

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
 Data File : VX037144.D
 Acq On : 21 Aug 2023 20:31
 Operator : JC/MD
 Sample : 03994-02 10X
 Misc : 6.46g/10.0mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NEVINS-SB06-Z36-37

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: VX037144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.037	804	812	828	rVB	451127	1202764	3.84%	1.302%
2	6.763	921	931	946	rBV	172197	408178	1.30%	0.442%
3	8.646	1235	1240	1249	rVB	359471	566903	1.81%	0.614%
4	10.055	1466	1471	1488	rVB	408099	551567	1.76%	0.597%
5	10.195	1488	1494	1501	rBV	1490276	1896647	6.06%	2.053%
6	10.640	1562	1567	1577	rVB	401806	510323	1.63%	0.552%
7	11.079	1634	1639	1651	rVB	383763	541711	1.73%	0.586%
8	11.609	1722	1726	1734	rVB	254023	340557	1.09%	0.369%
9	11.750	1745	1749	1755	rVB	712805	884093	2.83%	0.957%
10	12.024	1788	1794	1799	rBV2	470230	668454	2.14%	0.723%
11	12.085	1799	1804	1808	rBV	314043	421912	1.35%	0.457%
12	12.243	1824	1830	1837	rBV	5629573	6898738	22.05%	7.466%
13	12.317	1837	1842	1848	rVV2	347513	451524	1.44%	0.489%
14	12.609	1886	1890	1894	rBV	386782	458425	1.47%	0.496%
15	12.695	1899	1904	1910	rBV	285755	454029	1.45%	0.491%
16	12.963	1944	1948	1954	rBV	249133	340884	1.09%	0.369%
17	13.170	1974	1982	1986	rBV	816306	986831	3.15%	1.068%
18	13.286	1997	2001	2006	rBV2	469796	651514	2.08%	0.705%
19	13.341	2006	2010	2014	rVB	777608	915973	2.93%	0.991%
20	13.426	2019	2024	2029	rVB	1940392	2524663	8.07%	2.732%
21	13.786	2076	2083	2088	rVV	20090195	31288073	100.00%	33.862%
22	13.871	2089	2097	2101	rVV	766476	1080656	3.45%	1.170%
23	13.926	2101	2106	2111	rVB3	242278	358355	1.15%	0.388%
24	14.219	2149	2154	2157	rVV2	375733	535318	1.71%	0.579%
25	14.316	2164	2170	2176	rVV	351161	568867	1.82%	0.616%
26	14.639	2218	2223	2233	rVB	10956583	13995050	44.73%	15.146%
27	14.780	2240	2246	2255	rVB	6841879	8637283	27.61%	9.348%
28	15.206	2308	2316	2320	rBV	866797	1173502	3.75%	1.270%
29	15.371	2331	2343	2347	rBV	1758515	2749056	8.79%	2.975%
30	15.475	2354	2360	2365	rBV	1445376	2294872	7.33%	2.484%
31	15.615	2377	2383	2386	rBV	1506849	2395321	7.66%	2.592%
32	15.651	2386	2389	2395	rVB	897634	1277533	4.08%	1.383%
33	15.834	2409	2419	2424	rBV	411379	1080663	3.45%	1.170%
34	15.987	2438	2444	2454	rVB	259316	467447	1.49%	0.506%
35	16.084	2454	2460	2466	rBV	193442	324951	1.04%	0.352%
36	16.328	2490	2500	2509	rBV2	1217546	2496721	7.98%	2.702%

