

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
 Data File : VX037052.D
 Acq On : 17 Aug 2023 10:23
 Operator : JC/MD
 Sample : 03958-04
 Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB02-Z46-47

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX037052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.757	920	930	950	rBV	209154	500742	1.03%	0.272%
2	8.647	1234	1240	1249	rVB	436778	673962	1.38%	0.366%
3	10.055	1466	1471	1476	rBV	482224	635873	1.30%	0.345%
4	10.195	1488	1494	1500	rBV	2552722	3350661	6.86%	1.818%
5	10.640	1562	1567	1582	rVB	832001	1102753	2.26%	0.598%
6	10.963	1614	1620	1628	rBV	370828	493508	1.01%	0.268%
7	11.085	1634	1640	1651	rVB	464605	694601	1.42%	0.377%
8	11.396	1684	1691	1696	rBV	874697	1210376	2.48%	0.657%
9	11.451	1696	1700	1703	rBV	593020	731084	1.50%	0.397%
10	11.616	1722	1727	1734	rVB	557751	728894	1.49%	0.395%
11	11.750	1740	1749	1755	rBV	2141541	2844837	5.83%	1.544%
12	11.969	1777	1785	1789	rBV	396465	607951	1.24%	0.330%
13	12.024	1789	1794	1800	rVV2	704020	1172257	2.40%	0.636%
14	12.085	1800	1804	1808	rVV	828025	1043260	2.14%	0.566%
15	12.134	1808	1812	1816	rVB	478943	556443	1.14%	0.302%
16	12.244	1824	1830	1837	rBV	11714452	15072021	30.86%	8.178%
17	12.317	1837	1842	1848	rVV2	2134962	2749771	5.63%	1.492%
18	12.554	1878	1881	1885	rVB	555668	692300	1.42%	0.376%
19	12.615	1885	1891	1894	rBV	1968974	2392380	4.90%	1.298%
20	12.701	1900	1905	1910	rBV	1202092	1814476	3.72%	0.984%
21	12.750	1910	1913	1917	rVB	455725	527315	1.08%	0.286%
22	12.792	1917	1920	1925	rBV	528413	671700	1.38%	0.364%
23	12.963	1944	1948	1953	rBV	996831	1214879	2.49%	0.659%
24	13.048	1959	1962	1967	rVV2	719430	1188100	2.43%	0.645%
25	13.170	1977	1982	1986	rVB	2826352	3338639	6.84%	1.811%
26	13.286	1998	2001	2006	rVV2	1390743	1861092	3.81%	1.010%
27	13.341	2006	2010	2016	rVB	2004564	2318786	4.75%	1.258%
28	13.426	2018	2024	2029	rVB	5146008	6660313	13.64%	3.614%
29	13.499	2034	2036	2040	rVB	480975	523918	1.07%	0.284%
30	13.548	2040	2044	2048	rBV	674713	997753	2.04%	0.541%
31	13.682	2061	2066	2069	rBV2	585113	759532	1.56%	0.412%
32	13.792	2075	2084	2089	rBV	27078029	48835024	100.00%	26.497%
33	13.871	2089	2097	2101	rVV	1476267	2185572	4.48%	1.186%
34	13.926	2101	2106	2111	rVB3	561517	846824	1.73%	0.459%
35	14.097	2131	2134	2137	rVV	853625	1082712	2.22%	0.587%
36	14.127	2137	2139	2148	rVB3	427861	825642	1.69%	0.448%

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

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37	14.219	2149	2154	2158	rBV2	1228531	1972103	4.04%	1.070%
38	14.255	2158	2160	2164	rVV2	479779	566762	1.16%	0.308%
39	14.316	2164	2170	2176	rVV	1157060	1845739	3.78%	1.001%
40	14.524	2200	2204	2211	rVV2	526936	860600	1.76%	0.467%
41	14.597	2211	2216	2218	rVV	365611	517867	1.06%	0.281%
42	14.639	2218	2223	2233	rVV	17577570	25006369	51.21%	13.568%
43	14.780	2240	2246	2256	rVV	12811283	17865778	36.58%	9.694%
44	15.206	2308	2316	2320	rBV	1429034	2034243	4.17%	1.104%
45	15.371	2331	2343	2347	rBV	3167911	4878511	9.99%	2.647%
46	15.475	2354	2360	2365	rBV	2539436	3865013	7.91%	2.097%
47	15.615	2377	2383	2386	rBV	2685501	4294078	8.79%	2.330%
48	15.652	2386	2389	2394	rVB	1367591	1928359	3.95%	1.046%
49	15.834	2409	2419	2424	rBV	645756	1761177	3.61%	0.956%
50	15.987	2438	2444	2453	rVB	407124	712531	1.46%	0.387%
51	16.322	2491	2499	2512	rBV2	1641690	3290001	6.74%	1.785%

