

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
 Data File : VX035443.D
 Acq On : 01 May 2023 16:18
 Operator : JC/MD
 Sample : 02522-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14

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: VX035443.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	715	732	739	rBV3	235302	972595	1.64%	0.433%
2	5.830	765	778	790	rBV4	250021	818658	1.38%	0.364%
3	6.763	919	931	941	rBV	358725	855050	1.44%	0.381%
4	8.647	1235	1240	1248	rVB	744384	1145247	1.93%	0.510%
5	10.055	1462	1471	1476	rBV	726581	990236	1.67%	0.441%
6	10.195	1489	1494	1503	rVB	449921	618044	1.04%	0.275%
7	10.963	1614	1620	1625	rBV	2477048	3212313	5.41%	1.430%
8	11.079	1634	1639	1644	rBV	630852	813212	1.37%	0.362%
9	11.305	1671	1676	1682	rVV	2321052	2778064	4.68%	1.236%
10	11.396	1684	1691	1696	rVV	1452333	1882930	3.17%	0.838%
11	11.451	1696	1700	1707	rVB	845520	1025226	1.73%	0.456%
12	11.610	1719	1726	1737	rBV	4793584	6145504	10.35%	2.735%
13	11.756	1739	1750	1755	rBV	15790166	20112224	33.87%	8.950%
14	11.811	1755	1759	1763	rVB	588020	697425	1.17%	0.310%
15	12.018	1789	1793	1799	rVB2	1227938	1794483	3.02%	0.799%
16	12.085	1799	1804	1809	rBV	5612202	7224423	12.17%	3.215%
17	12.244	1824	1830	1837	rBV	11589999	14906650	25.10%	6.634%