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NEVINS-SB06-Z36-37

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

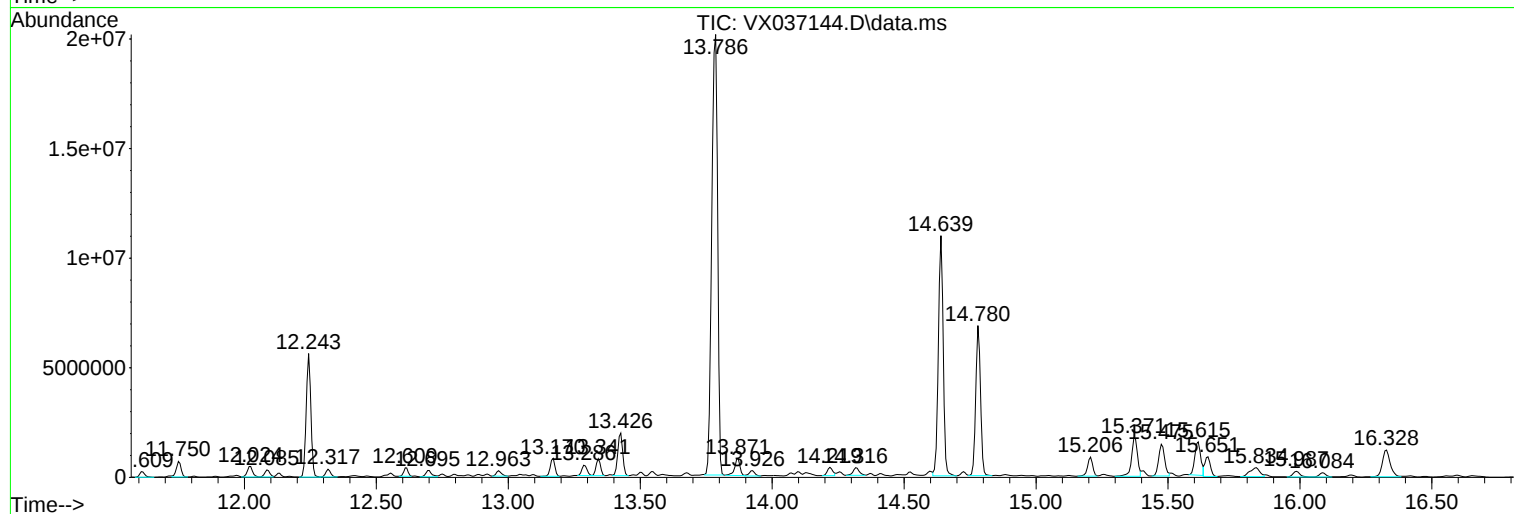
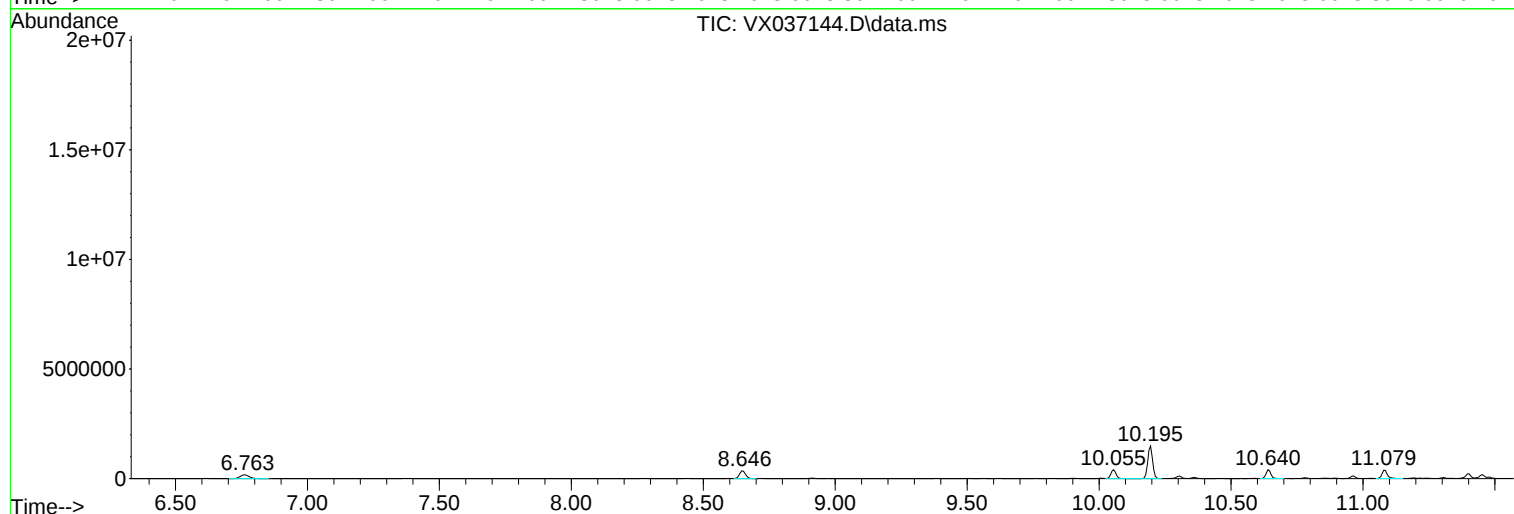
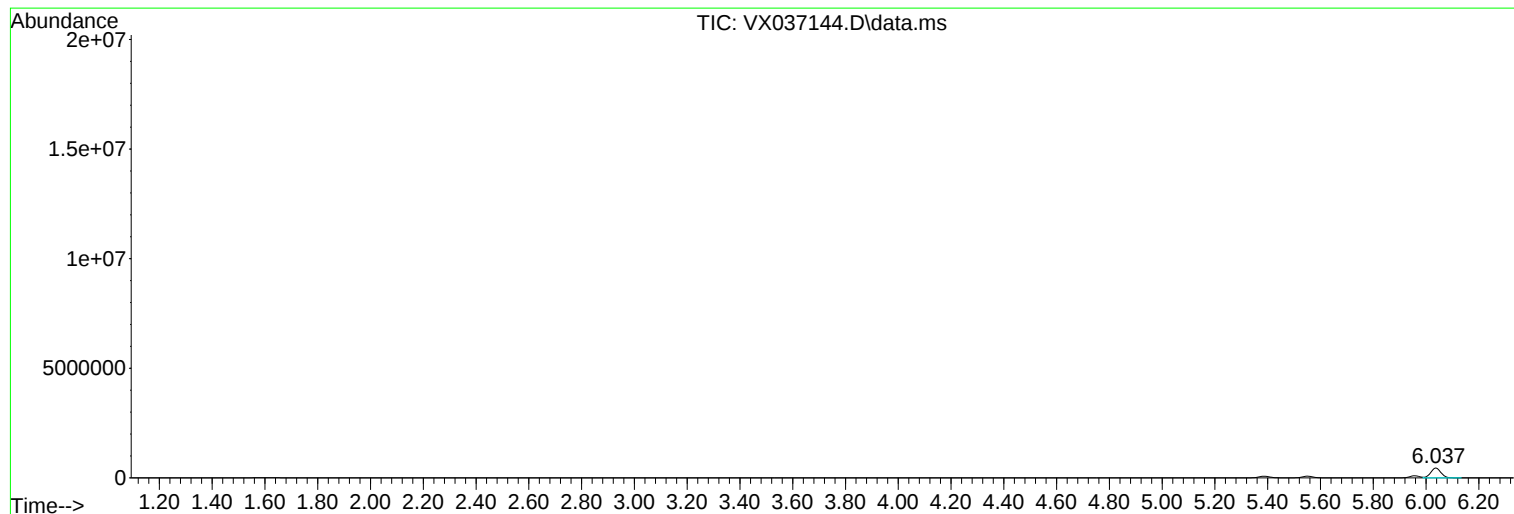
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



