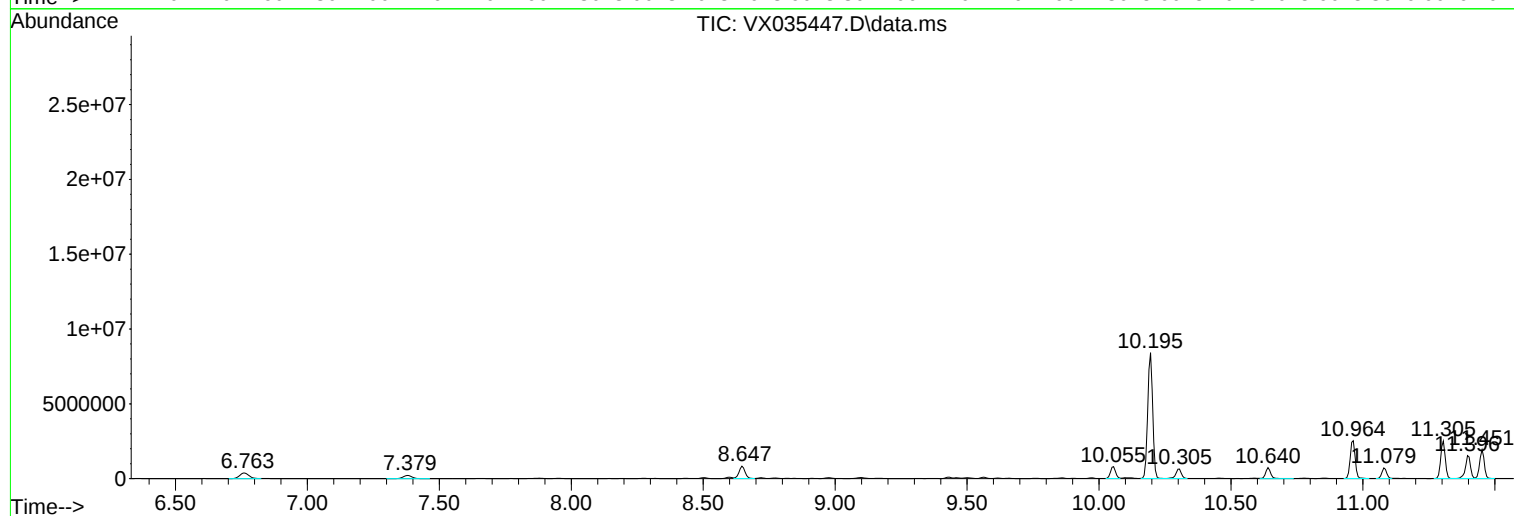
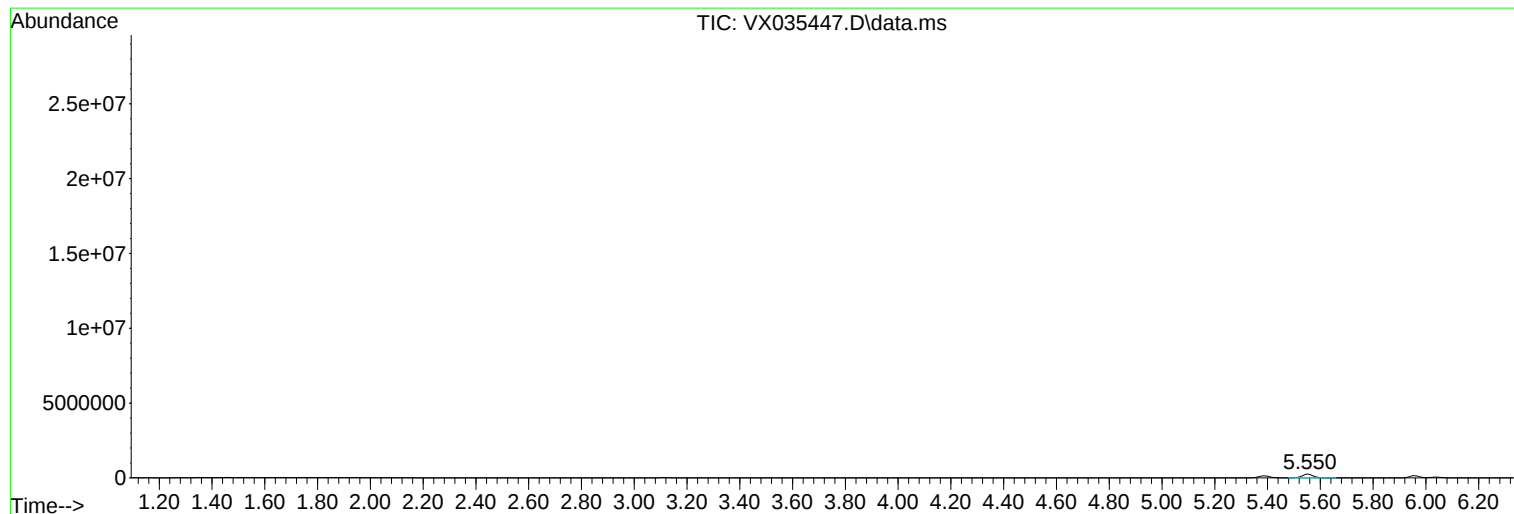
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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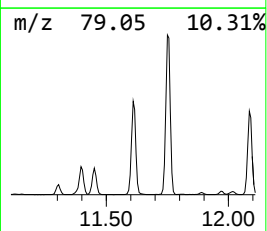
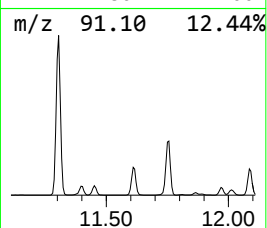
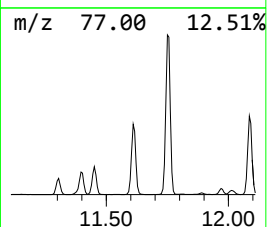
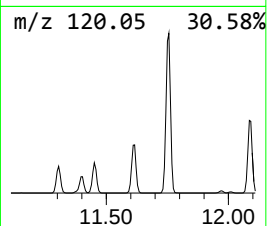
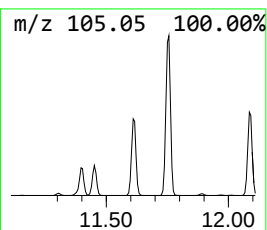
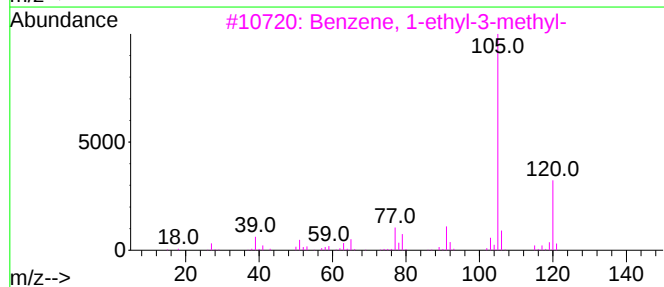
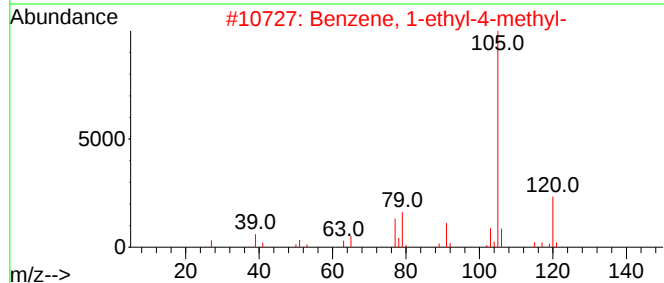
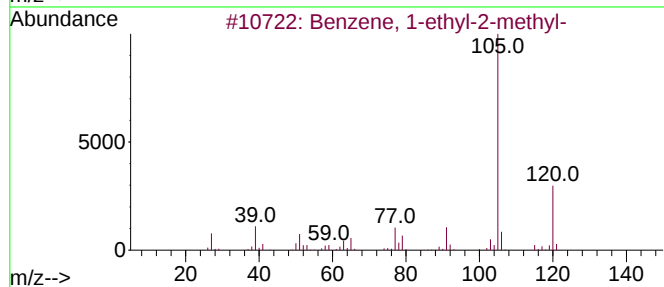
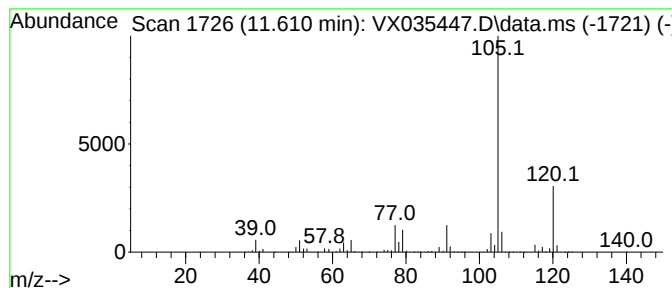
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	171.26 ug/l	5621400	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-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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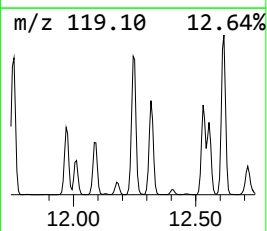
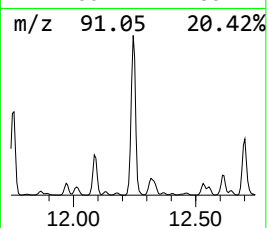
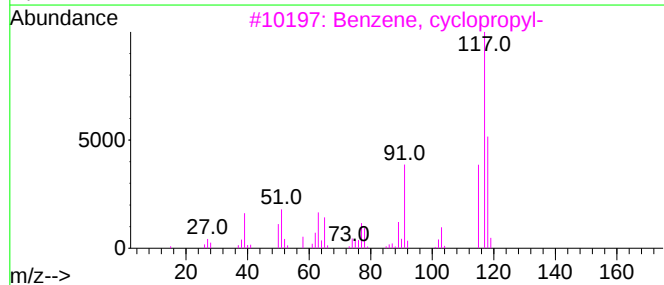
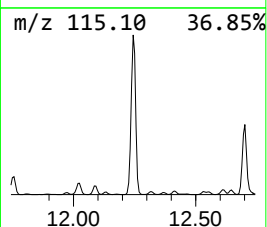