18	12.317	1837	1842	1847	rVV2	1839145	2466600	4.15%	1.098%
19	12.530	1872	1877	1879	rBV	1051686	1403220	2.36%	0.624%
20	12.555	1879	1881	1885	rVV	1289524	1379758	2.32%	0.614%
21	12.616	1885	1891	1894	rVV	2682136	3353789	5.65%	1.493%
22	12.701	1900	1905	1911	rBV	5729489	7678709	12.93%	3.417%
23	12.847	1924	1929	1934	rVB	624296	763741	1.29%	0.340%
24	12.920	1934	1941	1944	rBV	1027609	1287821	2.17%	0.573%
25	12.963	1944	1948	1953	rVV	2130687	2625255	4.42%	1.168%
26	13.067	1960	1965	1967	rVV2	553220	833639	1.40%	0.371%
27	13.170	1977	1982	1987	rVB	3649633	4346091	7.32%	1.934%
28	13.286	1993	2001	2006	rBV2	3889557	5459075	9.19%	2.429%
29	13.341	2006	2010	2018	rVV	3221010	3937223	6.63%	1.752%
30	13.426	2018	2024	2030	rVB	10885794	13900420	23.41%	6.186%
31	13.506	2030	2037	2040	rBV	1633291	2059323	3.47%	0.916%
32	13.548	2040	2044	2047	rVV	688801	901314	1.52%	0.401%
33	13.676	2058	2065	2070	rVB2	547404	887421	1.49%	0.395%
34	13.792	2073	2084	2089	rBV	36087007	59385475	100.00%	26.428%
35	14.225	2149	2155	2158	rBV2	870941	1411444	2.38%	0.628%
36	14.262	2158	2161	2165	rVV2	377524	703417	1.18%	0.313%

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37	14.316	2166	2170	2177	rVB	1085736	1853408	3.12%	0.825%
38	14.524	2200	2204	2211	rVB	516980	798787	1.35%	0.355%
