

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
 Data File : VX037145.D
 Acq On : 21 Aug 2023 20:55
 Operator : JC/MD
 Sample : 03994-01 10X
 Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB06-Z22-23

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\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.043	803	813	828	rVB	4969124	13368385	19.66%	4.428%
2	8.647	1235	1240	1247	rVB	522712	809642	1.19%	0.268%
3	10.195	1488	1494	1500	rBV	12288647	17272138	25.40%	5.722%
4	10.305	1503	1512	1518	rVV	3008591	4114819	6.05%	1.363%
5	10.640	1562	1567	1582	rVB	3890774	5044210	7.42%	1.671%
6	10.963	1612	1620	1625	rBV	1149597	1473580	2.17%	0.488%
7	11.079	1634	1639	1651	rVB	492763	690522	1.02%	0.229%
8	11.402	1684	1692	1696	rVV	3304125	4716036	6.94%	1.562%
9	11.451	1696	1700	1712	rVB	1274984	1668930	2.45%	0.553%
10	11.610	1721	1726	1734	rVB	1607392	2103478	3.09%	0.697%
11	11.750	1740	1749	1755	rBV	4643812	6128767	9.01%	2.030%
12	11.969	1777	1785	1789	rBV	711646	1029450	1.51%	0.341%
13	12.018	1789	1793	1799	rVV3	880964	1394723	2.05%	0.462%
14	12.085	1799	1804	1809	rVV	1850076	2373790	3.49%	0.786%
15	12.134	1809	1812	1817	rVB	1123042	1269451	1.87%	0.421%
16	12.250	1824	1831	1837	rBV	24187380	35352913	52.00%	11.711%
17	12.317	1837	1842	1848	rVV	2493124	3175547	4.67%	1.052%
18	12.555	1873	1881	1885	rBV	1119342	1739141	2.56%	0.576%
19	12.616	1885	1891	1894	rBV	2649296	3299857	4.85%	1.093%
20	12.701	1900	1905	1910	rBV	1477094	2330918	3.43%	0.772%
21	12.750	1910	1913	1917	rVV	1082213	1258697	1.85%	0.417%
22	12.963	1944	1948	1953	rBV	1232485	1567621	2.31%	0.519%
23	13.170	1977	1982	1987	rVB	5039990	6015603	8.85%	1.993%
24	13.292	1997	2002	2006	rBV2	2060369	2723509	4.01%	0.902%
25	13.341	2006	2010	2015	rVB	3795204	4582487	6.74%	1.518%
26	13.426	2017	2024	2030	rVB	9272137	12856068	18.91%	4.259%
27	13.506	2030	2037	2040	rBV2	912637	1588142	2.34%	0.526%
28	13.548	2040	2044	2049	rBV	843964	1348873	1.98%	0.447%
29	13.695	2062	2068	2076	rBV2	474714	806356	1.19%	0.267%
30	13.804	2076	2086	2087	rBV3	29000262	67992319	100.00%	22.523%
31	13.877	2092	2098	2102	rVV	4459154	5832613	8.58%	1.932%
32	13.926	2102	2106	2111	rVB2	1216445	1629249	2.40%	0.540%
33	14.073	2125	2130	2132	rBV2	559994	804950	1.18%	0.267%
34	14.097	2132	2134	2137	rVV	898116	1123451	1.65%	0.372%
35	14.127	2137	2139	2149	rVV2	691865	1256903	1.85%	0.416%
36	14.219	2149	2154	2158	rVV	1488480	2375908	3.49%	0.787%

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Stop Thrs : 0

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

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37	14.255	2158	2160	2164	rVV2	745248	979676	1.44%	0.325%
38	14.316	2164	2170	2176	rVV	1467483	2554498	3.76%	0.846%
39	14.524	2200	2204	2211	rVB3	506219	829564	1.22%	0.275%
40	14.597	2211	2216	2219	rVV	976029	1421902	2.09%	0.471%
41	14.652	2219	2225	2233	rVV	25276355	42008150	61.78%	13.916%
42	14.725	2233	2237	2241	rVV	552769	723292	1.06%	0.240%
43	14.786	2241	2247	2259	rVB	17399297	24550095	36.11%	8.133%
44	15.206	2308	2316	2320	rBV	661133	888358	1.31%	0.294%
45	15.371	2331	2343	2348	rBV	1681857	2564110	3.77%	0.849%
46	15.475	2354	2360	2365	rBV	803370	1228903	1.81%	0.407%
47	15.609	2371	2382	2386	rBV	610258	1007365	1.48%	0.334%