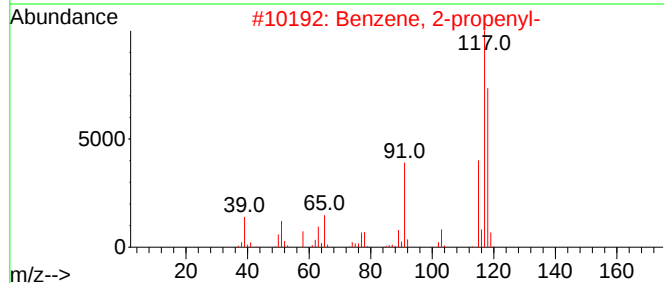
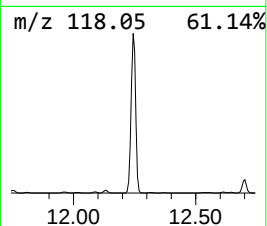
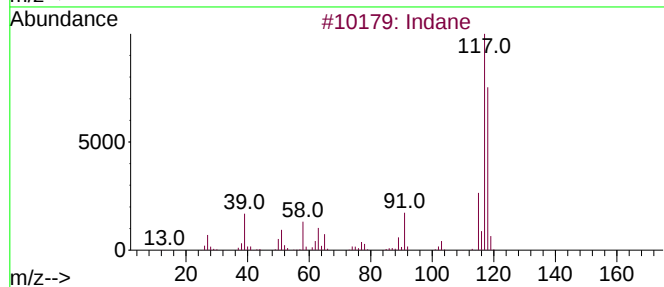
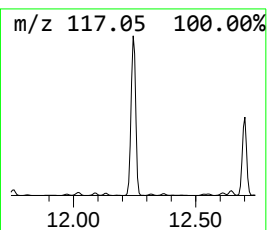
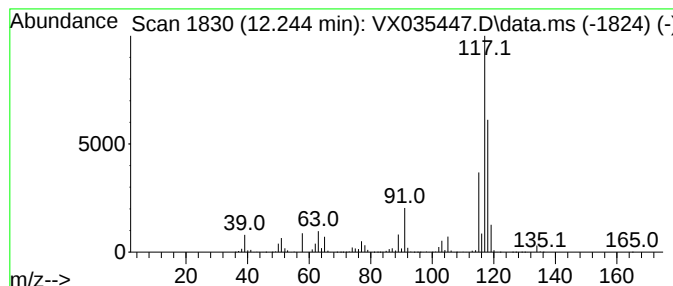
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	552.57 ug/l	18137700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	68
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	53



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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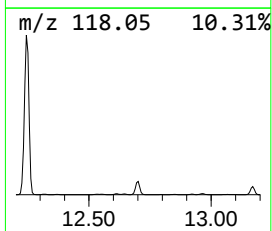
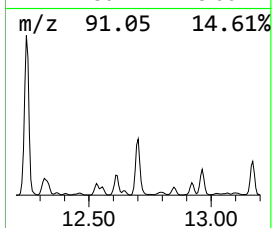
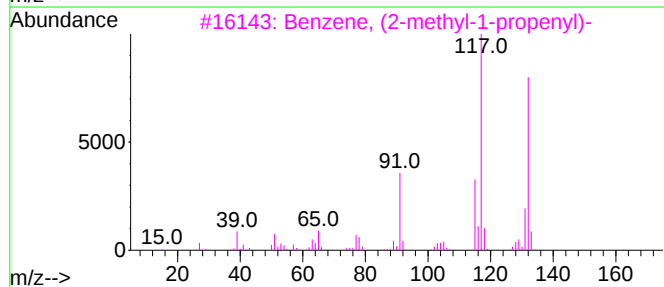
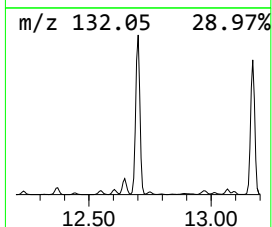
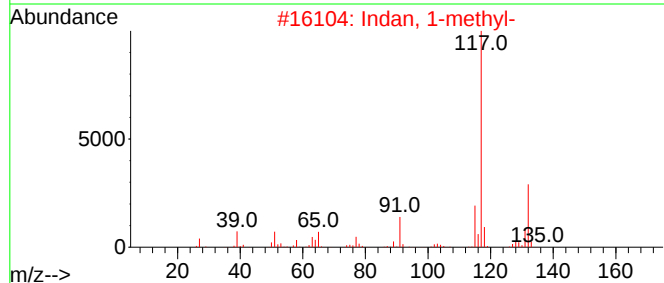
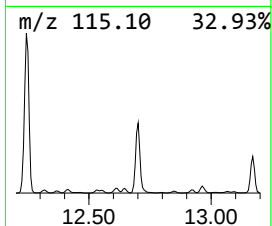
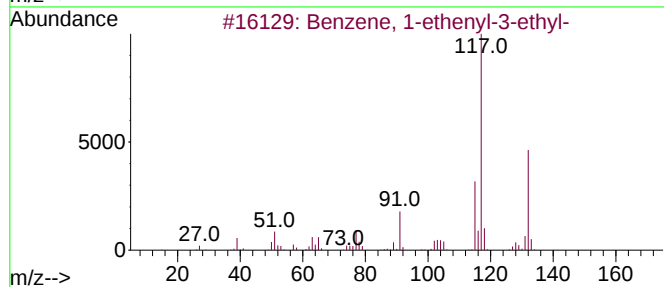
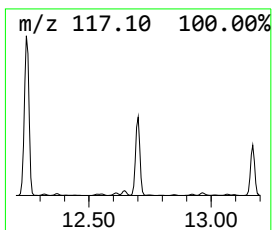
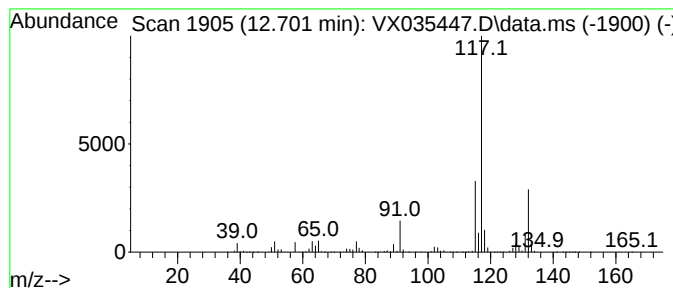