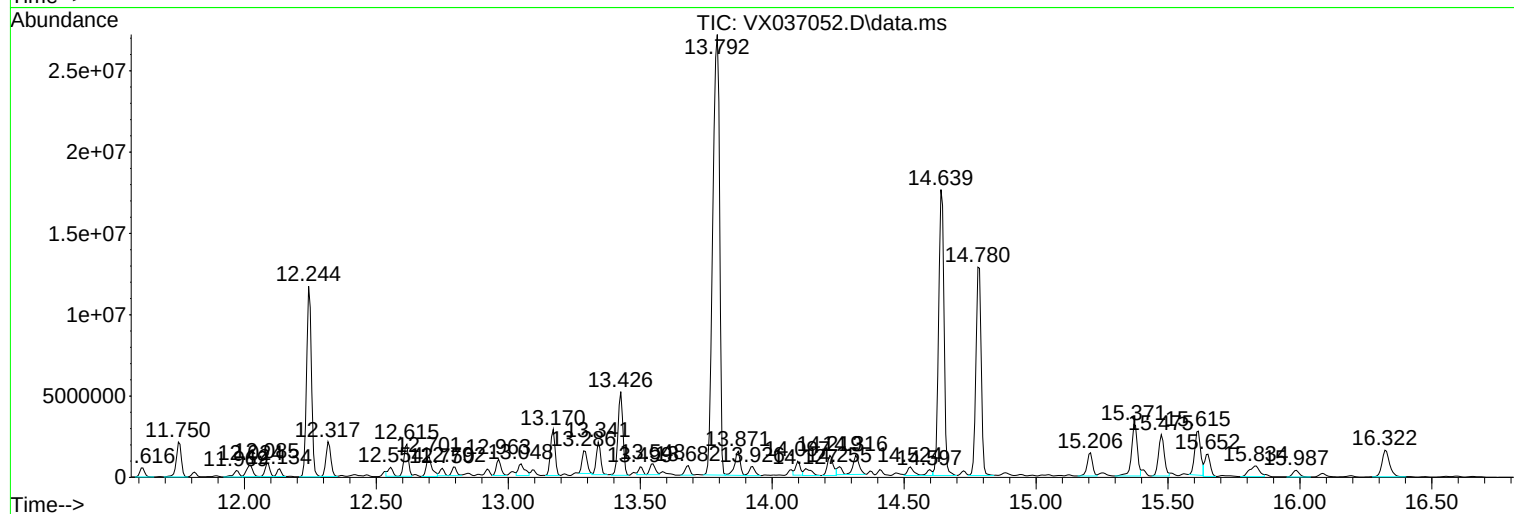
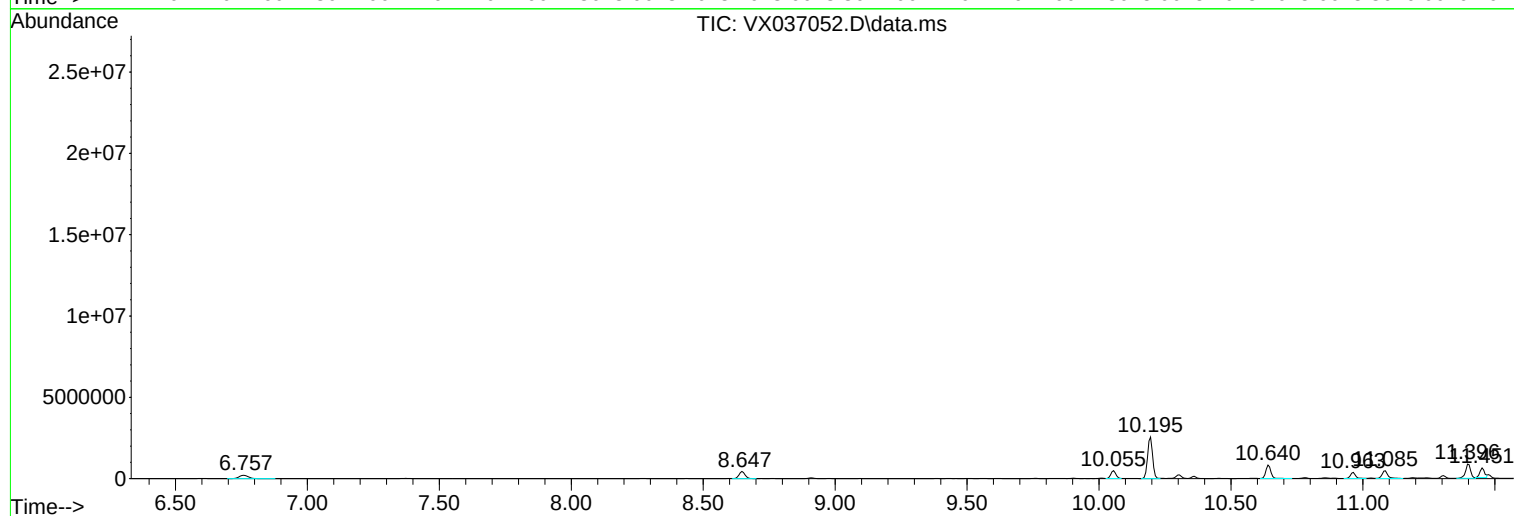
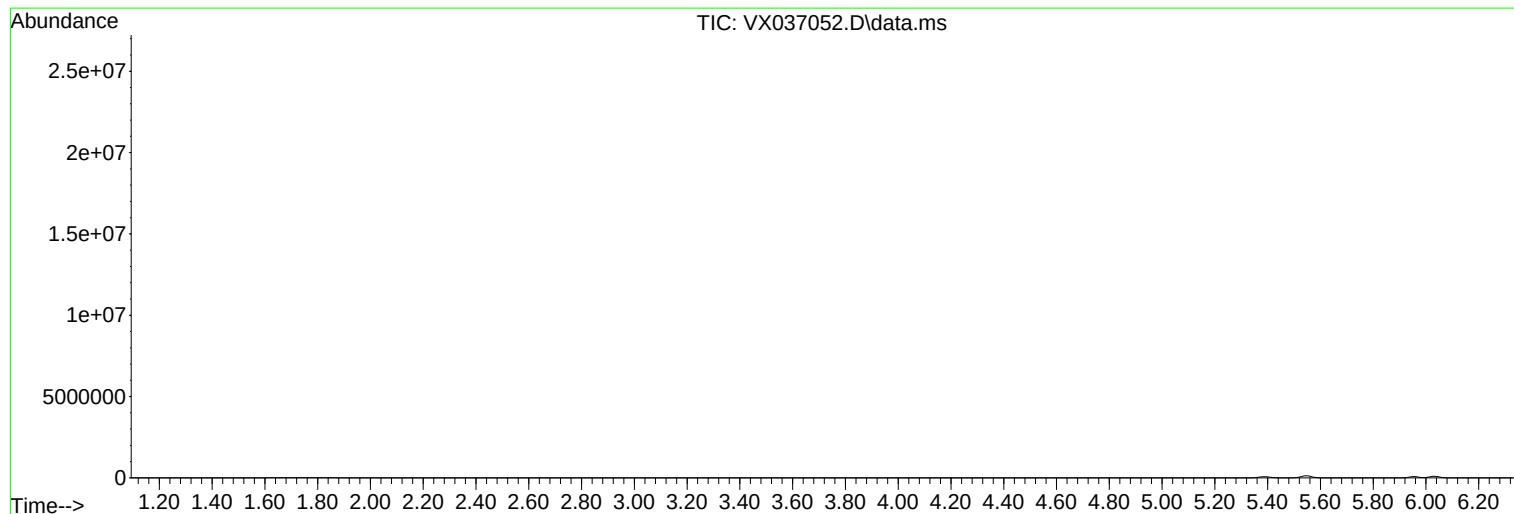
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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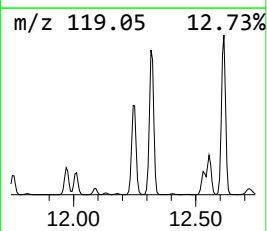
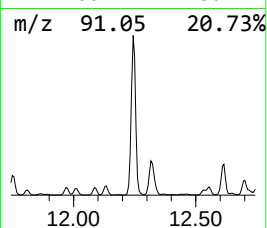
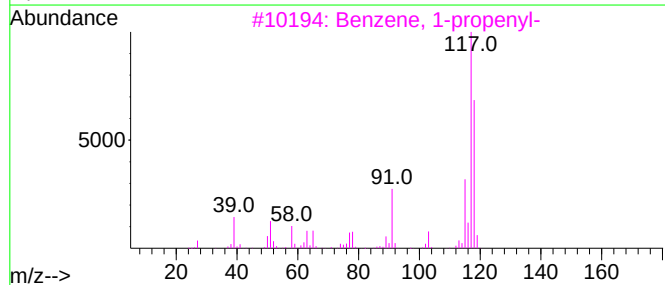
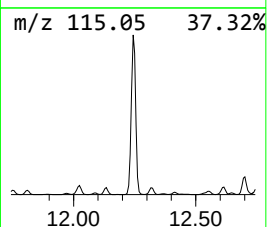