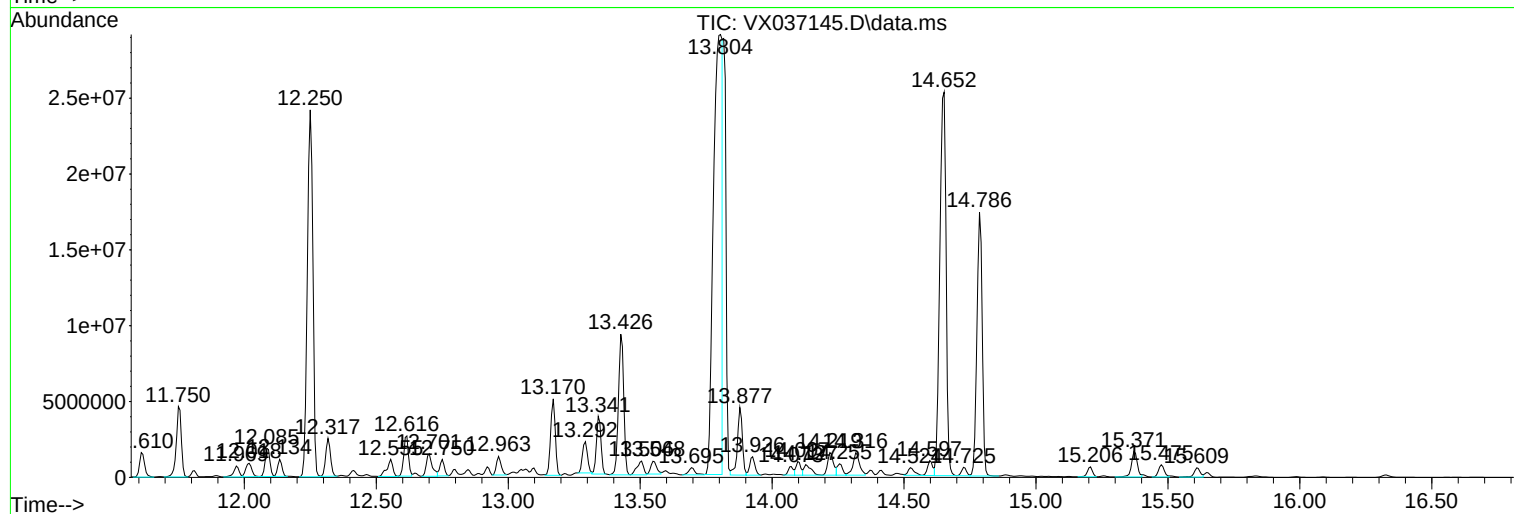
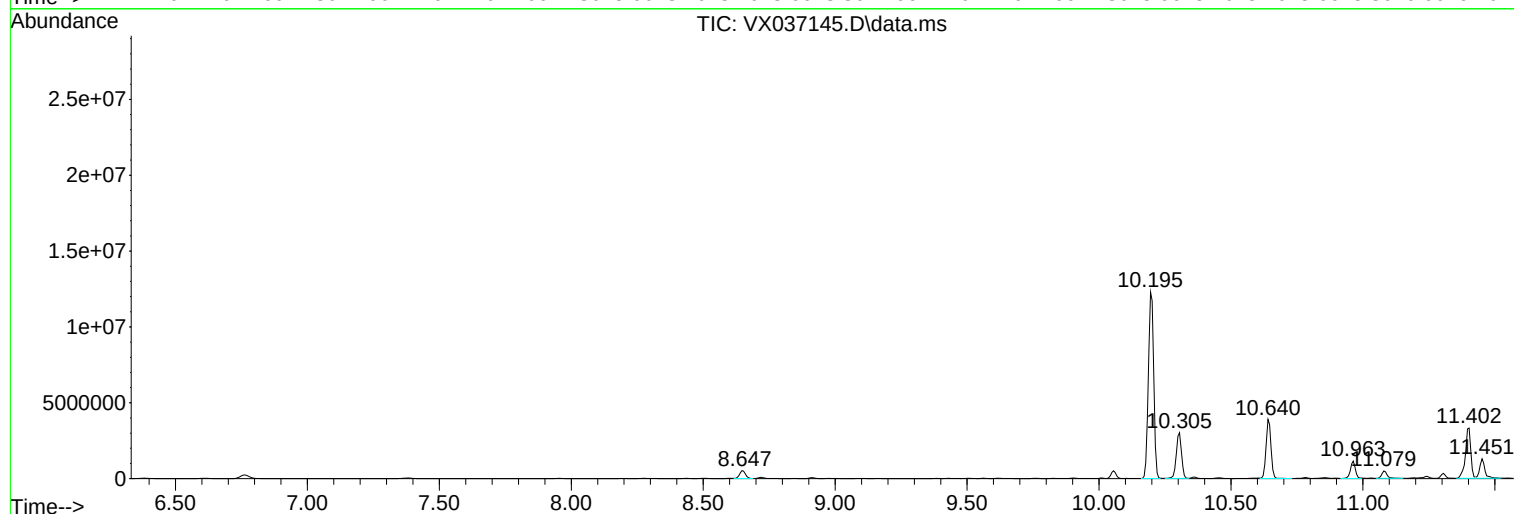
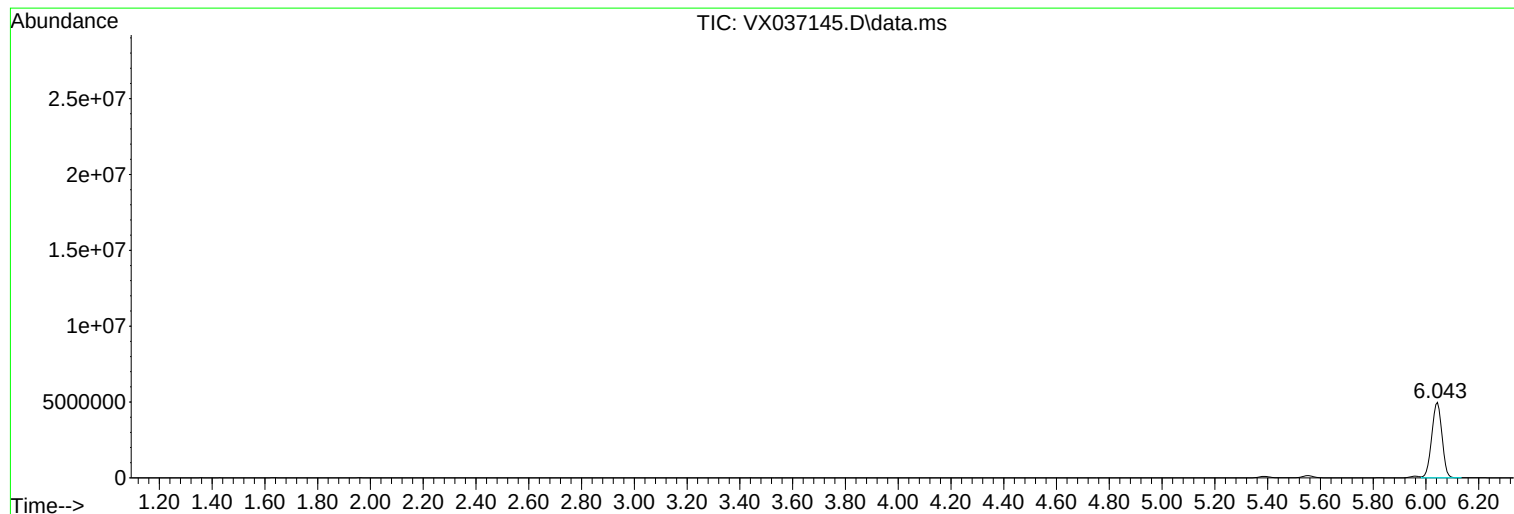
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Quant Title : SW846 8260