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	220.54 ug/l	7238960	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	91
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



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Instrument :
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ClientSampleId :
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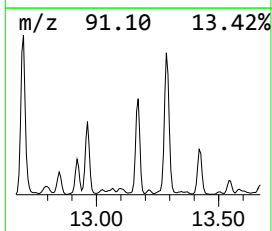
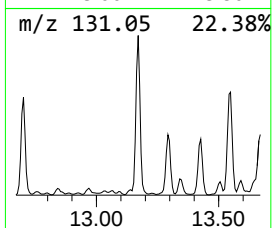
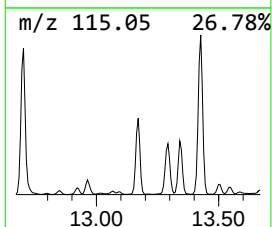
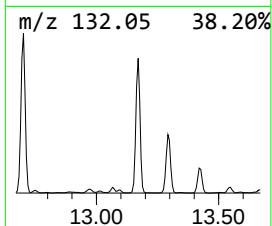
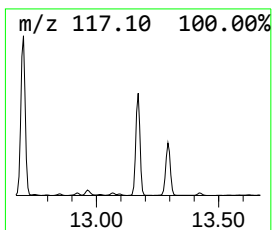
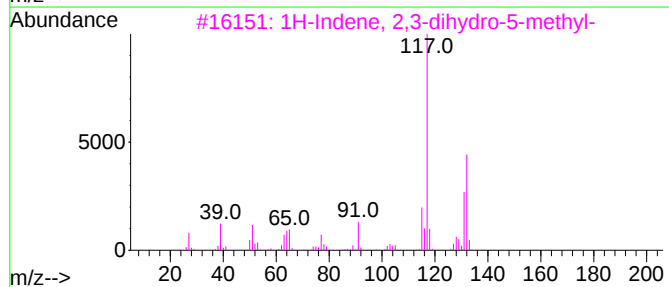
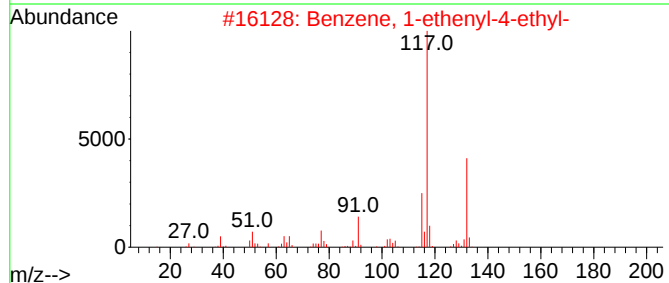
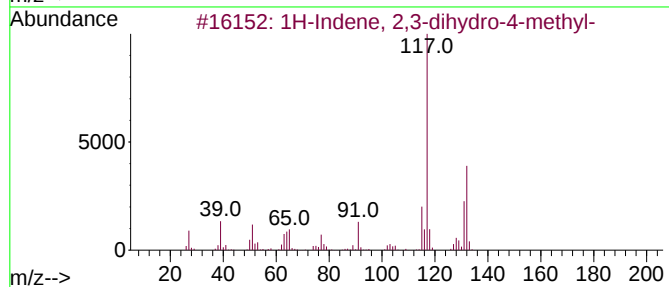
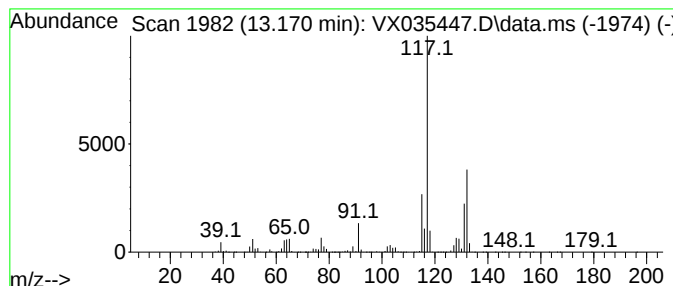
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Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.171	144.10 ug/l	4730090	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	95	
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94	