39	14.640	2218	2223	2233	rVB	12905053	16036199	27.00%	7.137%
40	14.786	2241	2247	2252	rBV	12430574	16222065	27.32%	7.219%
41	15.207	2308	2316	2321	rBV	691102	952890	1.60%	0.424%
42	15.377	2338	2344	2347	rBV	779622	1129144	1.90%	0.502%
43	15.475	2355	2360	2366	rBV	700615	1140655	1.92%	0.508%
44	15.615	2376	2383	2386	rBV	1275850	1983877	3.34%	0.883%
45	15.652	2386	2389	2395	rVB	480371	704237	1.19%	0.313%
46	15.834	2410	2419	2432	rVB	372068	1041502	1.75%	0.463%
47	16.328	2492	2500	2510	rBV	1110925	2067514	3.48%	0.920%

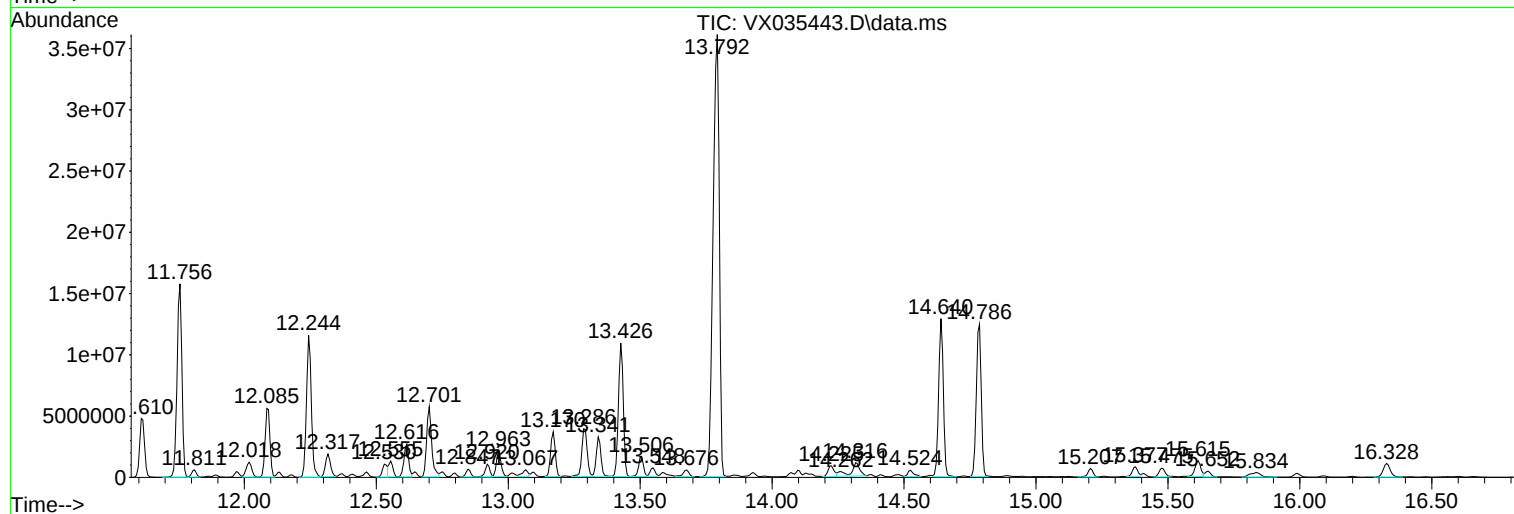
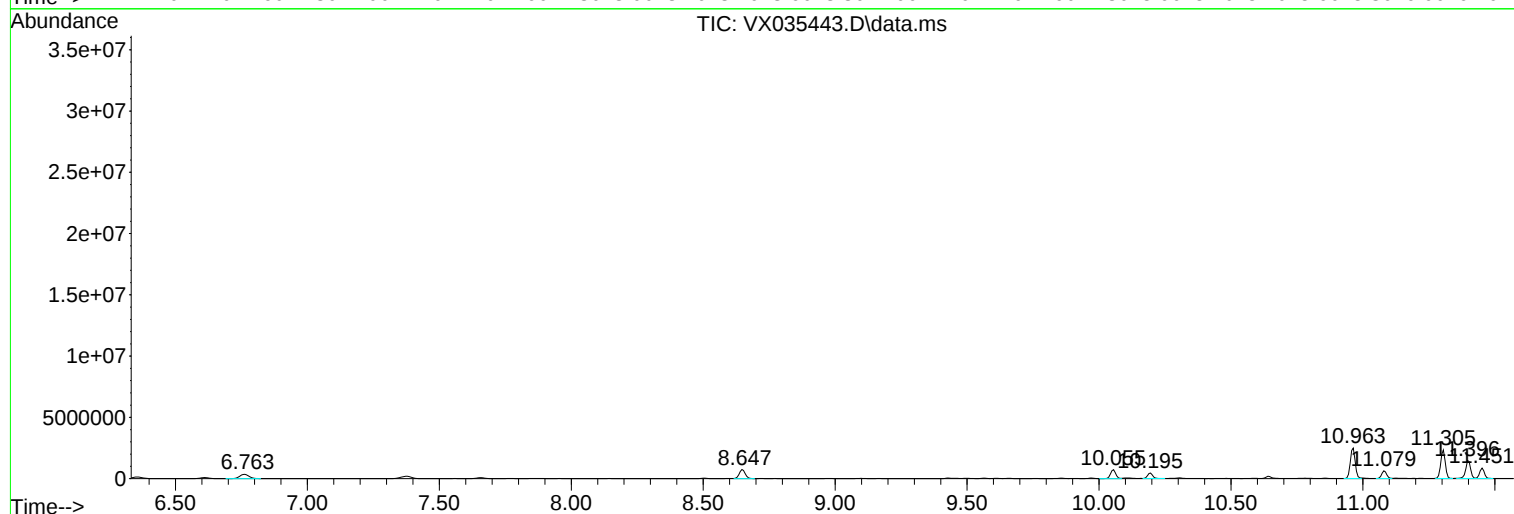
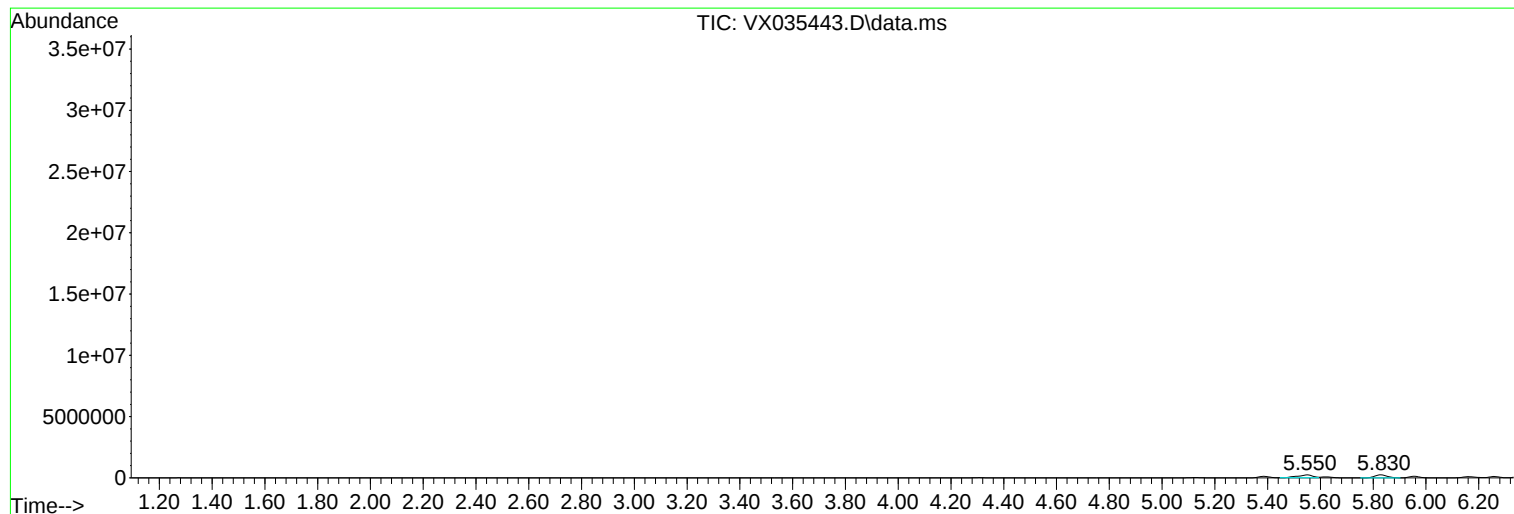
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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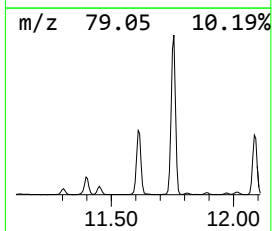
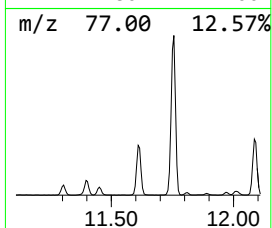
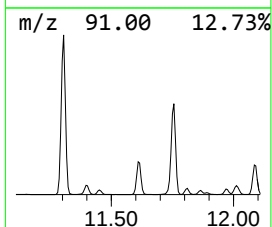
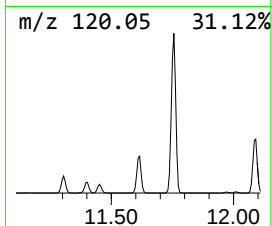
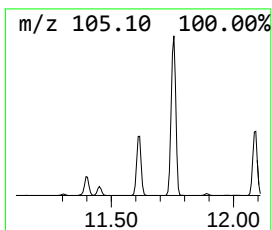
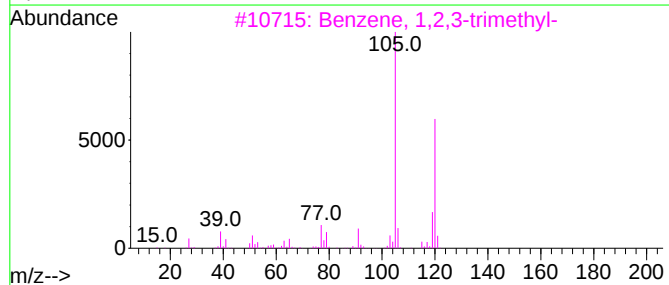
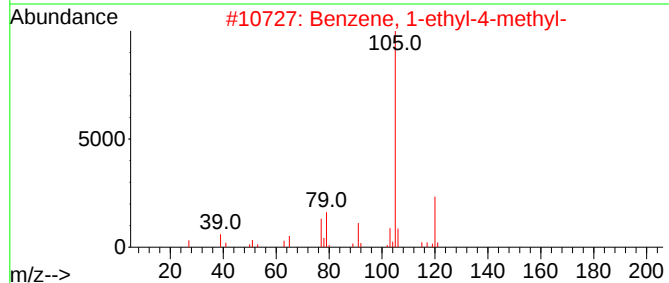
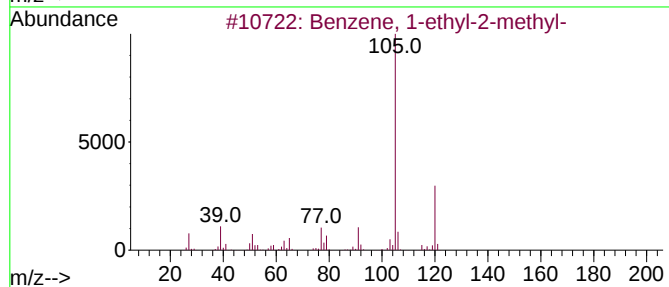
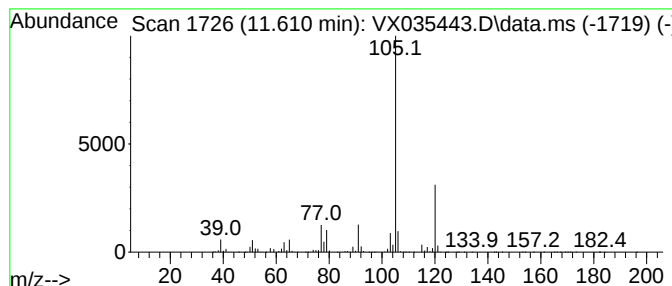
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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	171.23 ug/l	6145500	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	93