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



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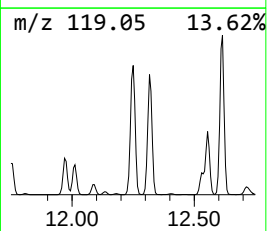
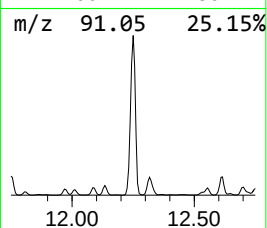
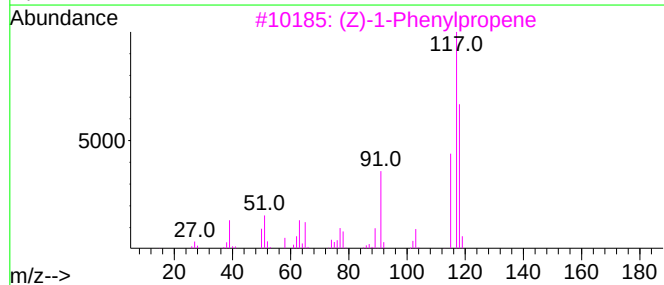
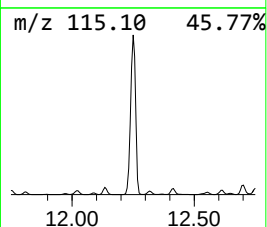
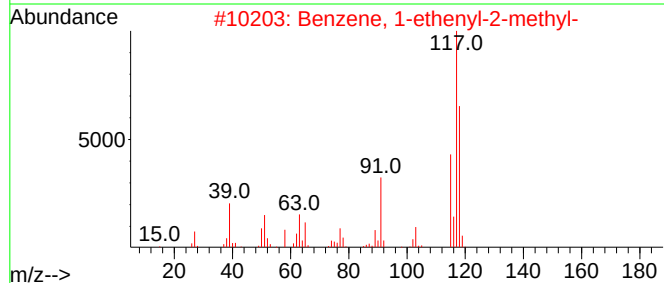
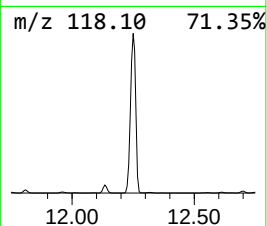
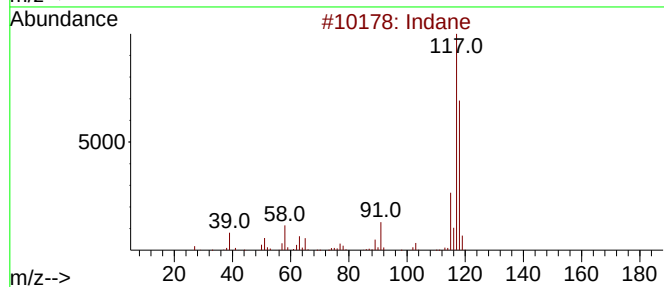
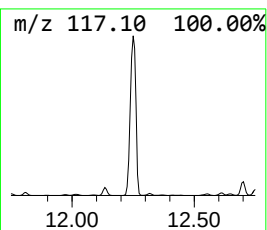
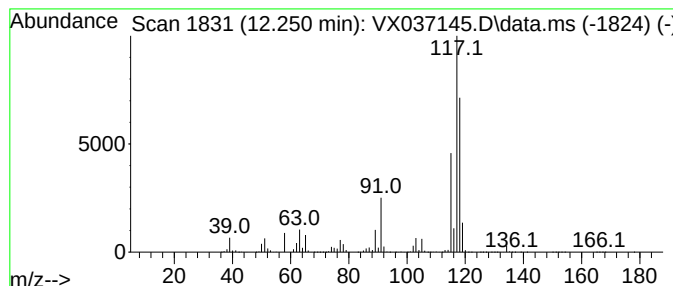
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	1267.38 ug/l	35352900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	92
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	64