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93	
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92	
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90	



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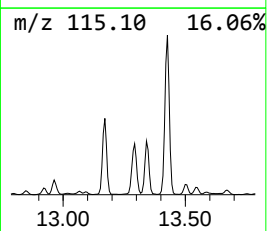
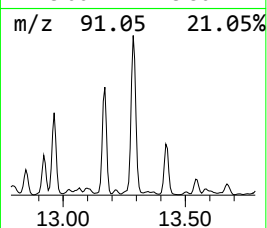
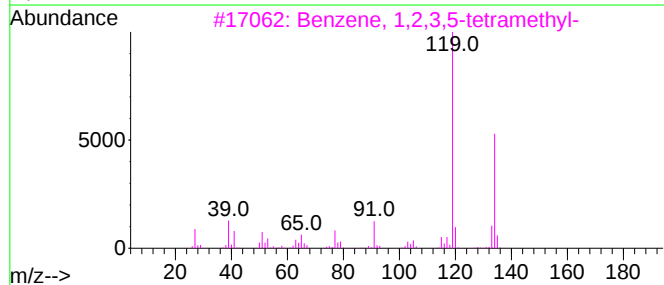
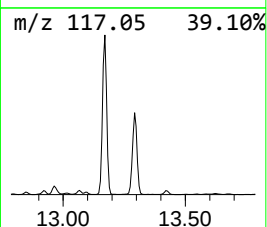
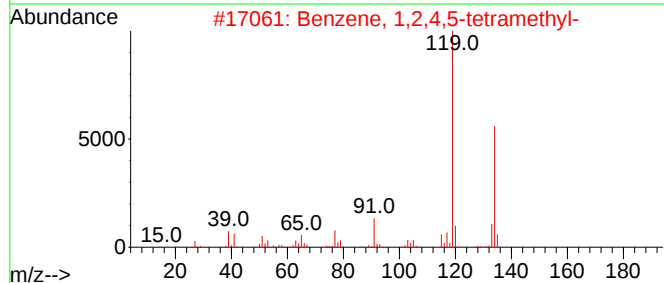
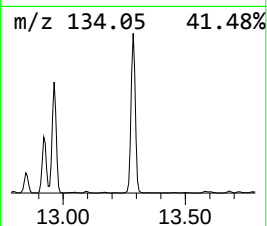
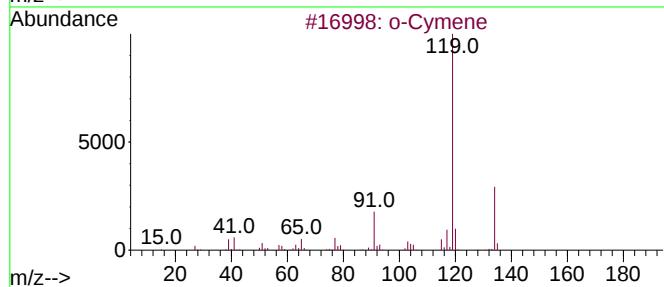
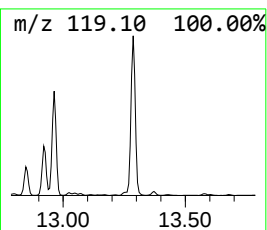
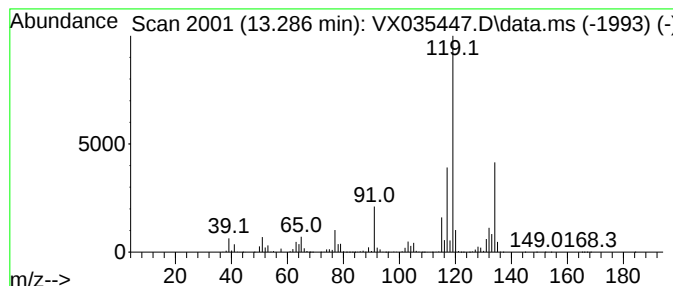
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	190.13 ug/l	6240730	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	70
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	70
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035447.D
Acq On : 01 May 2023 17:51
Operator : JC/MD
Sample : 02522-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