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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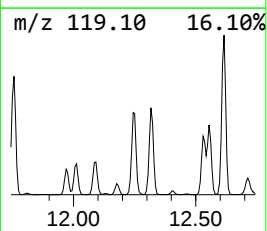
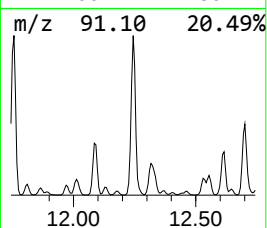
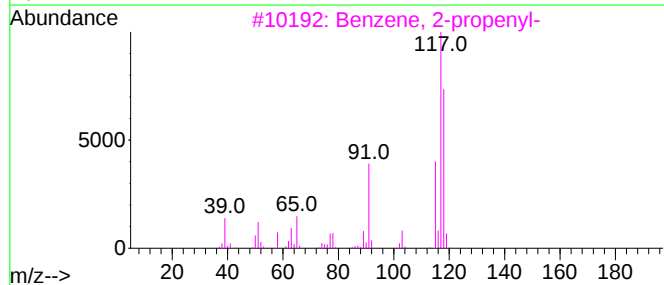
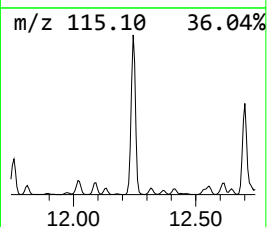
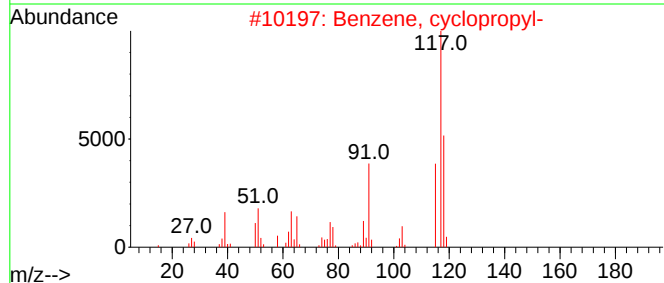
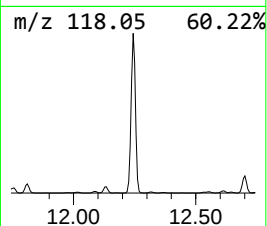
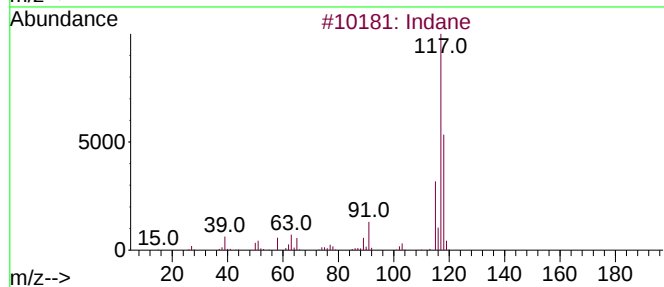
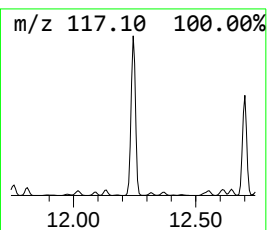
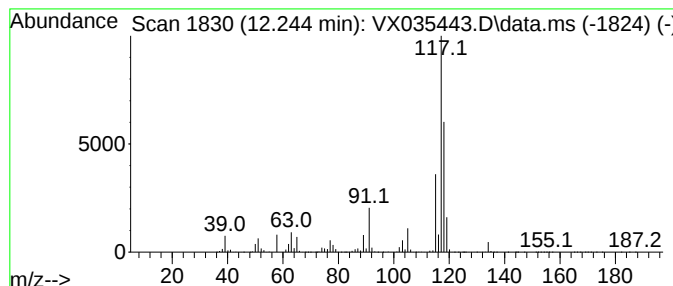
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	415.35 ug/l	14906700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	62
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55



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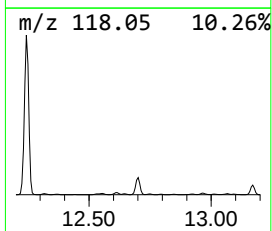
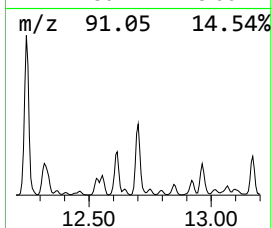
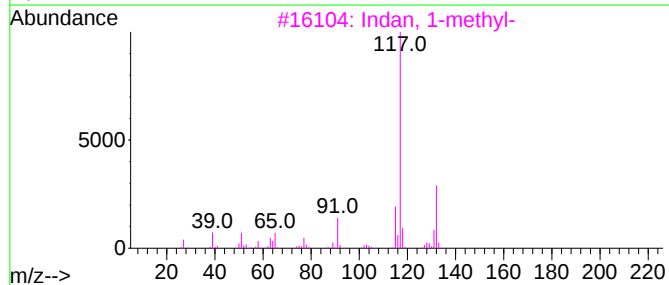
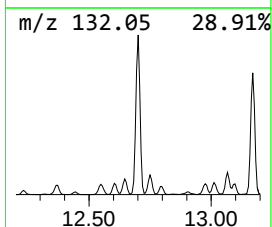
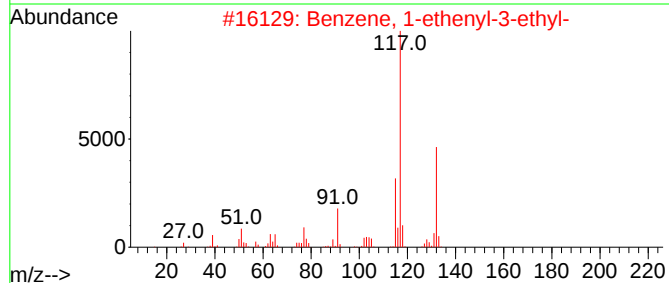
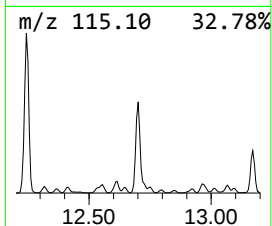
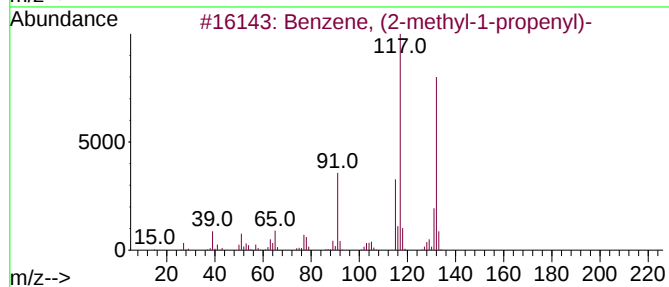
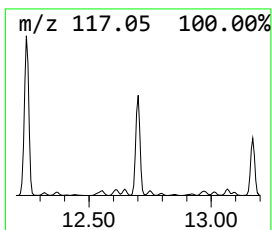
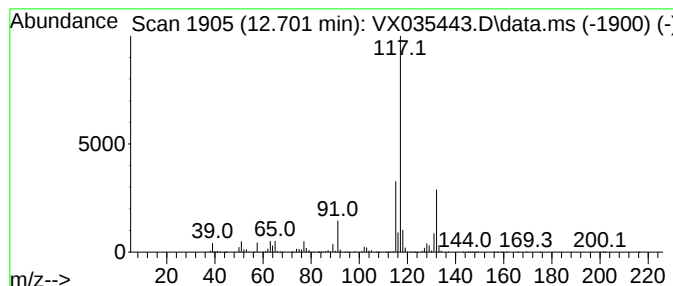
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	213.95 ug/l	7678710	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	91