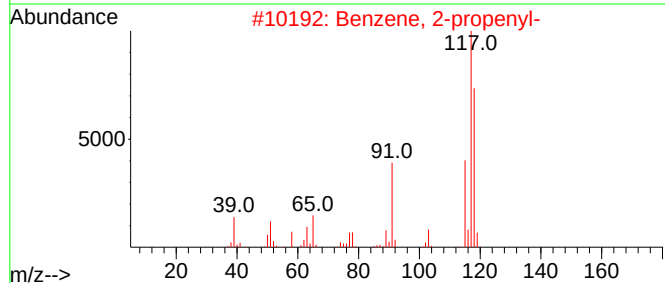
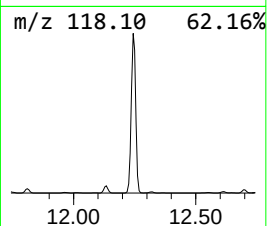
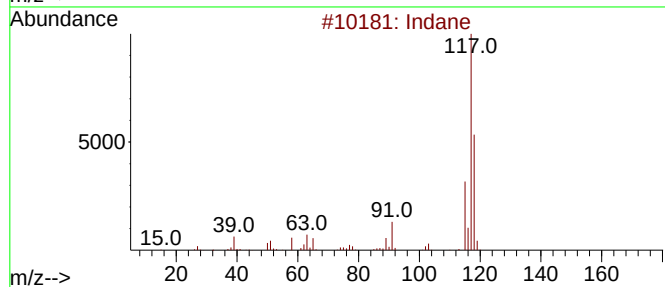
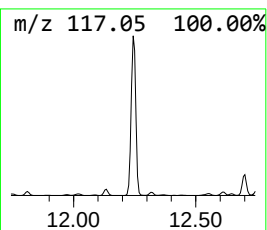
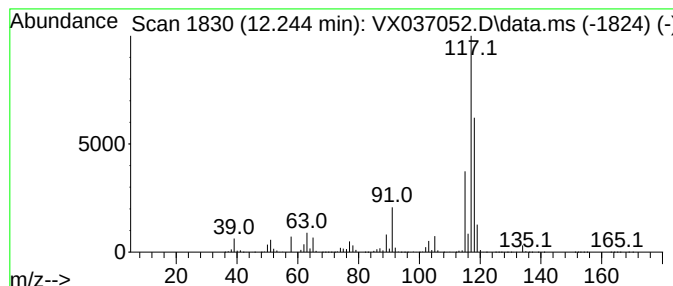
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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.
12.244	642.86 ug/l	15072000	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49