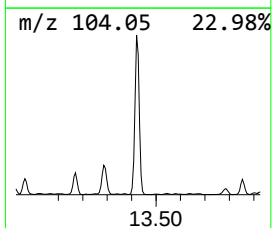
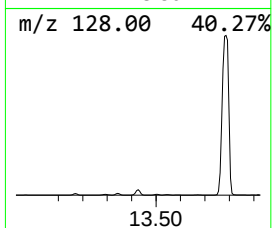
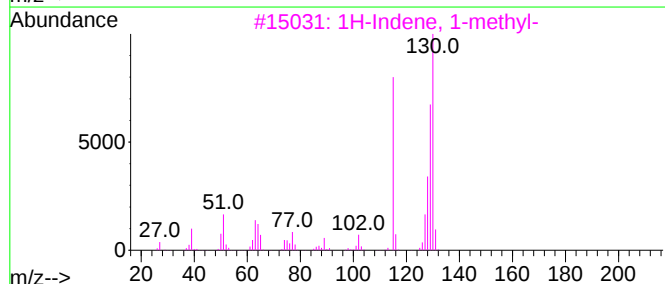
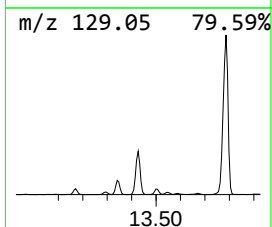
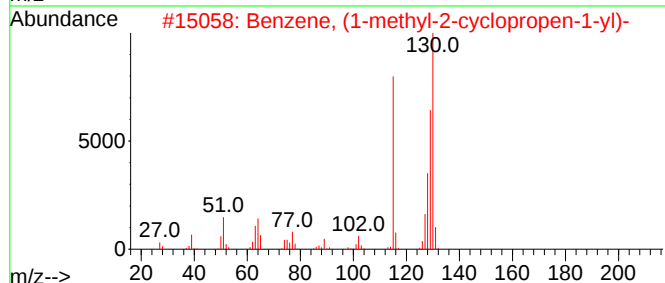
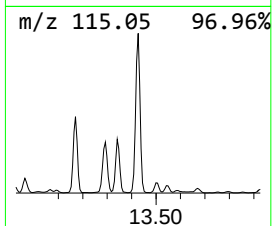
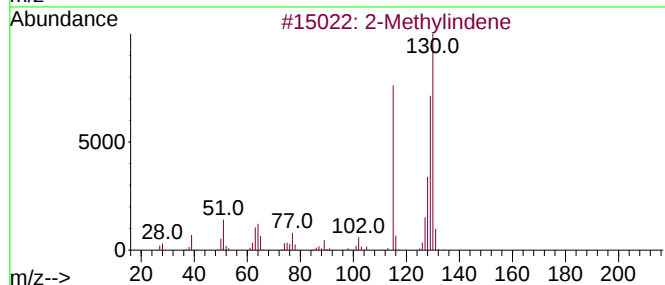
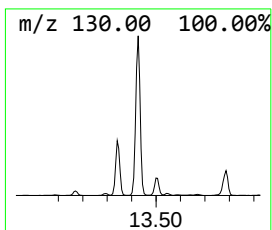
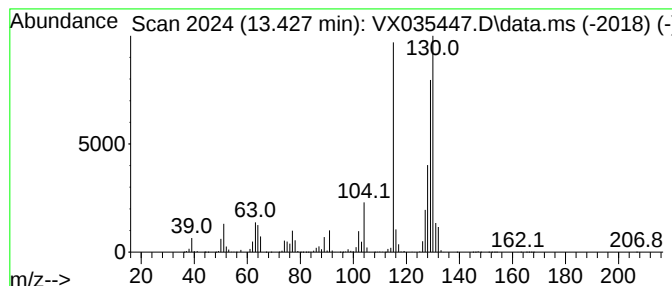
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	157.25 ug/l	5161390	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene			130	C10H10	002177-47-1	96
2	Benzene, (1-methyl-2-cyclopropen...			130	C10H10	065051-83-4	96
3	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	95
4	Benzene,1-methyl-1,2-propadienyl-			130	C10H10	022433-39-2	94
5	1H-Indene, 3-methyl-			130	C10H10	000767-60-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035447.D
Acq On : 01 May 2023 17:51
Operator : JC/MD
Sample : 02522-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