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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ClientSampleId :
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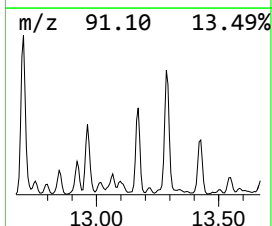
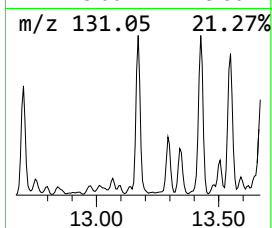
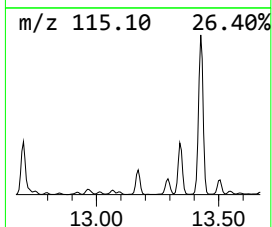
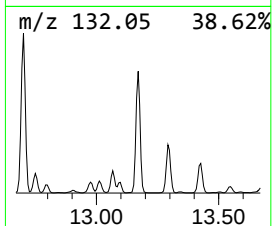
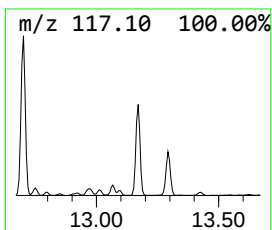
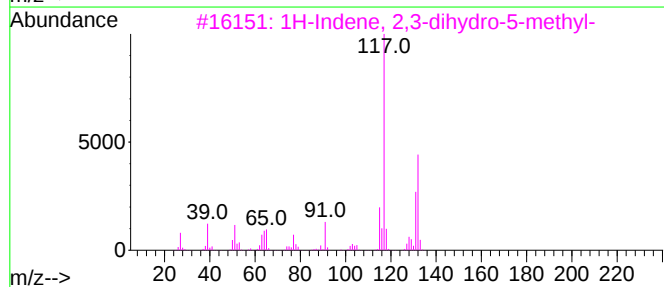
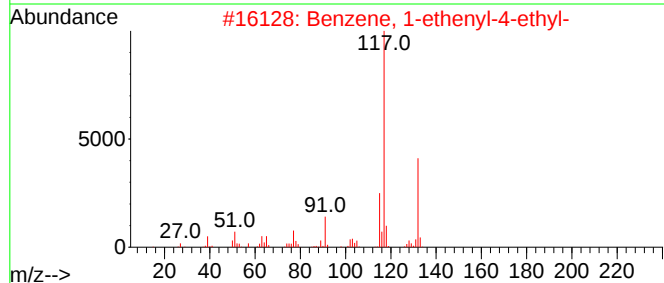
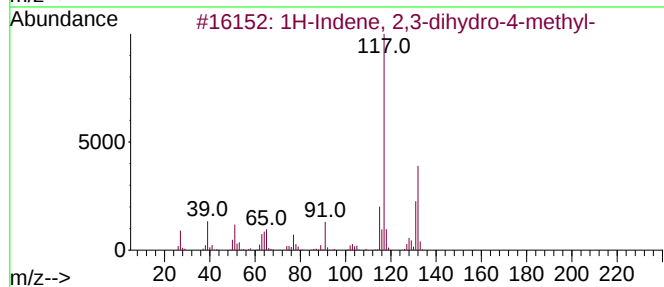
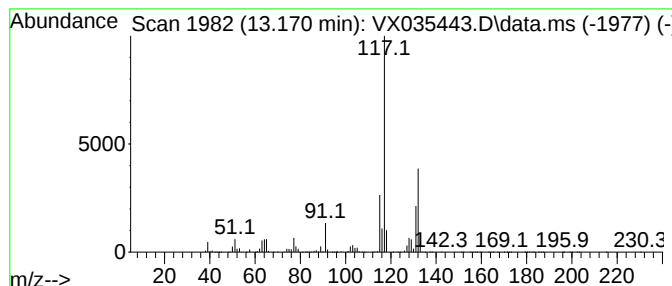
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Quant Title : SW846 8260

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.
13.170	121.10 ug/l	4346090	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, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



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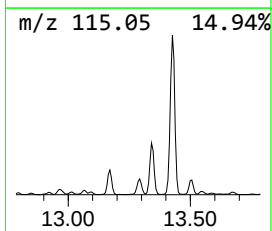
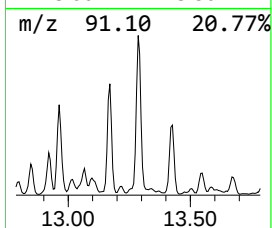
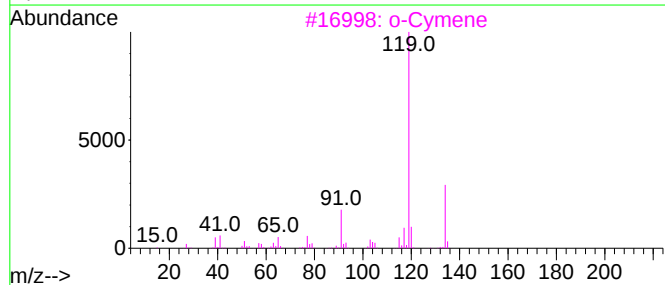
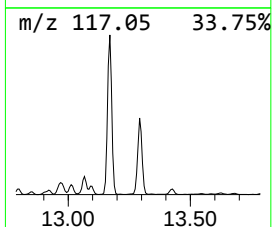
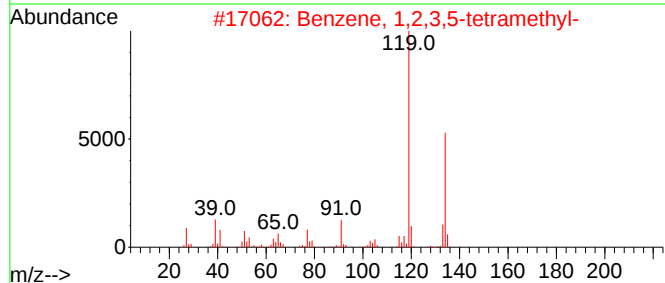
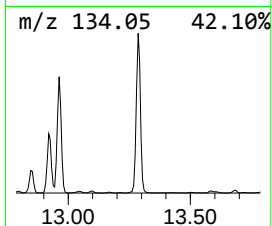
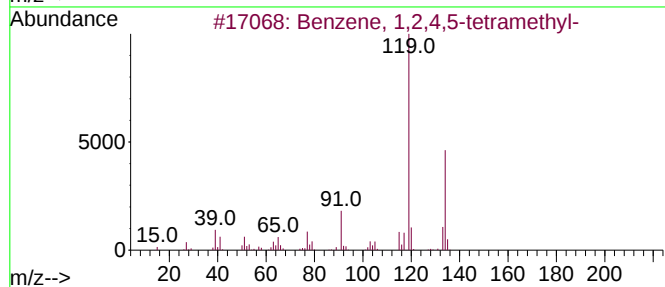
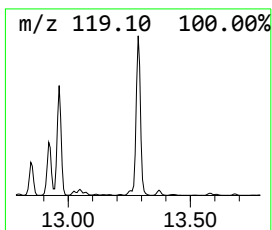
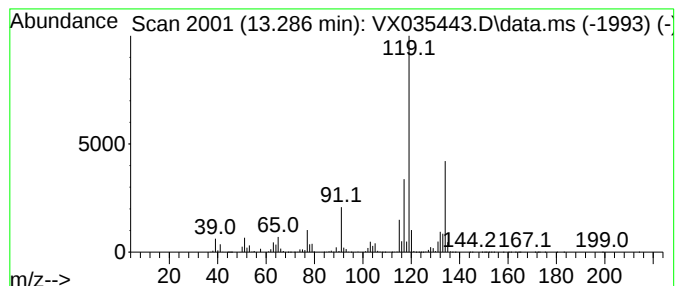
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	152.11 ug/l	5459080	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	90