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Instrument :
MSVOA_X
ClientSampleId :
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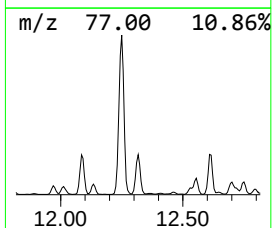
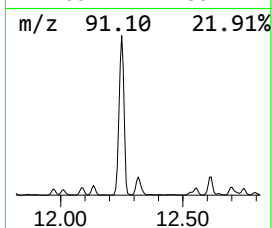
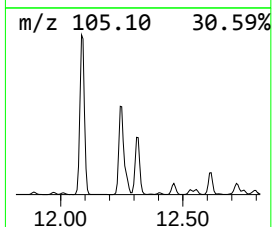
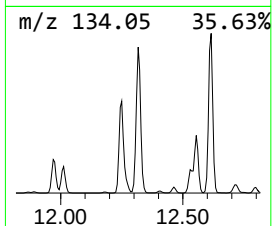
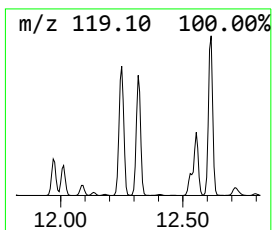
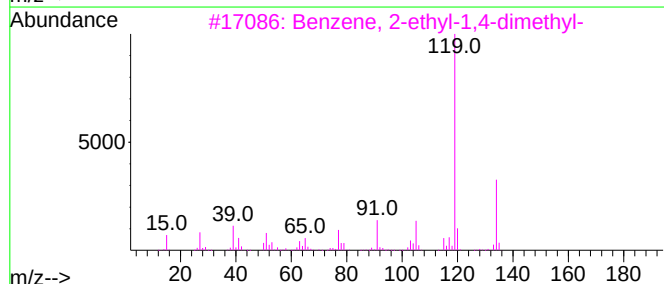
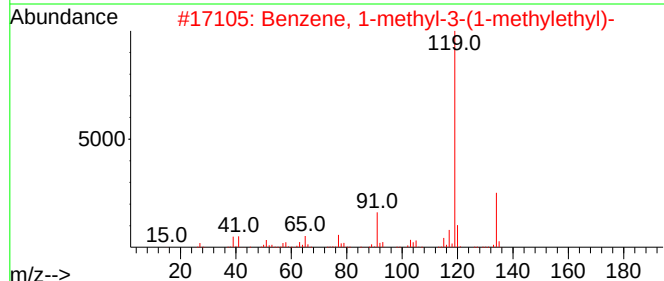
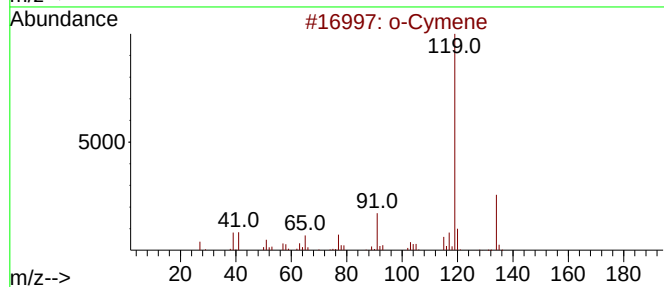
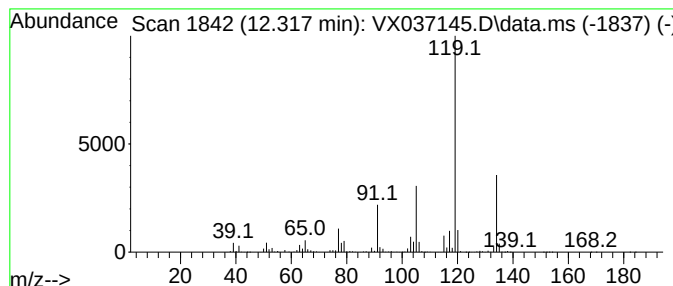
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	113.84 ug/l	3175550	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	93
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



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Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB06-Z22-23

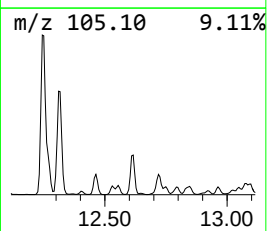
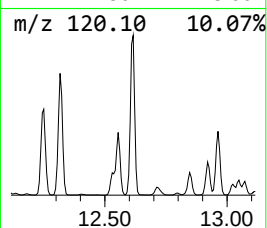
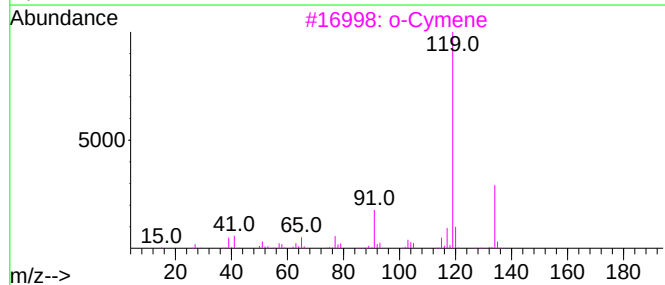
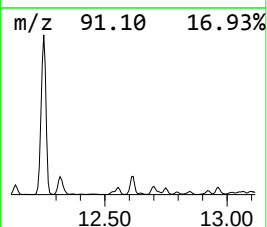
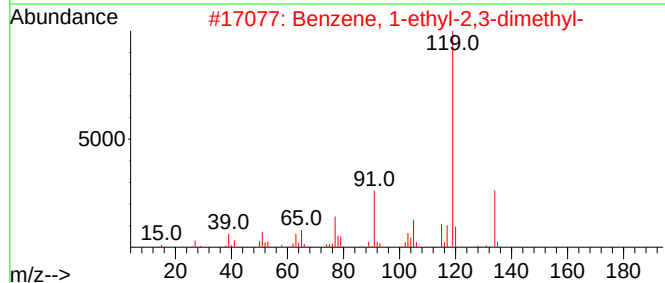
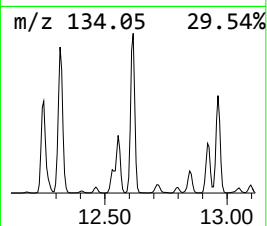
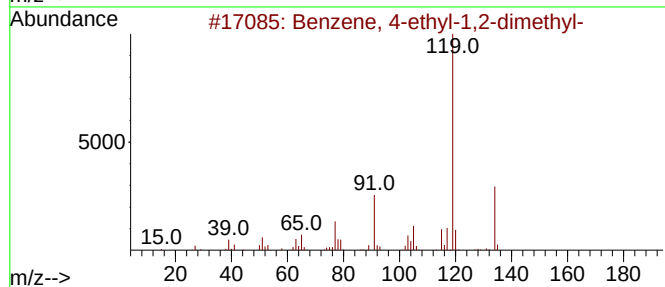
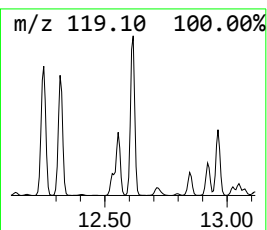
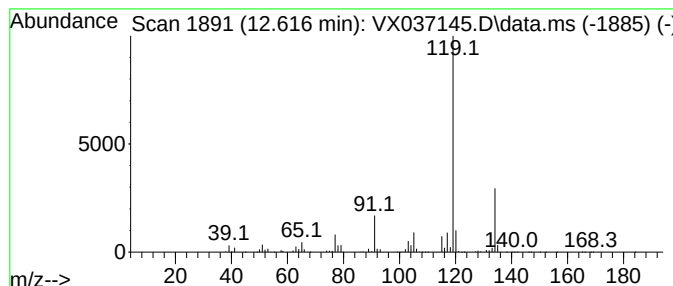
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	118.30 ug/l	3299860	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