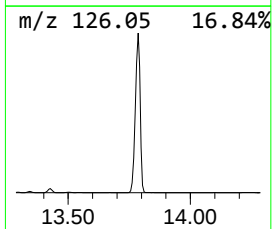
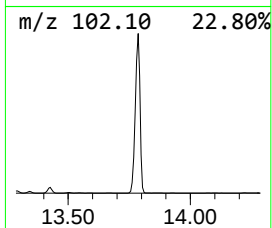
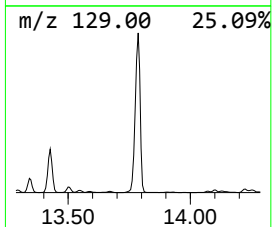
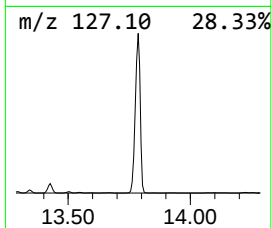
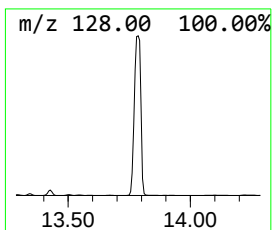
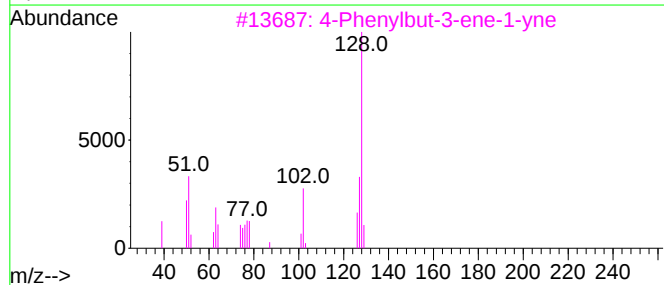
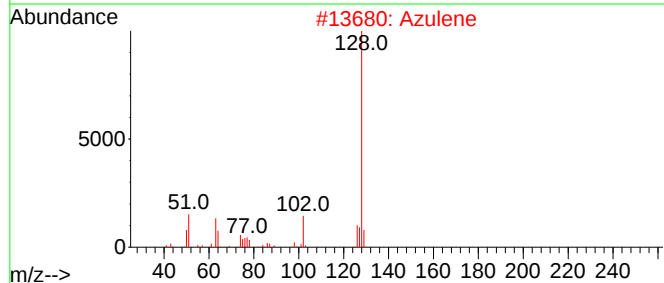
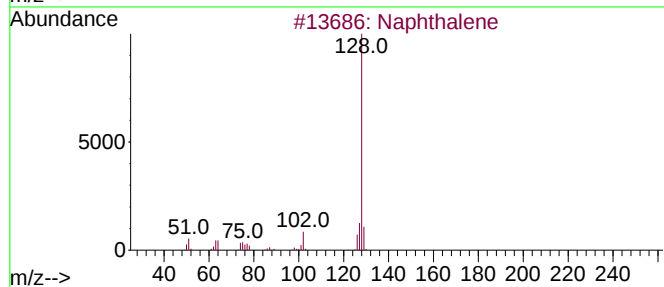
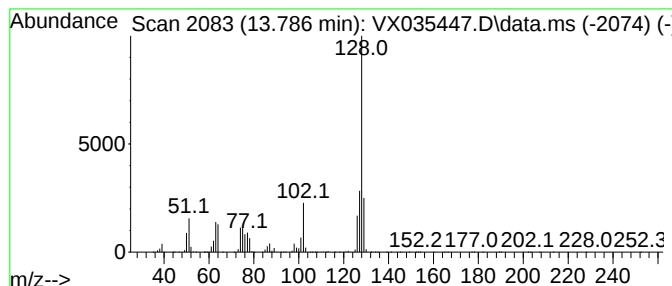
Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.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	1333.85 ug/l	43782100	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	90
2	Azulene	128	C10H8	000275-51-4	81
3	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	76
4	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	74
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX050123\
Data File : VX035447.D
Acq On : 01 May 2023 17:51
Operator : JC/MD
Sample : 02522-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