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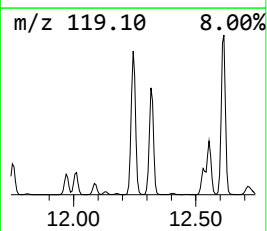
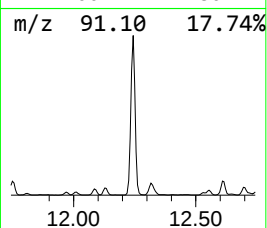
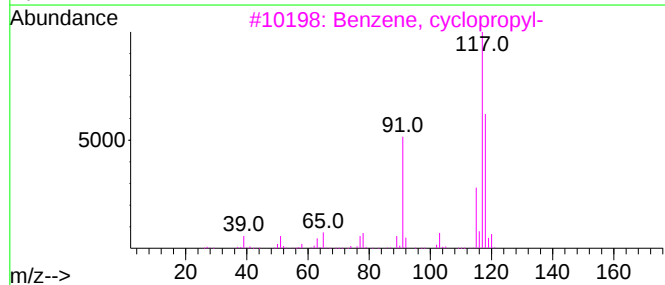
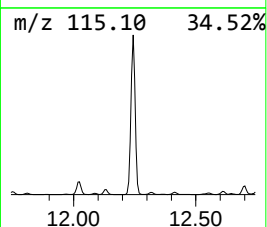
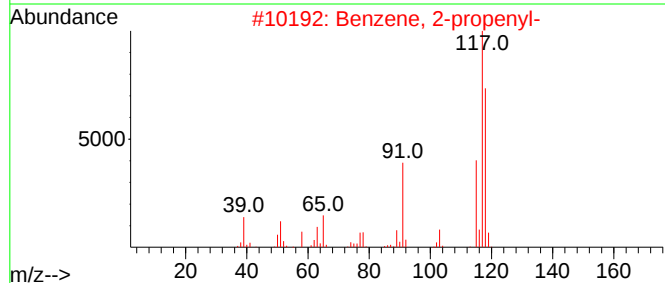
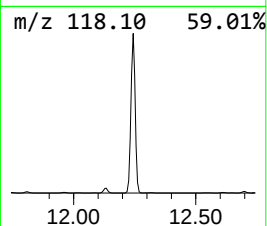
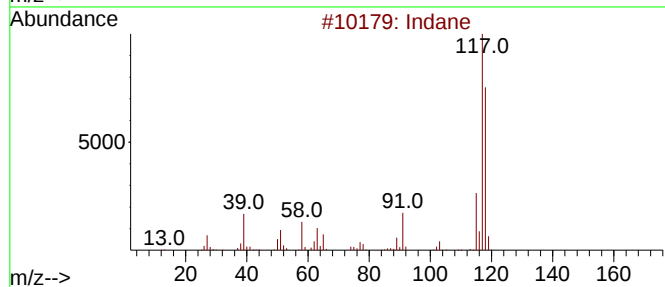
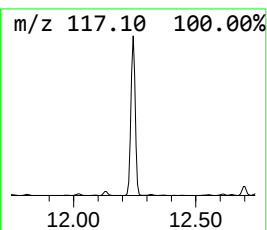
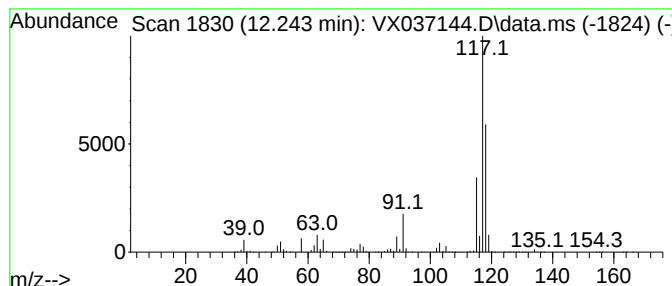
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	516.02 ug/l	6898740	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	72