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Instrument :
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ClientSampleId :
NEVINS-SB06-Z22-23

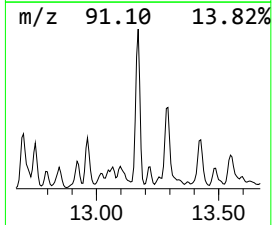
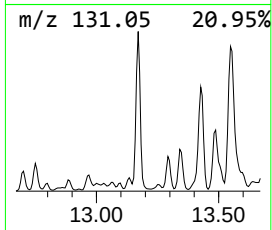
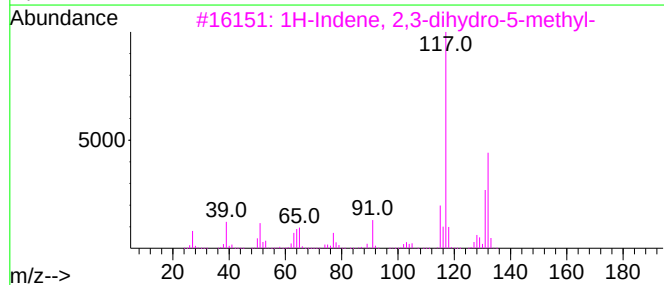
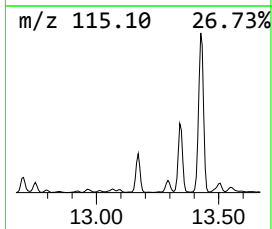
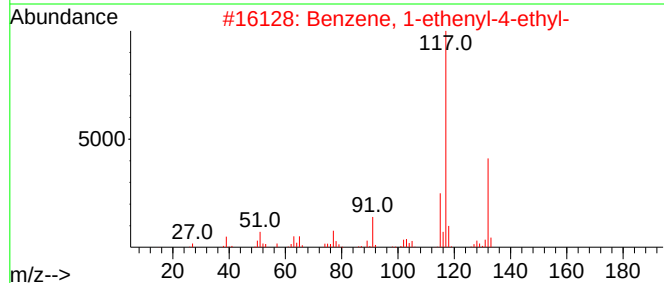
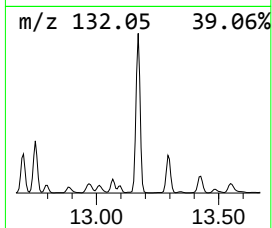
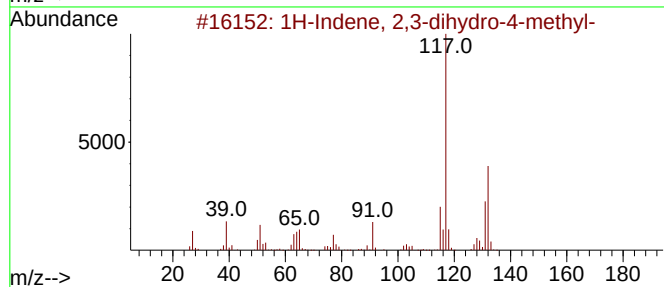
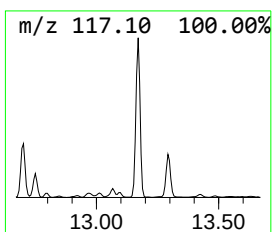
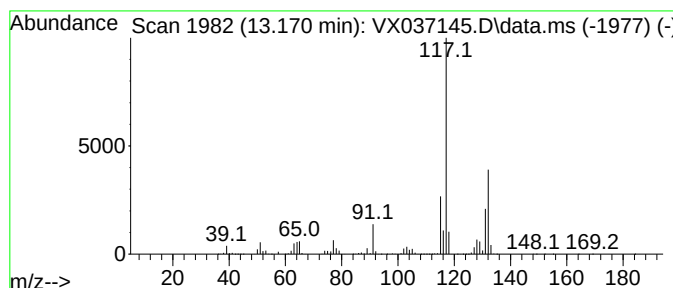
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	215.66 ug/l	6015600	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	3-Phenylbut-1-ene			132	C10H12	000934-10-1	90
5	Benzene, 1-ethenyl-3-ethyl-			132	C10H12	007525-62-4	90