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, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035443.D
Acq On : 01 May 2023 16:18
Operator : JC/MD
Sample : 02522-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

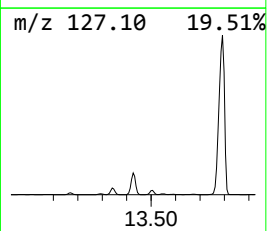
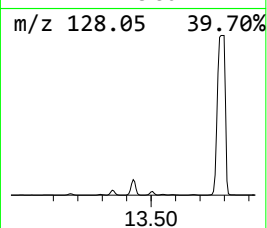
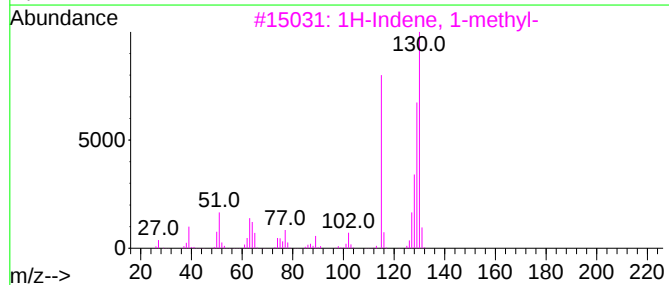
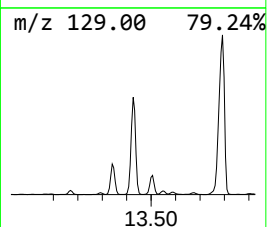
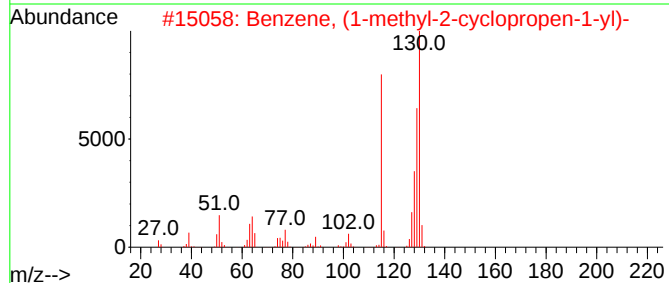
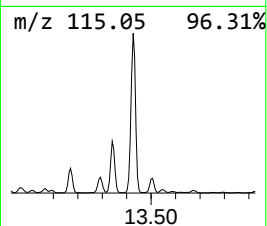
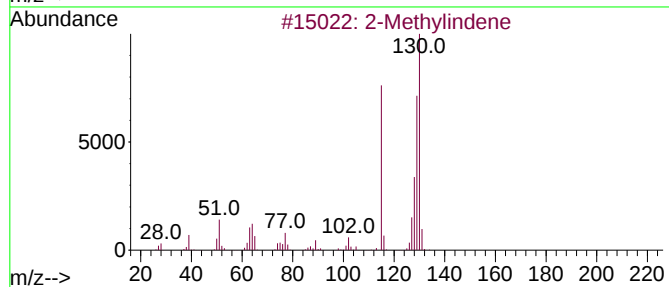
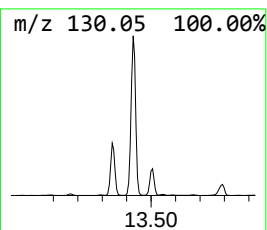
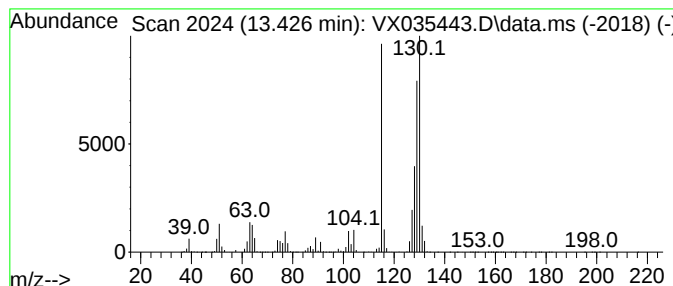
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	387.31 ug/l	13900400	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 : VX035443.D
Acq On : 01 May 2023 16:18
Operator : JC/MD
Sample : 02522-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

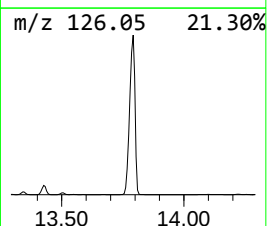
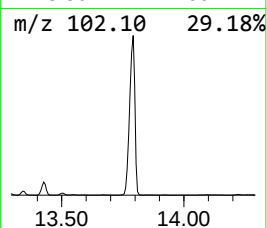
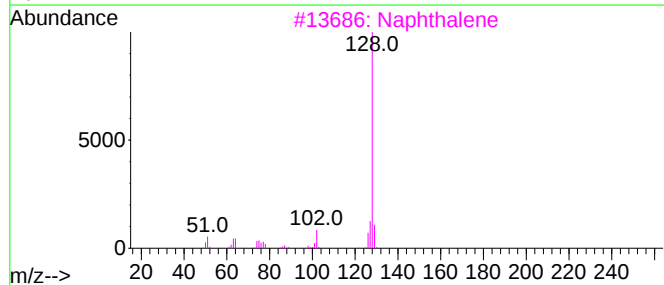
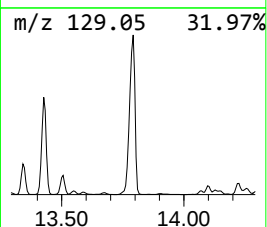
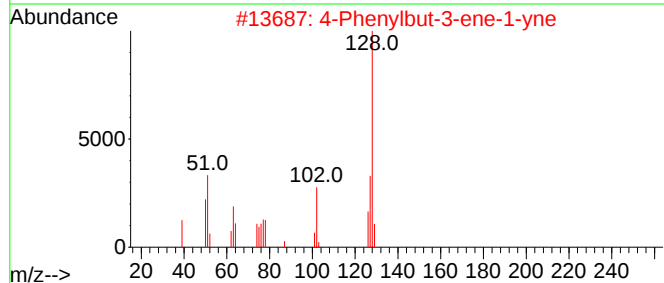
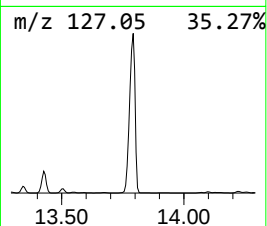
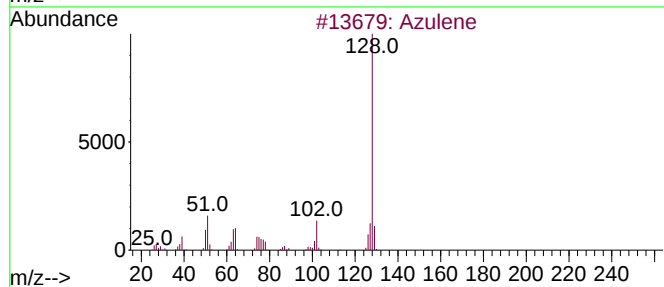
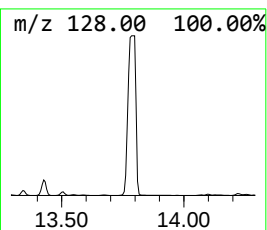
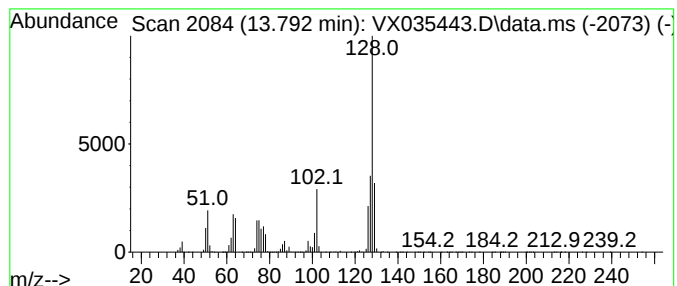