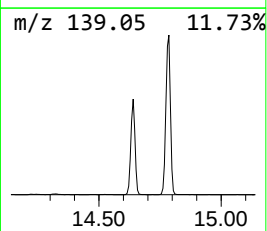
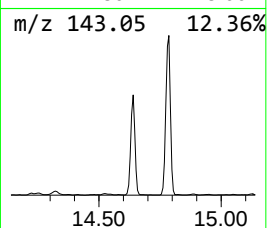
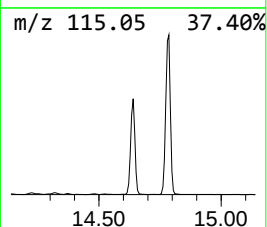
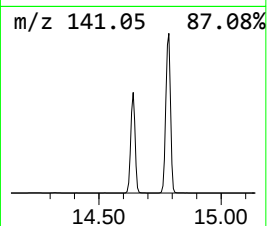
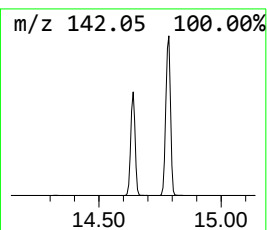
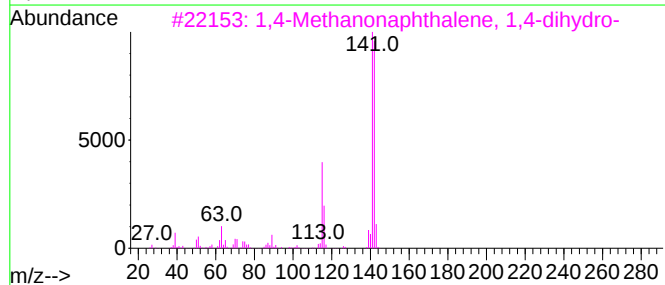
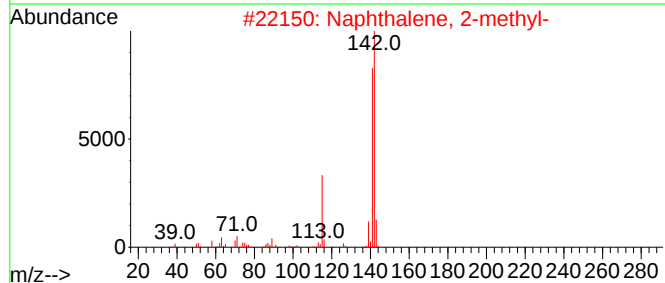
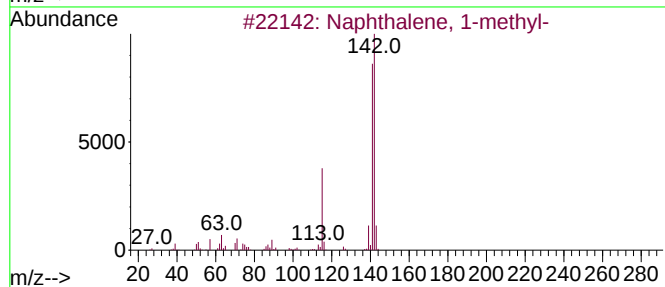
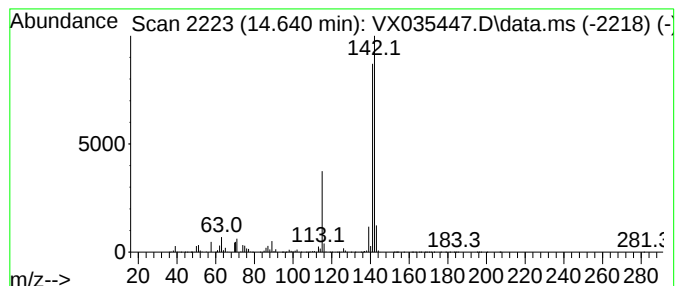
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	301.32 ug/l	9890540	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035447.D
Acq On : 01 May 2023 17:51
Operator : JC/MD
Sample : 02522-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

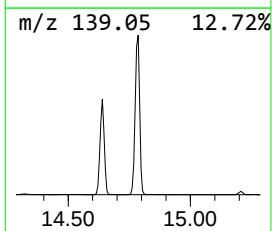
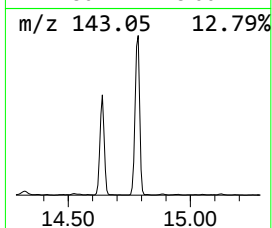
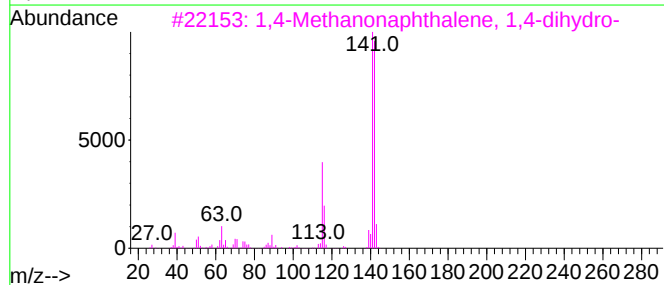
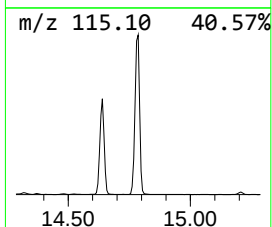
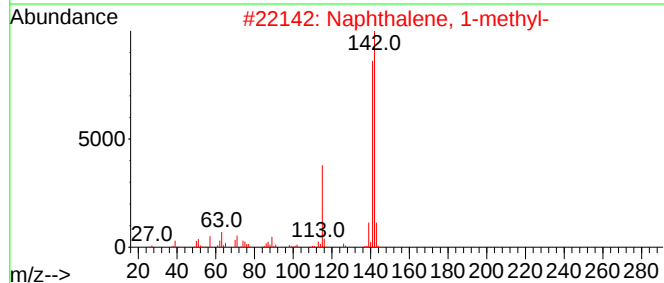
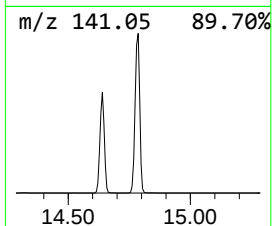
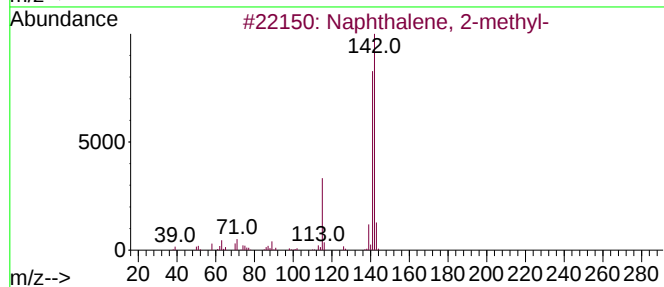
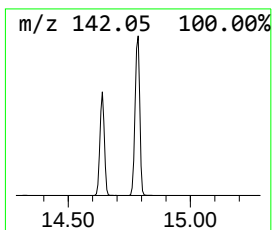