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ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

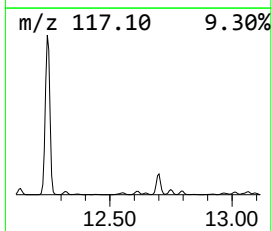
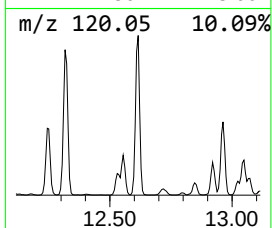
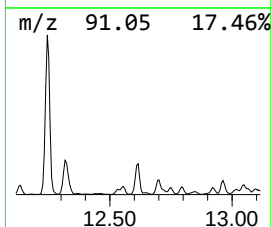
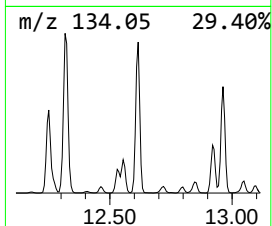
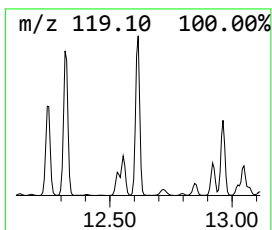
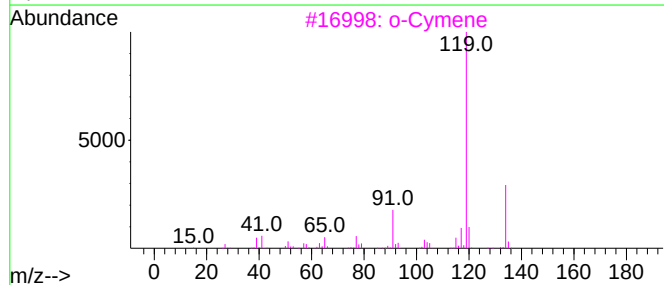
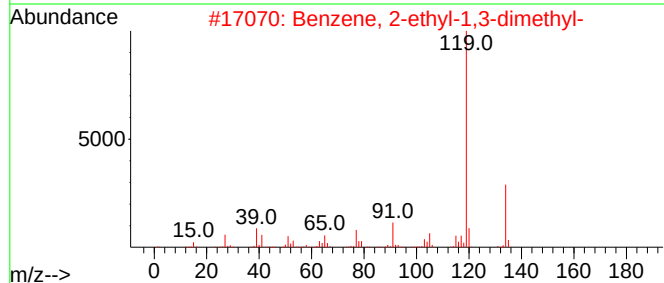
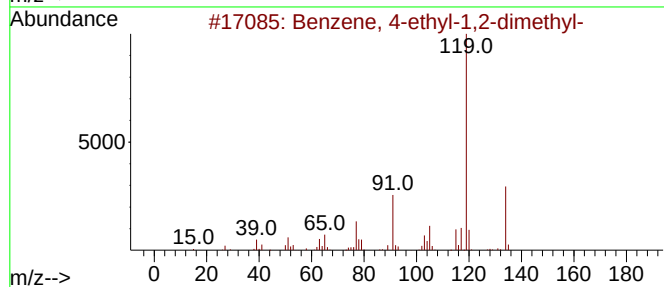
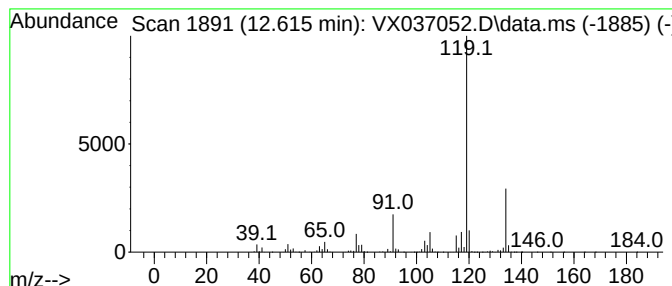
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	102.04 ug/l	2392380	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, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
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Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

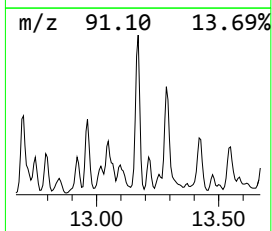
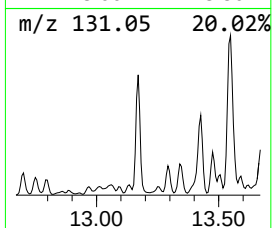
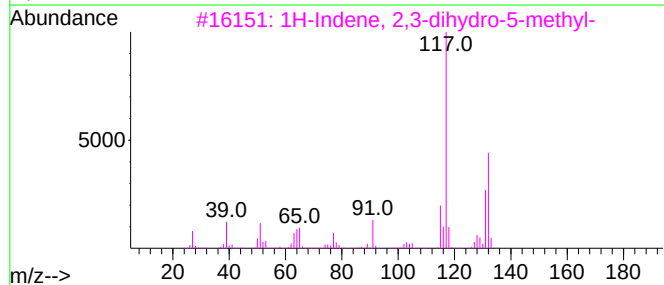
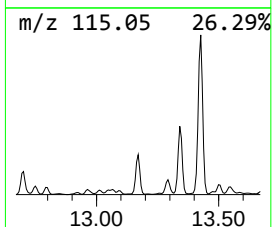
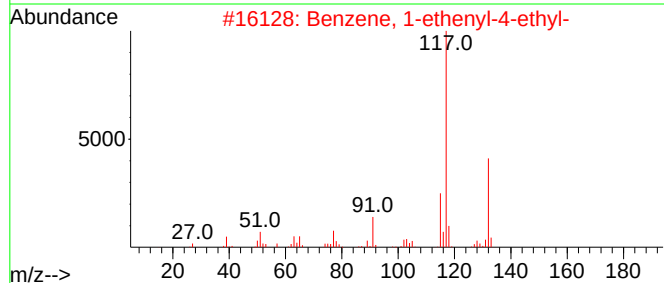
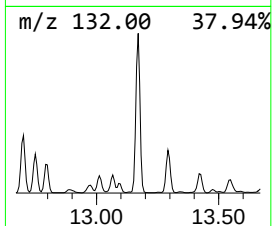
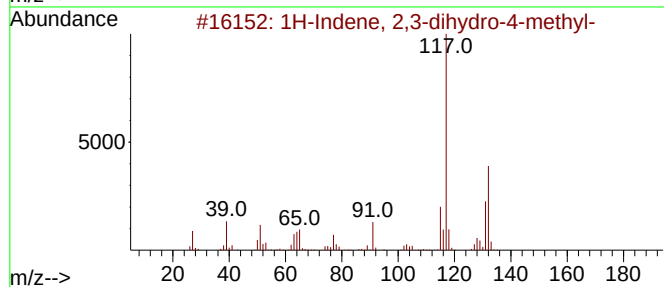
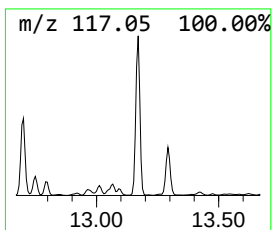
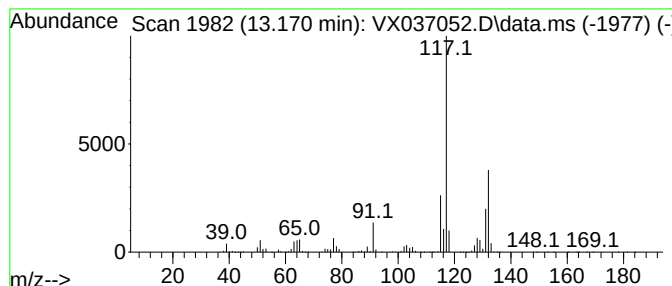
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	142.40 ug/l	3338640	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	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90	