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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z36-37

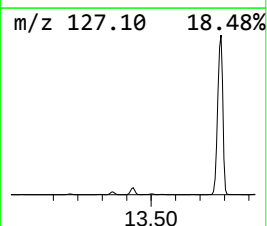
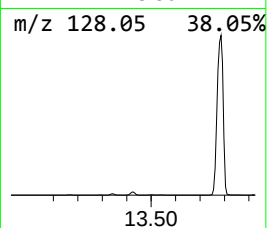
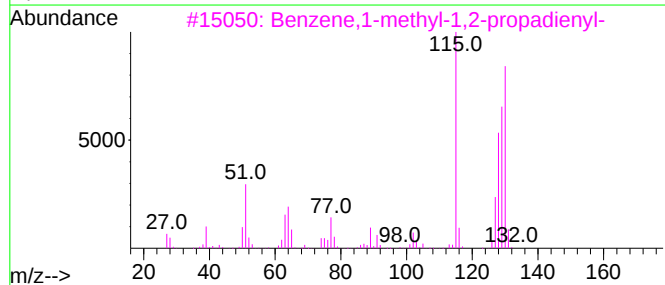
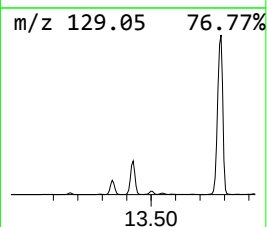
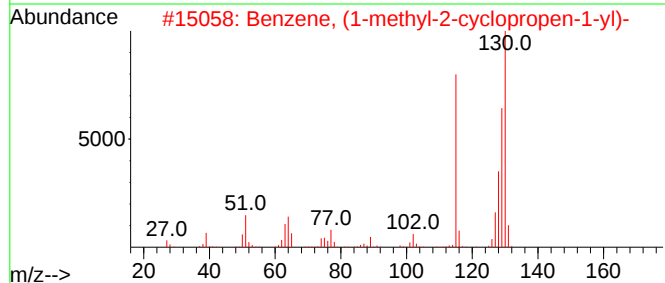
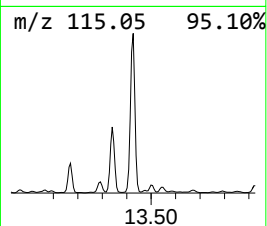
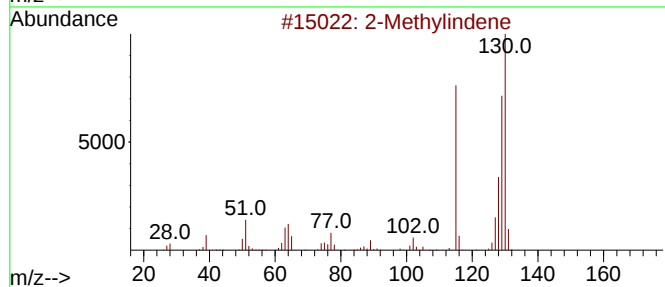
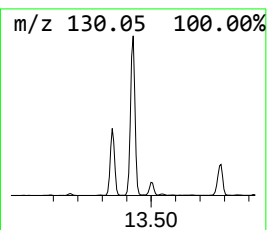
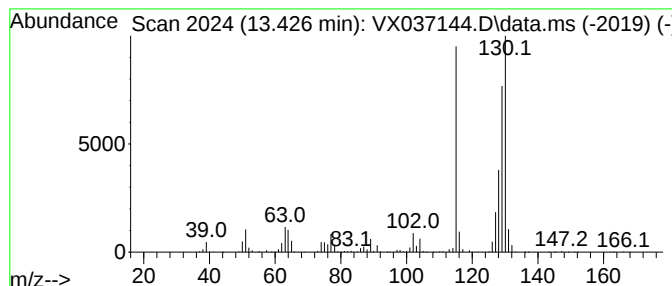
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Methylindene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	188.84 ug/l	2524660	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	95
2			Benzene, (1-methyl-2-cyclopropen-1-yl)-	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			Benzene, 1-butylnyl-	130	C10H10	000622-76-4	94