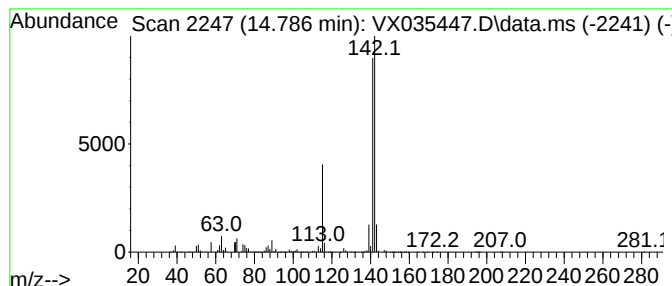
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	513.93 ug/l	16869400	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		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035447.D
Acq On : 01 May 2023 17:51
Operator : JC/MD
Sample : 02522-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.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	171.3	ug/l	5621400	4	12.024	1641200	50.0
Indane	12.244	552.6	ug/l	18137700	4	12.024	1641200	50.0
Benzene, 1-ethe...	12.701	220.5	ug/l	7238960	4	12.024	1641200	50.0
1H-Indene, 2,3-...	13.171	144.1	ug/l	4730090	4	12.024	1641200	50.0
o-Cymene	13.286	190.1	ug/l	6240730	4	12.024	1641200	50.0
2-Methylindene	13.427	157.3	ug/l	5161390	4	12.024	1641200	50.0
Azulene	13.786	1333.8	ug/l	43782100	4	12.024	1641200	50.0
1,4-Methanonaph...	14.640	301.3	ug/l	9890540	4	12.024	1641200	50.0
Bicyclo[4.4.1]u...	14.786	513.9	ug/l	16869400	4	12.024	1641200	50.0