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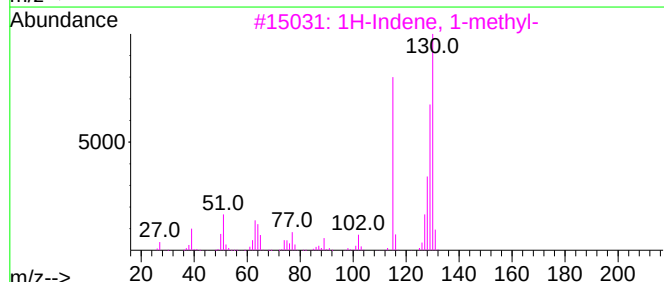
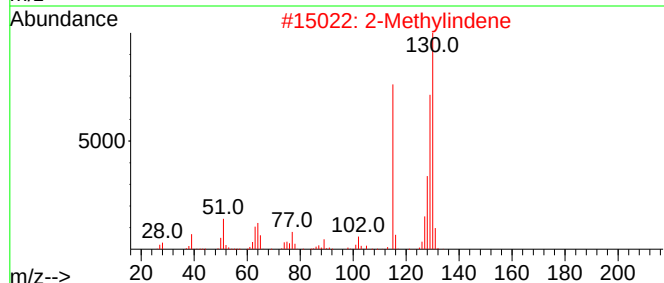
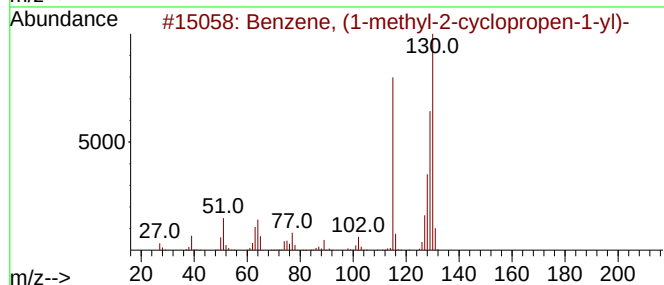
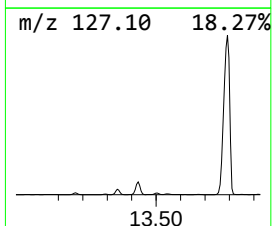
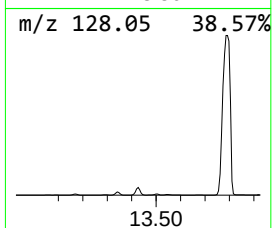
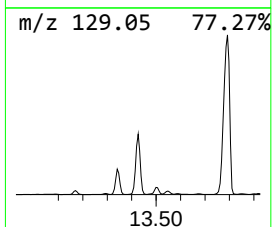
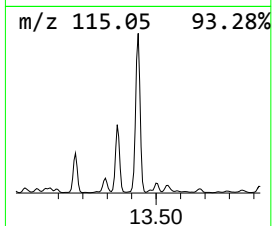
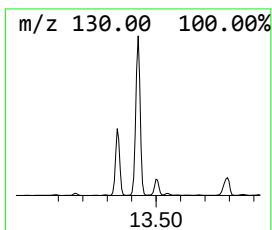
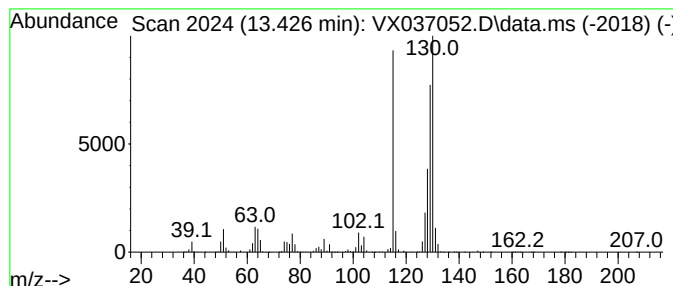
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	284.08 ug/l	6660310	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			2-Methylindene	130	C10H10	002177-47-1	94
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4			Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



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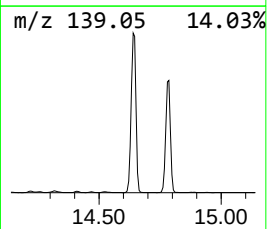
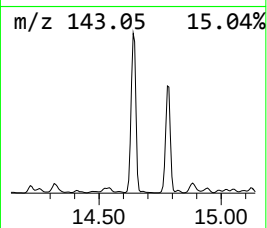
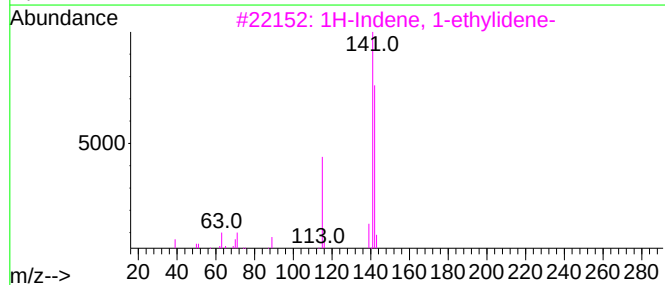
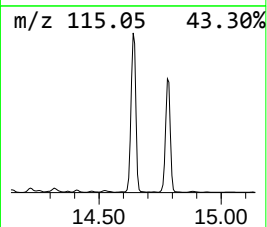
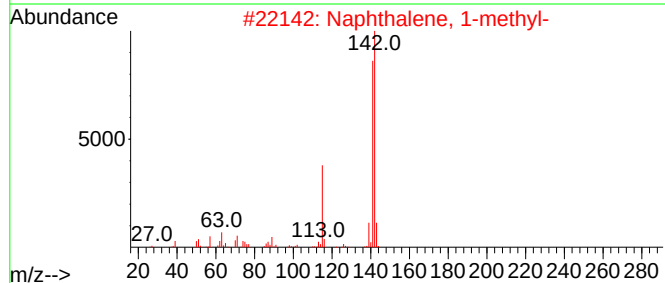
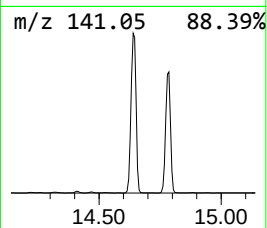
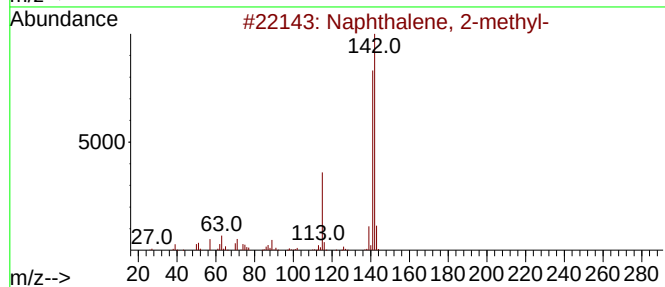
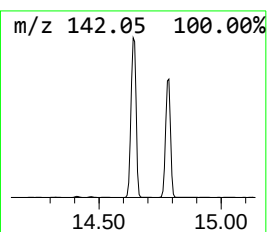
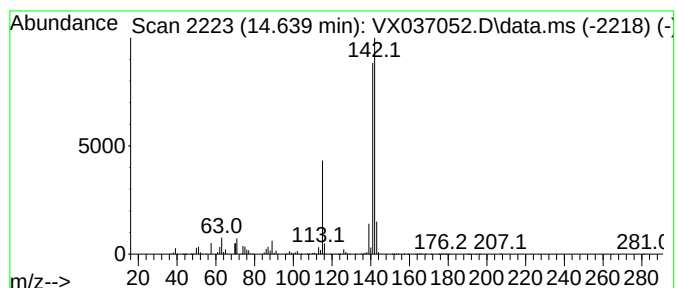
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	1066.59 ug/l	25006400	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
Acq On : 17 Aug 2023 10:23
Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