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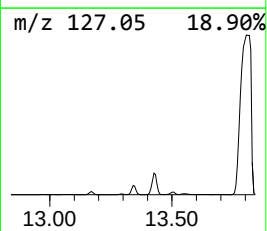
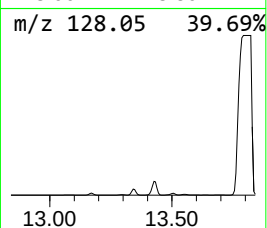
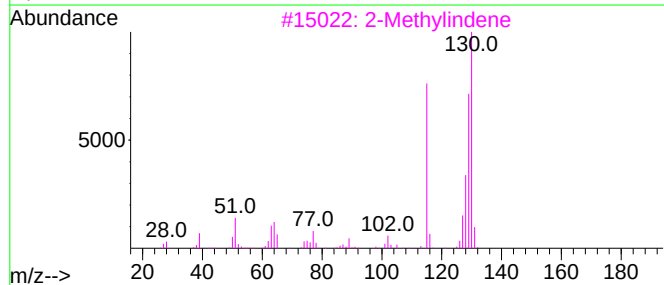
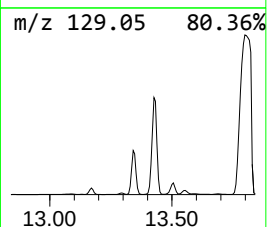
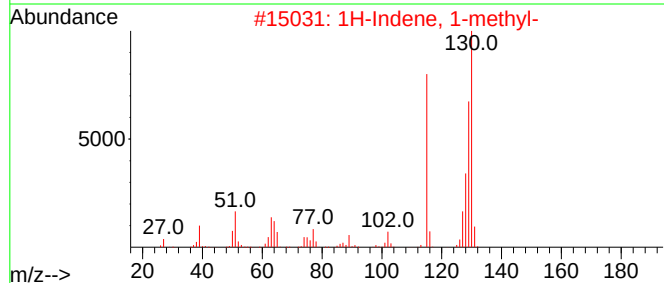
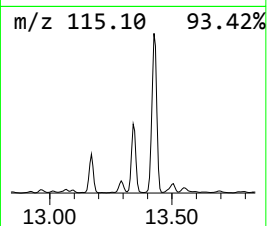
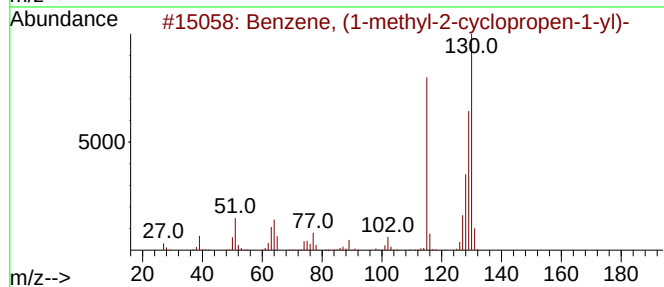
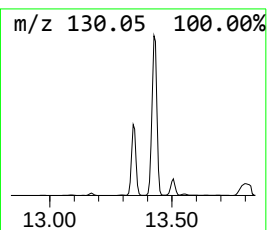
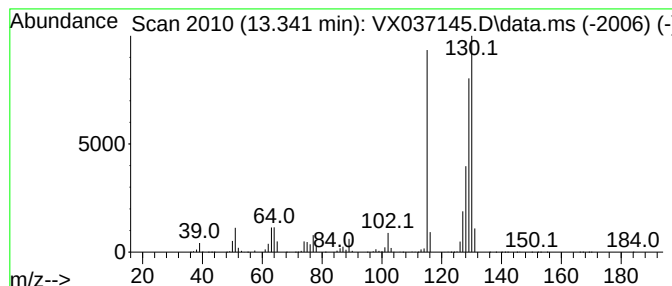
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1-methyl-2-cyclop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	164.28 ug/l	4582490	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
3			2-Methylindene	130	C10H10	002177-47-1	94
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037145.D
Acq On : 21 Aug 2023 20:55
Operator : JC/MD
Sample : 03994-01 10X
Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