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z36-37

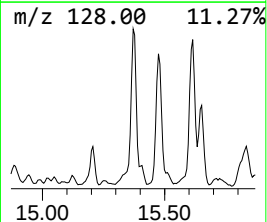
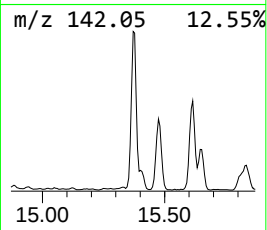
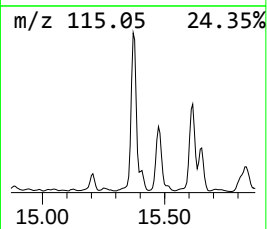
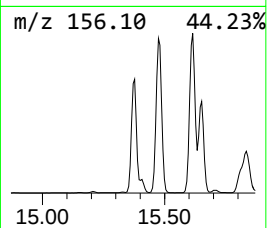
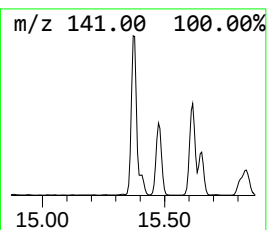
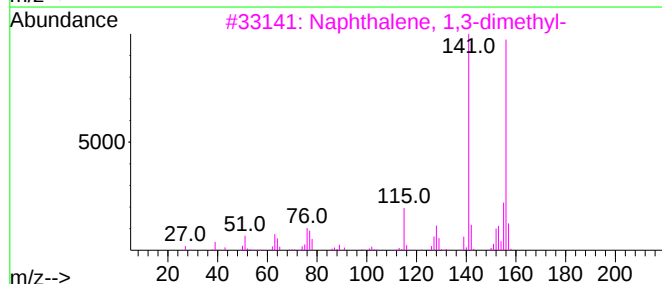
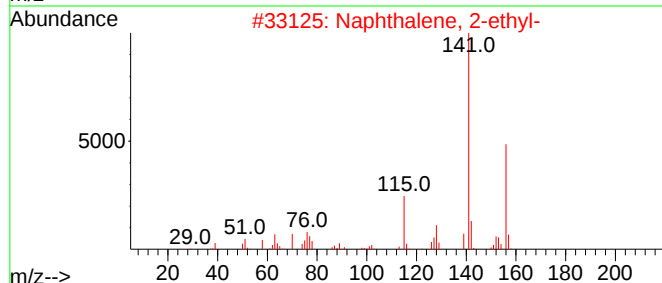
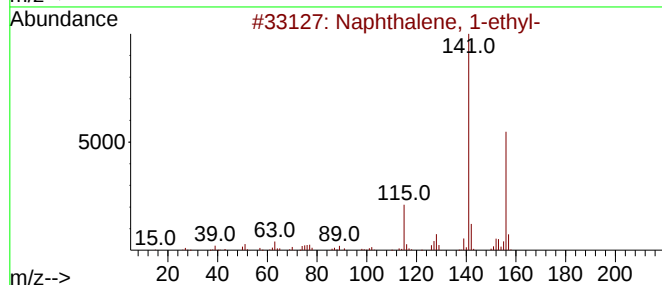
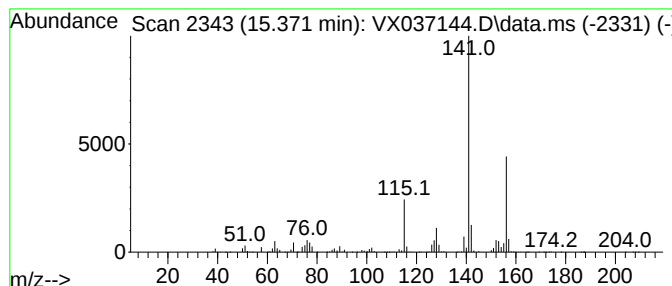
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	205.63 ug/l	2749060	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, 1,3-dimethyl-	156	C12H12	000575-41-7	91
4			2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59
5			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59