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Quant Title : SW846 8260

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.
13.792	1654.67 ug/l	59385500	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	93
2			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	90
3			Naphthalene	128	C10H8	000091-20-3	90
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	64
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035443.D
Acq On : 01 May 2023 16:18
Operator : JC/MD
Sample : 02522-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

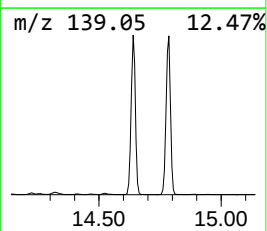
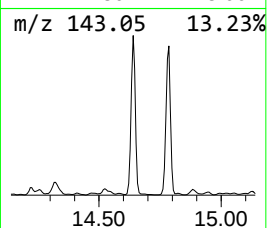
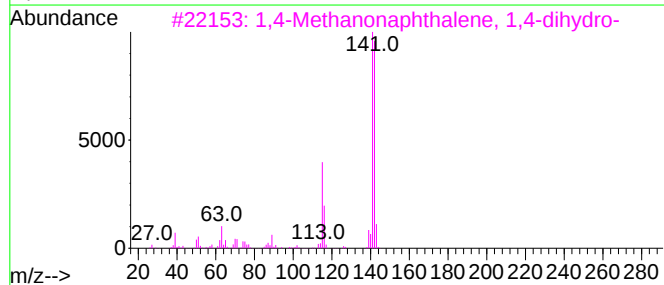
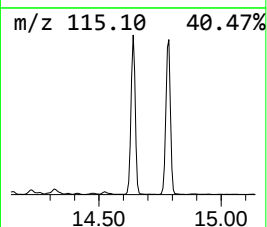
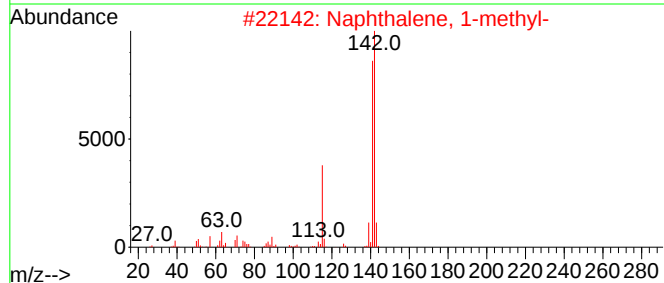
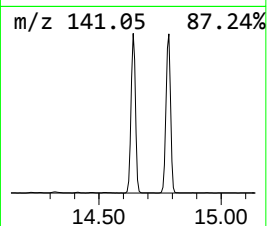
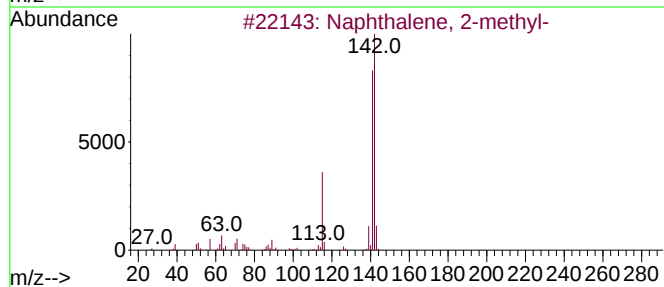
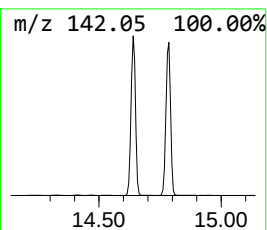
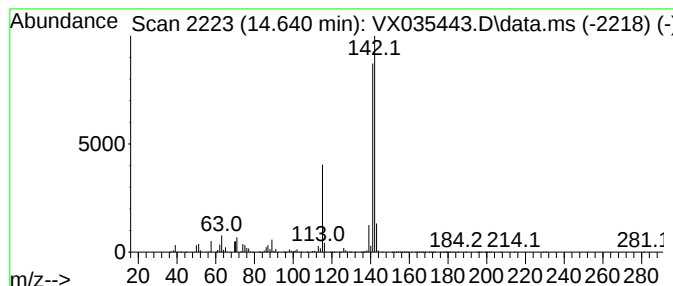
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	446.82 ug/l	16036200	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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035443.D
Acq On : 01 May 2023 16:18
Operator : JC/MD
Sample : 02522-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

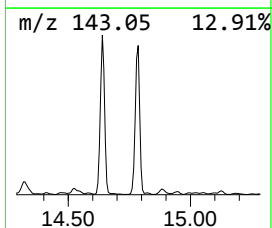
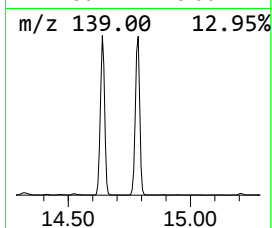