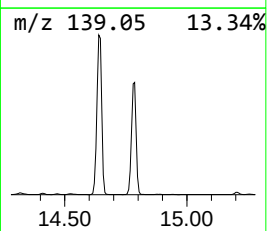
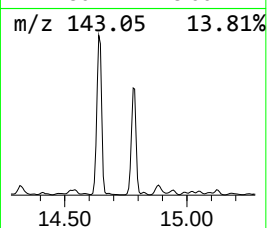
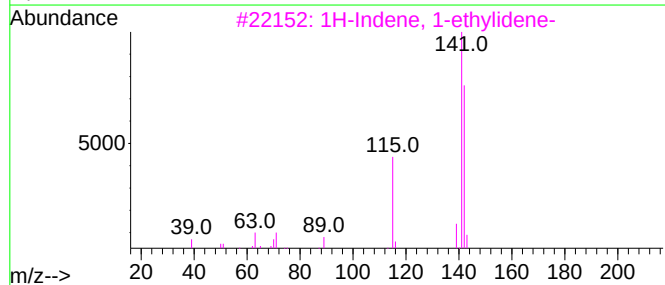
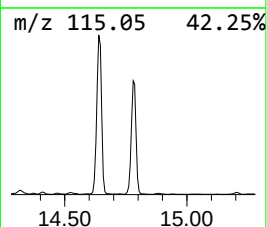
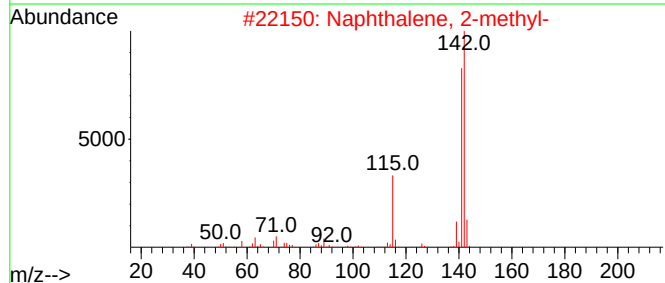
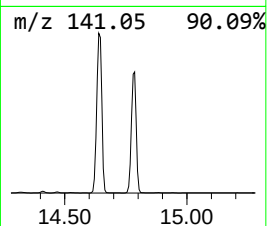
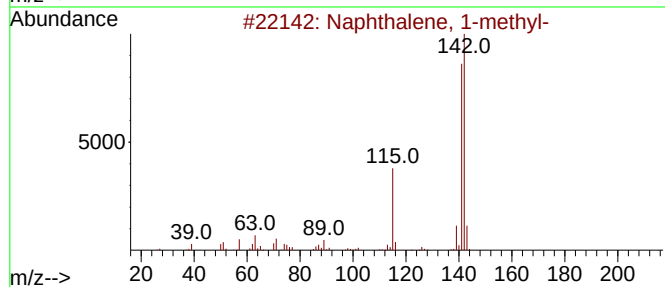
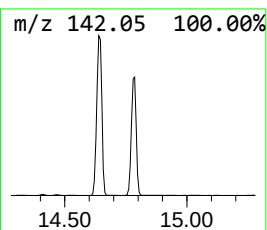
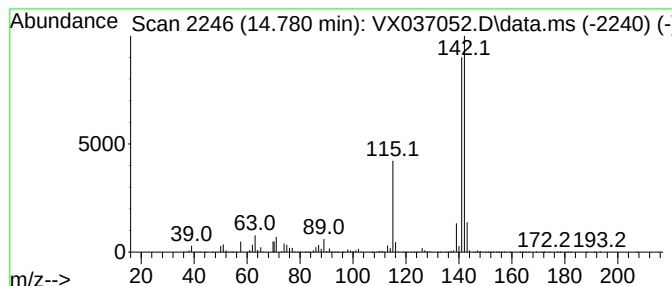
Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 1-ethylidene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.780	762.02 ug/l	17865800	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	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	94
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
Acq On : 17 Aug 2023 10:23
Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