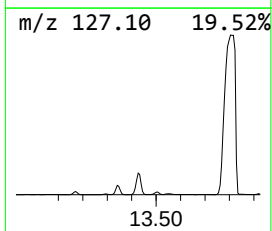
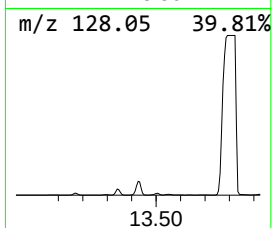
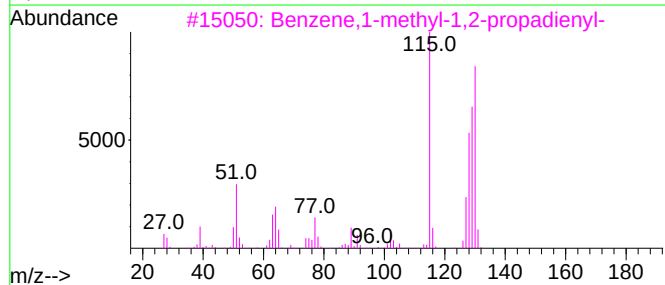
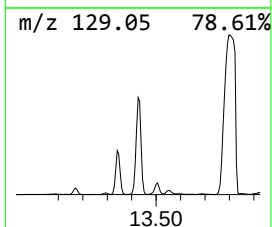
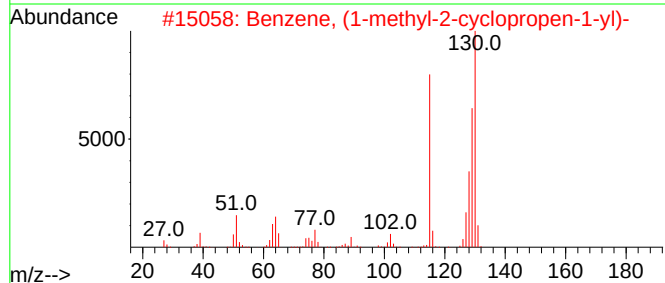
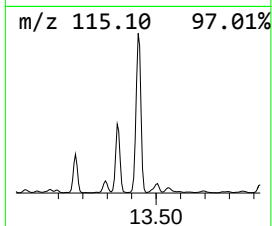
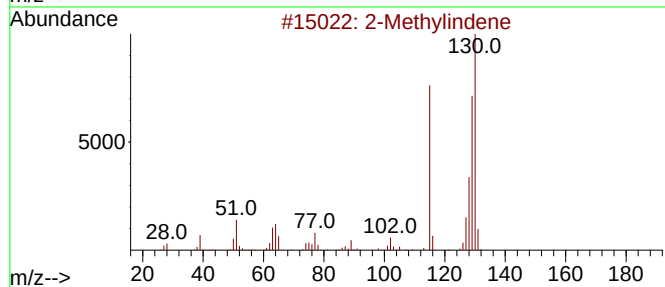
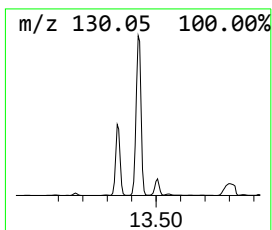
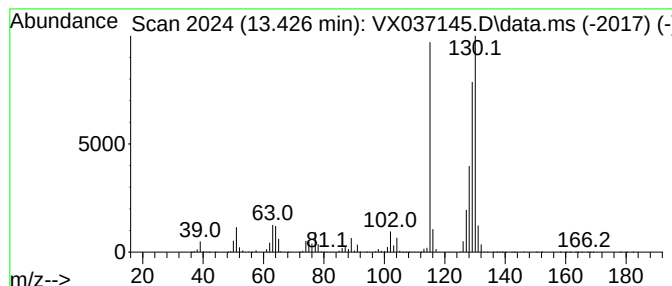
Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z22-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.426	460.88 ug/l	12856100	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	95
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037145.D
Acq On : 21 Aug 2023 20:55
Operator : JC/MD
Sample : 03994-01 10X
Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z22-23

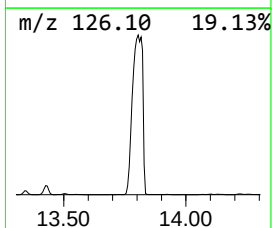
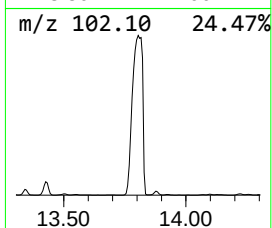
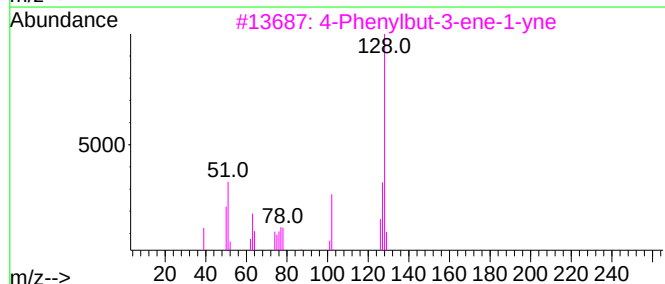
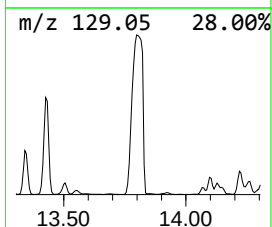
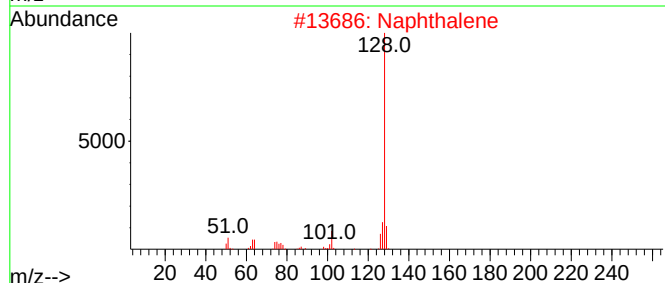
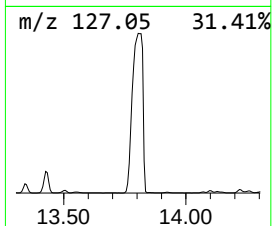
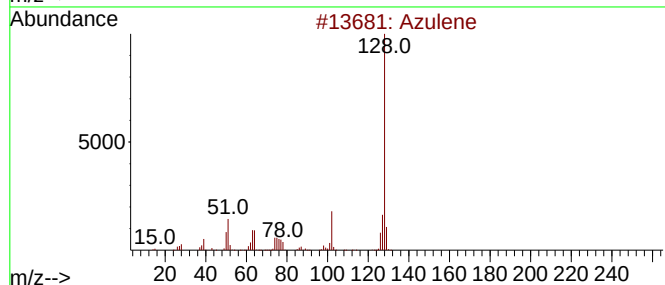
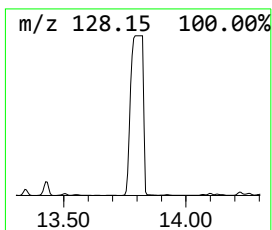
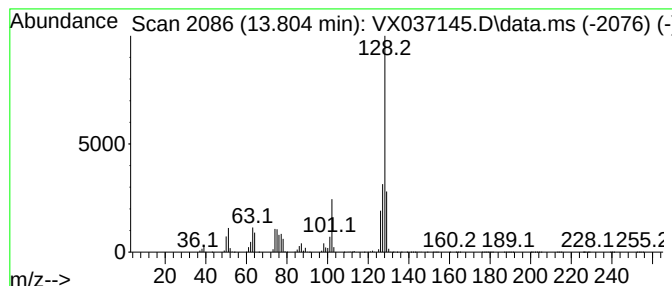
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Quant Title : SW846 8260