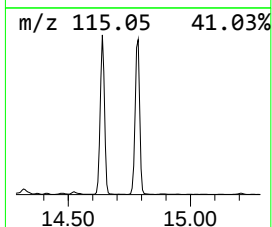
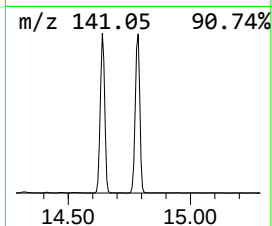
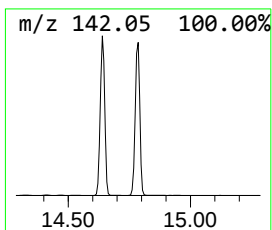
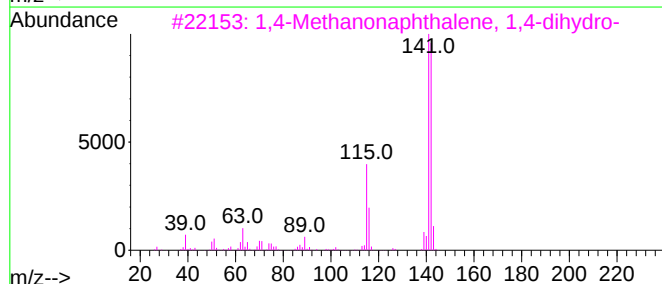
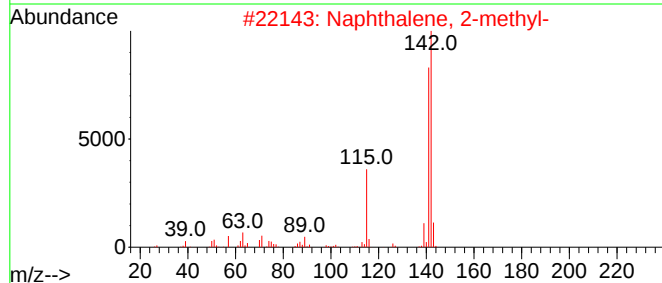
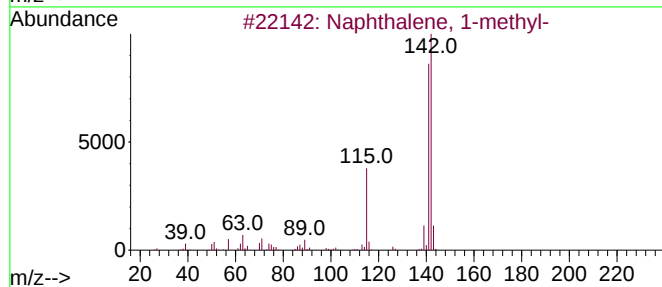
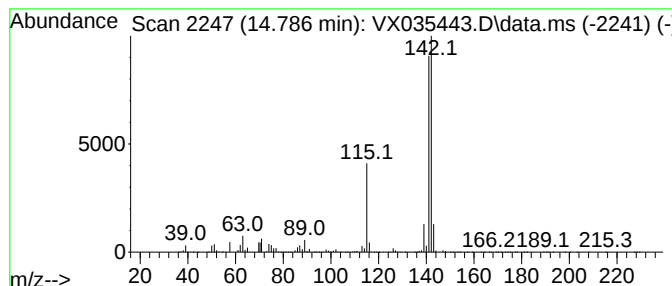
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	452.00 ug/l	16222100	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	94
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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050123\
Data File : VX035443.D
Acq On : 01 May 2023 16:18
Operator : JC/MD
Sample : 02522-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

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	171.2	ug/l	6145500	4	12.024	1794480	50.0
Indane	12.244	415.4	ug/l	14906700	4	12.024	1794480	50.0
Benzene, (2-met...	12.701	213.9	ug/l	7678710	4	12.024	1794480	50.0
1H-Indene, 2,3-...	13.170	121.1	ug/l	4346090	4	12.024	1794480	50.0
Benzene, 1,2,4,...	13.286	152.1	ug/l	5459080	4	12.024	1794480	50.0
2-Methylindene	13.426	387.3	ug/l	13900400	4	12.024	1794480	50.0
Azulene	13.792	1654.7	ug/l	59385500	4	12.024	1794480	50.0
1,4-Methanonaph...	14.640	446.8	ug/l	16036200	4	12.024	1794480	50.0
Bicyclo[4.4.1]u...	14.786	452.0	ug/l	16222100	4	12.024	1794480	50.0