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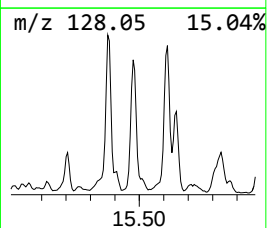
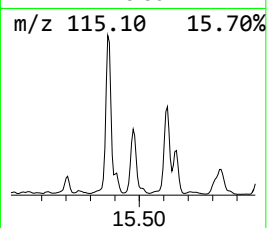
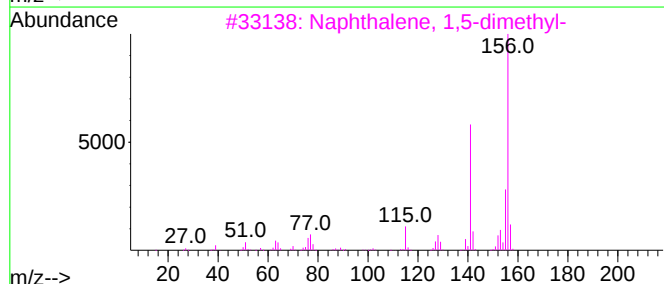
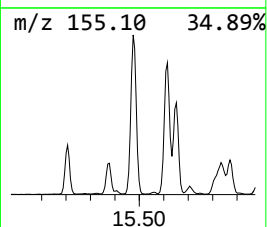
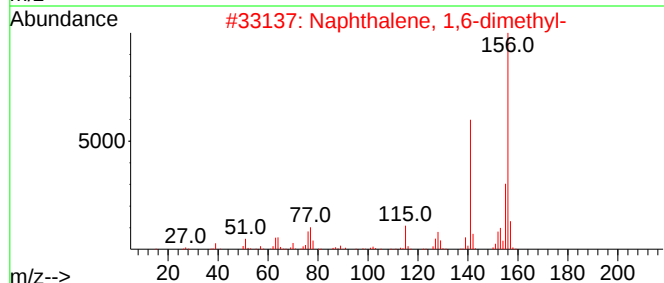
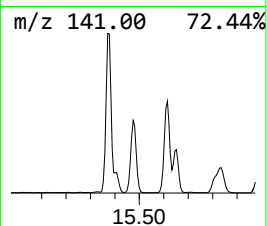
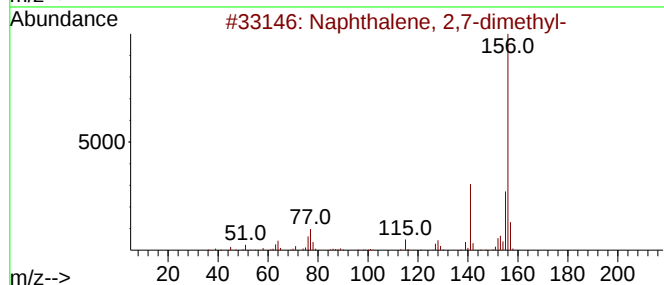
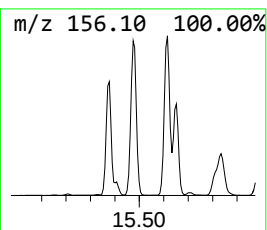
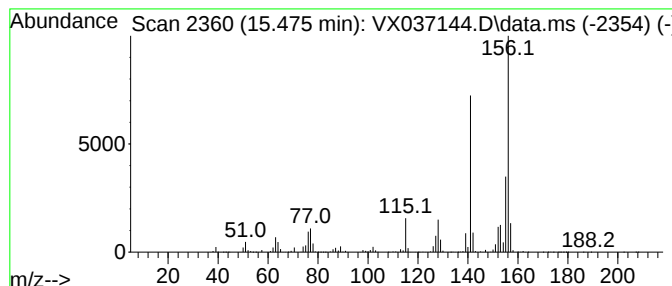
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	171.66 ug/l	2294870	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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97



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NEVINS-SB06-Z36-37

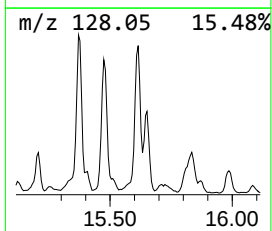
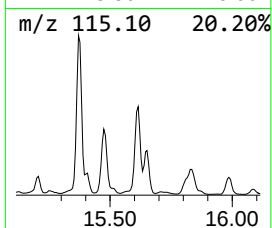
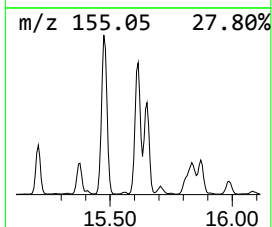
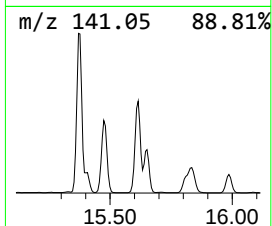
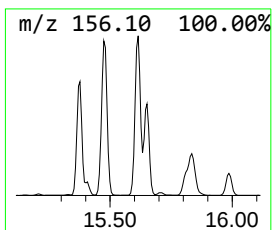
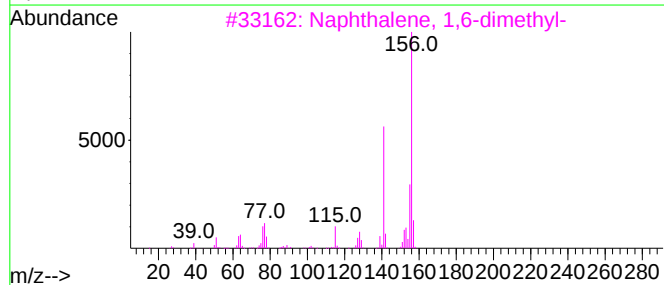
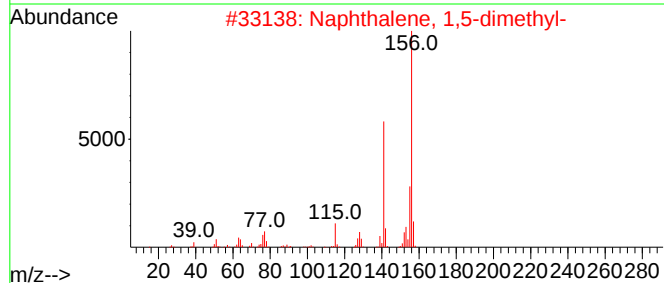
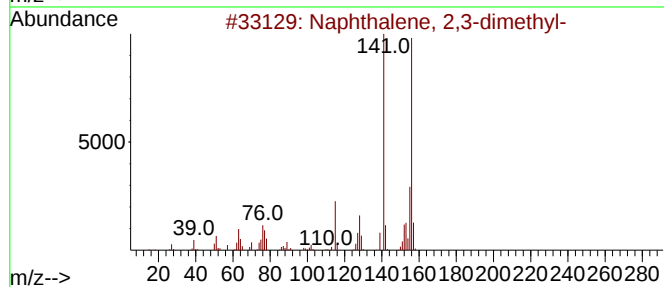
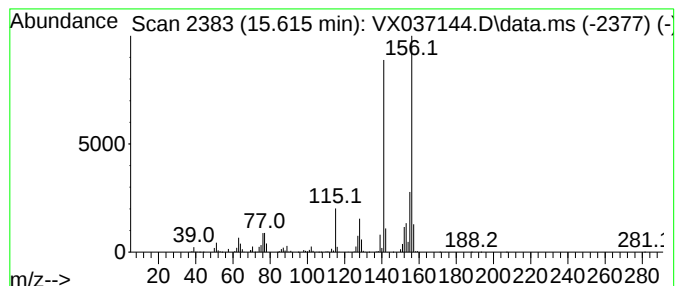
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	179.17 ug/l	2395320	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037144.D
Acq On : 21 Aug 2023 20:31
Operator : JC/MD
Sample : 03994-02 10X
Misc : 6.46g/10.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z36-37