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

Peak Number 7 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	2437.48 ug/l	67992300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	81
2			Naphthalene	128	C10H8	000091-20-3	76
3			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	76
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	52
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037145.D
Acq On : 21 Aug 2023 20:55
Operator : JC/MD
Sample : 03994-01 10X
Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z22-23

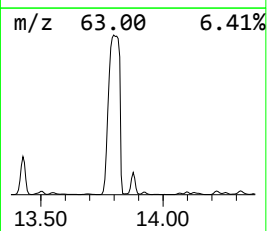
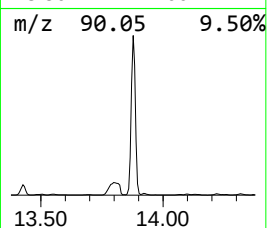
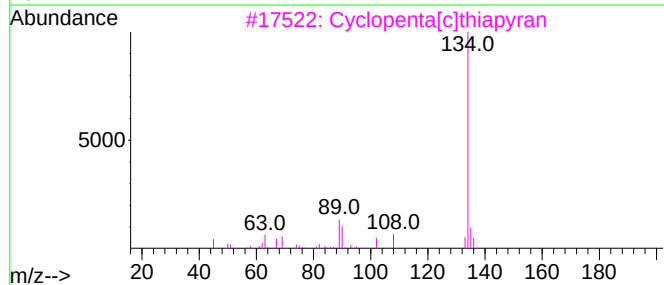
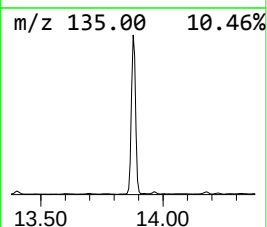
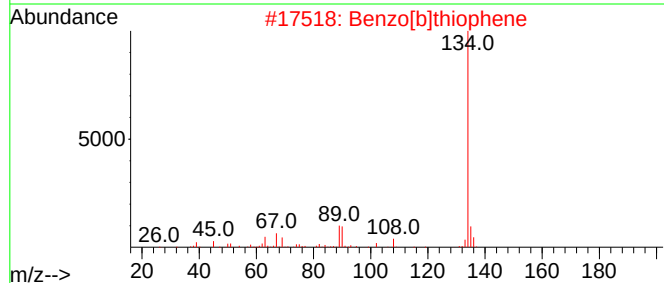
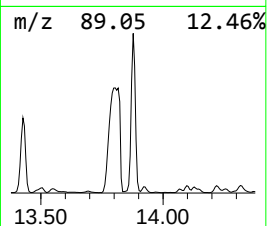
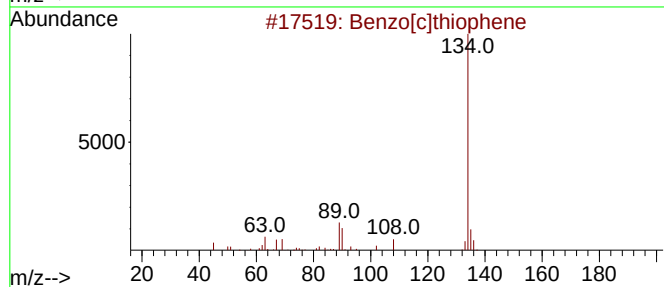
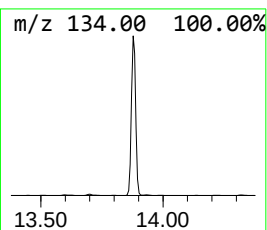
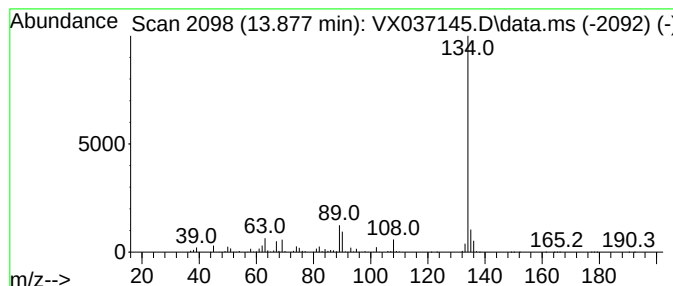
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.878	209.10 ug/l	5832610	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	38
5			2H-Benzimidazol-2-one, 1,3-dihydro-	134	C7H6N2O	000615-16-7	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037145.D
Acq On : 21 Aug 2023 20:55
Operator : JC/MD
Sample : 03994-01 10X
Misc : 6.76g/5.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z22-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.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
Indane	12.250	1267.4	ug/l	35352900	4	12.024	1394720	50.0
o-Cymene	12.317	113.8	ug/l	3175550	4	12.024	1394720	50.0
Benzene, 4-ethy...	12.616	118.3	ug/l	3299860	4	12.024	1394720	50.0
1H-Indene, 2,3-...	13.170	215.7	ug/l	6015600	4	12.024	1394720	50.0
Benzene, (1-met...	13.341	164.3	ug/l	4582490	4	12.024	1394720	50.0
2-Methylindene	13.426	460.9	ug/l	12856100	4	12.024	1394720	50.0
Azulene	13.804	2437.5	ug/l	67992300	4	12.024	1394720	50.0
Benzo[c]thiophene	13.878	209.1	ug/l	5832610	4	12.024	1394720	50.0