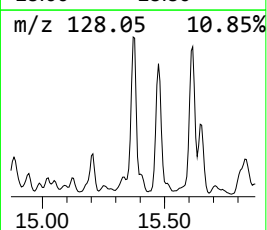
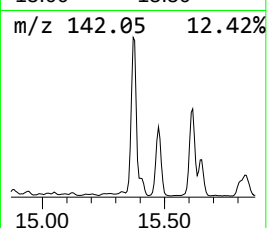
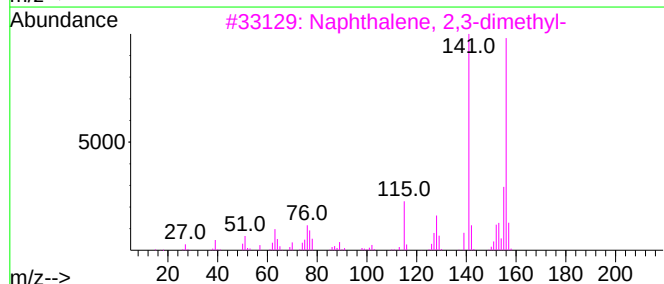
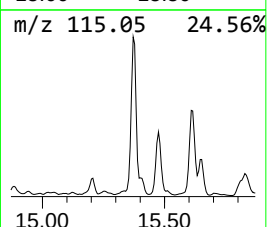
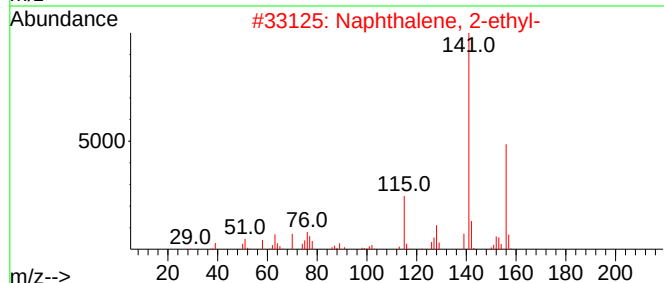
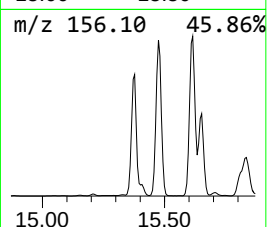
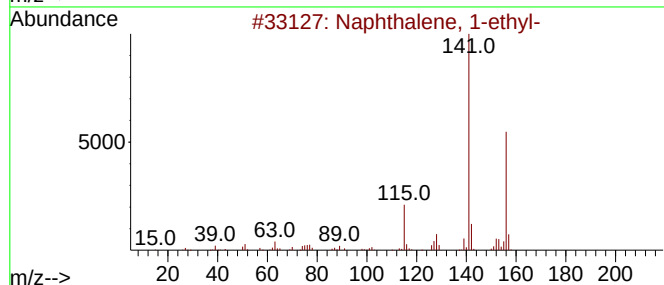
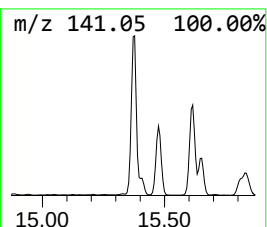
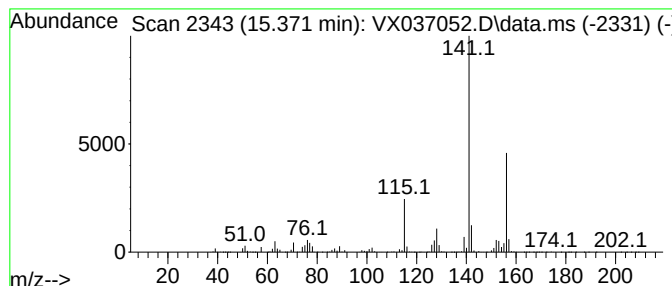
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	208.08 ug/l	4878510	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
4			5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53
5			Naphthalene, 1-propyl-	170	C13H14	002765-18-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
Acq On : 17 Aug 2023 10:23
Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

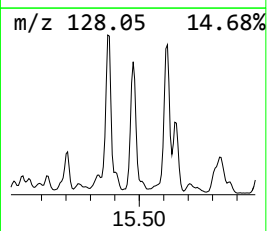
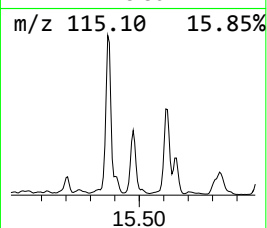
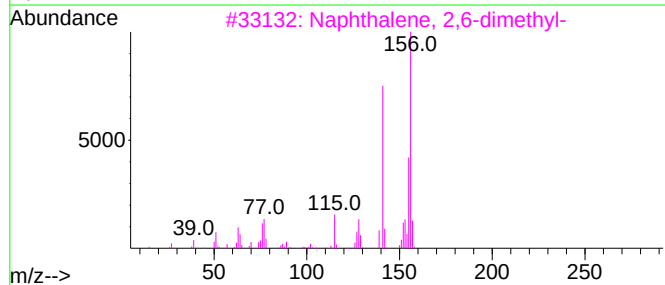
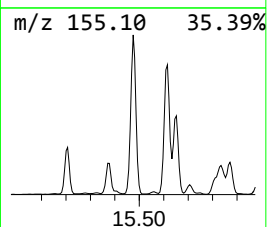
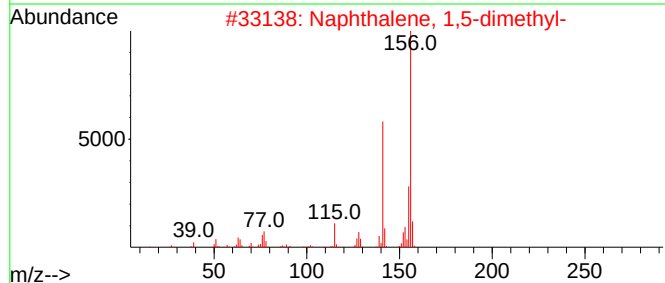
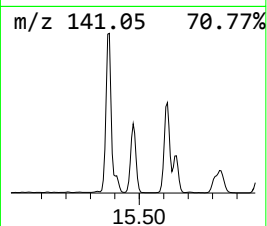
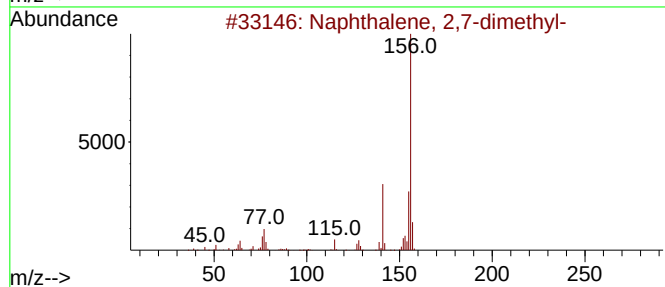
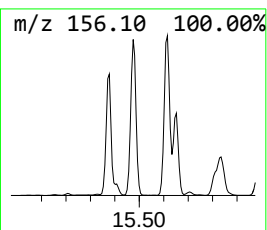
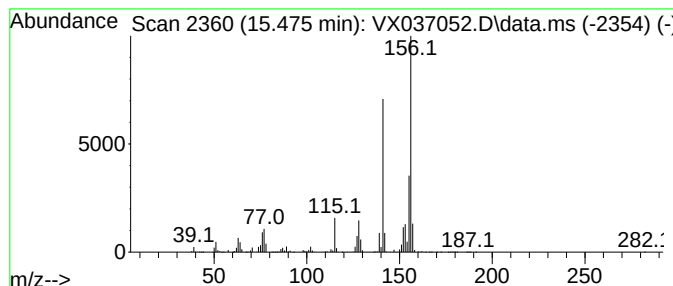
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	164.85 ug/l	3865010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
Acq On : 17 Aug 2023 10:23
Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