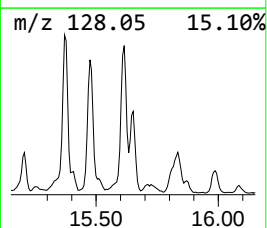
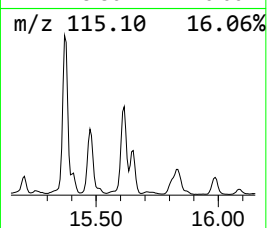
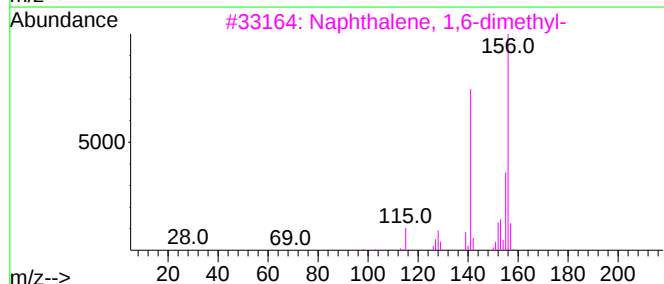
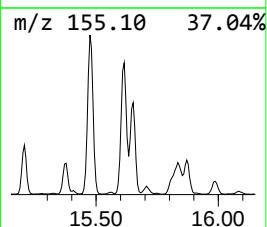
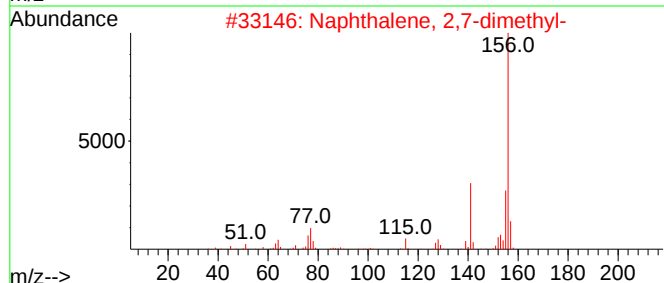
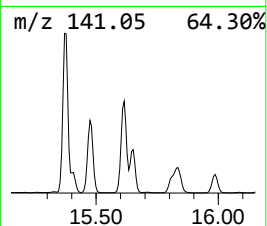
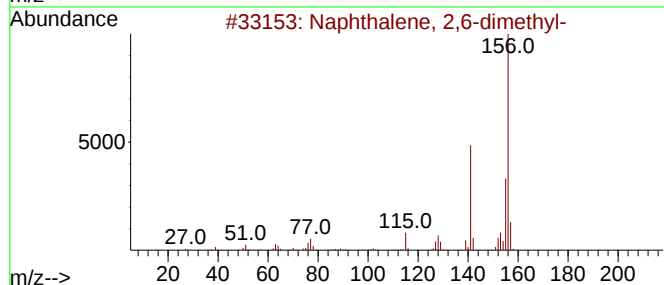
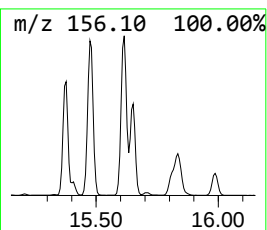
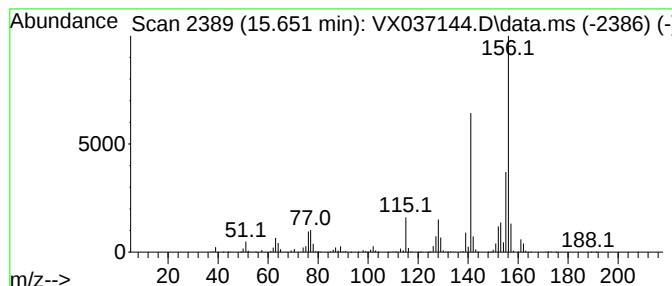
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.651	95.56 ug/l	1277530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037144.D
Acq On : 21 Aug 2023 20:31
Operator : JC/MD
Sample : 03994-02 10X
Misc : 6.46g/10.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z36-37

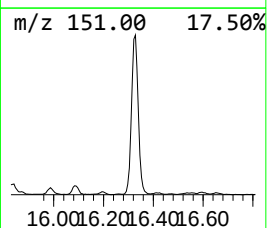
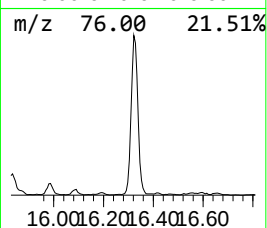
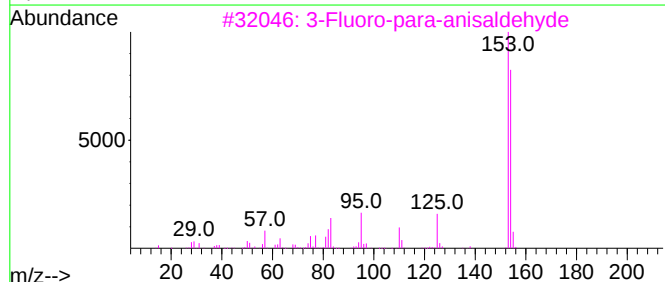
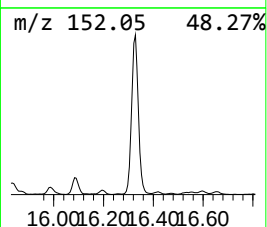
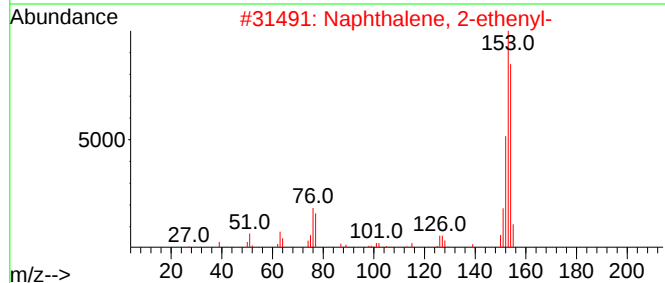
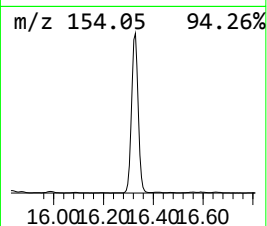
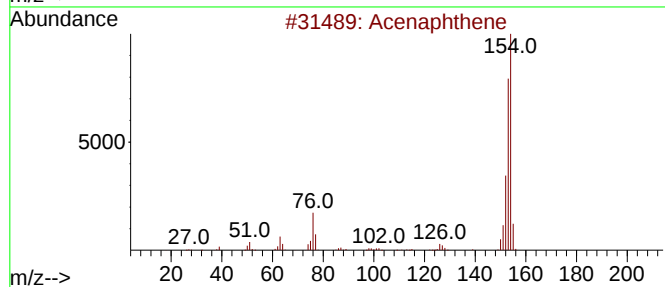
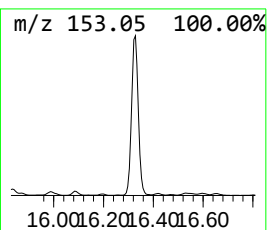
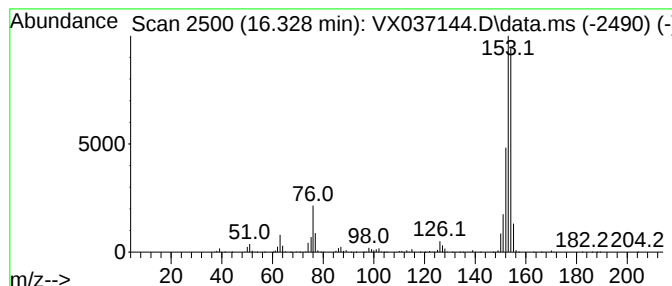
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-ethenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	186.75 ug/l	2496720	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	64
3		3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
4		2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	40
5		Biphenyl	154	C12H10	000092-52-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082123\
Data File : VX037144.D
Acq On : 21 Aug 2023 20:31
Operator : JC/MD
Sample : 03994-02 10X
Misc : 6.46g/10.0mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB06-Z36-37

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	12.243	516.0	ug/l	6898740	4	12.024	668454	50.0
2-Methylindene	13.426	188.8	ug/l	2524660	4	12.024	668454	50.0
Naphthalene, 1-...	15.371	205.6	ug/l	2749060	4	12.024	668454	50.0
Naphthalene, 2,...	15.475	171.7	ug/l	2294870	4	12.024	668454	50.0
Naphthalene, 2,...	15.615	179.2	ug/l	2395320	4	12.024	668454	50.0
Naphthalene, 2,...	15.651	95.6	ug/l	1277530	4	12.024	668454	50.0
Naphthalene, 2-...	16.328	186.8	ug/l	2496720	4	12.024	668454	50.0