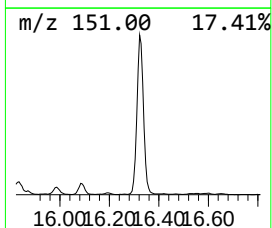
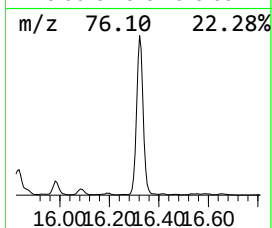
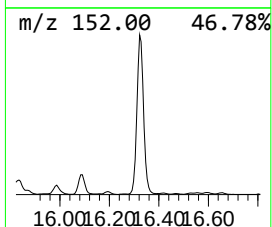
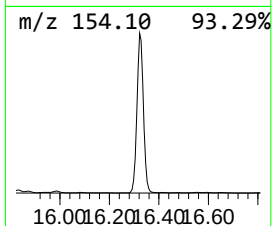
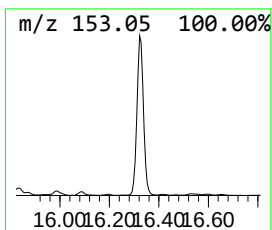
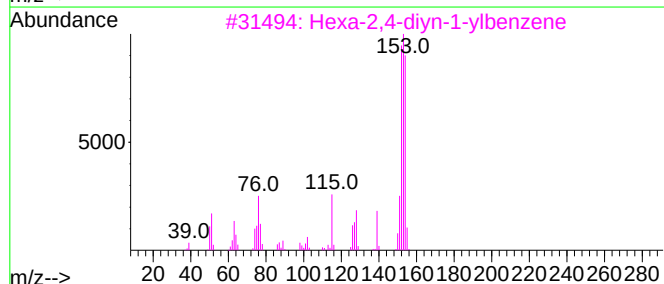
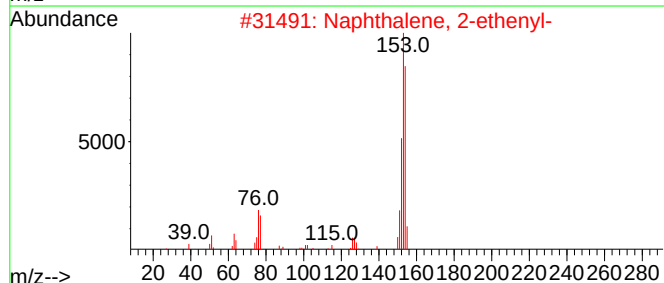
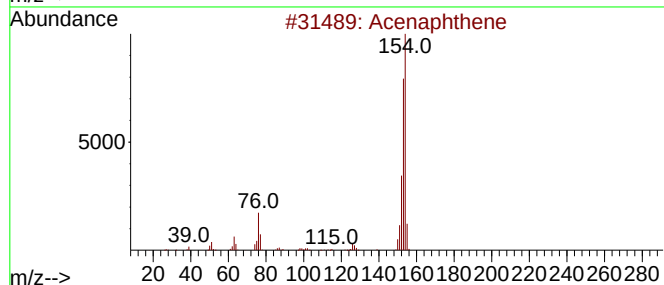
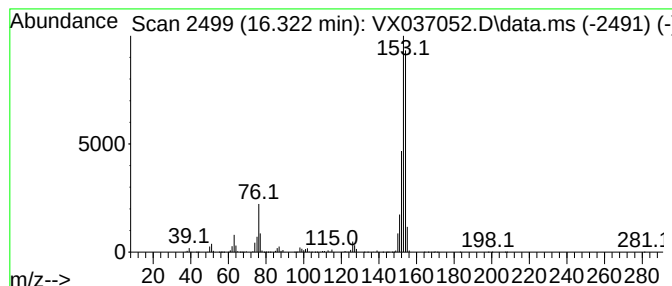
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 10 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	140.33 ug/l	3290000	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acenaphthene	154	C12H10	000083-32-9	94
2		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
3		Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4		3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5		1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037052.D
Acq On : 17 Aug 2023 10:23
Operator : JC/MD
Sample : 03958-04
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z46-47

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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	12.244	642.9	ug/l	15072000	4	12.024	1172260	50.0
Benzene, 4-ethy...	12.616	102.0	ug/l	2392380	4	12.024	1172260	50.0
1H-Indene, 2,3-...	13.170	142.4	ug/l	3338640	4	12.024	1172260	50.0
Benzene, (1-met...	13.426	284.1	ug/l	6660310	4	12.024	1172260	50.0
Naphthalene, 1-...	14.640	1066.6	ug/l	25006400	4	12.024	1172260	50.0
1H-Indene, 1-et...	14.780	762.0	ug/l	17865800	4	12.024	1172260	50.0
Naphthalene, 2,...	15.371	208.1	ug/l	4878510	4	12.024	1172260	50.0
Naphthalene, 2,...	15.475	164.8	ug/l	3865010	4	12.024	1172260	50.0
Hexa-2,4-diyne-1...	16.322	140.3	ug/l	3290000	4	12.024	1172260	50.0