

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062025\
 Data File : VN087143.D
 Acq On : 20 Jun 2025 16:31
 Operator : JC\MD
 Sample : Q2355-03 20X
 Misc : 3.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20071

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_N\methods\82N060625W.M
 Title : SW846 8260

Signal : TIC: VN087143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1048	1057	1062	rBV	128307	308507	31.56%	4.331%
2	8.230	1062	1067	1078	rVB	202424	465743	47.65%	6.539%
3	8.577	1118	1126	1140	rBV2	134879	313298	32.06%	4.398%
4	9.106	1207	1216	1229	rBV	361202	708754	72.52%	9.950%
5	10.565	1455	1464	1474	rBV	468662	877097	89.74%	12.314%
6	11.865	1677	1685	1694	rBV	490023	881508	90.19%	12.376%
7	12.065	1711	1719	1724	rBV6	5882	12763	1.31%	0.179%
8	12.482	1779	1790	1802	rVB5	22508	87622	8.97%	1.230%
9	12.771	1830	1839	1840	rBV9	9889	21391	2.19%	0.300%
10	12.847	1845	1852	1861	rVV	380128	658311	67.36%	9.242%
11	13.153	1900	1904	1911	rBV7	15534	33514	3.43%	0.471%
12	13.312	1926	1931	1932	rBV5	10784	15336	1.57%	0.215%
13	13.659	1988	1990	1992	rBV3	8723	9894	1.01%	0.139%
14	13.788	2005	2012	2028	rBV	540132	977375	100.00%	13.722%
15	14.106	2061	2066	2079	rVB	31795	104739	10.72%	1.470%
16	14.329	2100	2104	2111	rVB10	7129	10069	1.03%	0.141%
17	14.435	2118	2122	2125	rBV6	7810	11439	1.17%	0.161%
18	14.623	2150	2154	2157	rBV4	26264	42103	4.31%	0.591%
19	14.735	2168	2173	2175	rBV5	8761	14587	1.49%	0.205%
20	14.835	2188	2190	2194	rBV4	10298	17092	1.75%	0.240%
21	15.047	2219	2226	2231	rBV7	29878	80232	8.21%	1.126%
22	15.206	2249	2253	2259	rBV3	36116	65890	6.74%	0.925%
23	15.259	2260	2262	2267	rVV5	10400	14401	1.47%	0.202%
24	15.317	2267	2272	2277	rBV8	27739	57249	5.86%	0.804%
25	15.435	2287	2292	2298	rVB4	41969	86409	8.84%	1.213%
26	15.594	2314	2319	2323	rBV6	21921	52382	5.36%	0.735%
27	15.694	2331	2336	2340	rBV3	40761	81152	8.30%	1.139%
28	15.947	2370	2379	2385	rBV7	36902	131106	13.41%	1.841%
29	16.159	2410	2415	2421	rBV3	113041	208722	21.36%	2.930%
30	16.494	2465	2472	2479	rBV4	102658	245055	25.07%	3.440%
31	16.700	2501	2507	2514	rBV	171385	399492	40.87%	5.609%
32	16.782	2515	2521	2522	rBV2	70897	129708	13.27%	1.821%

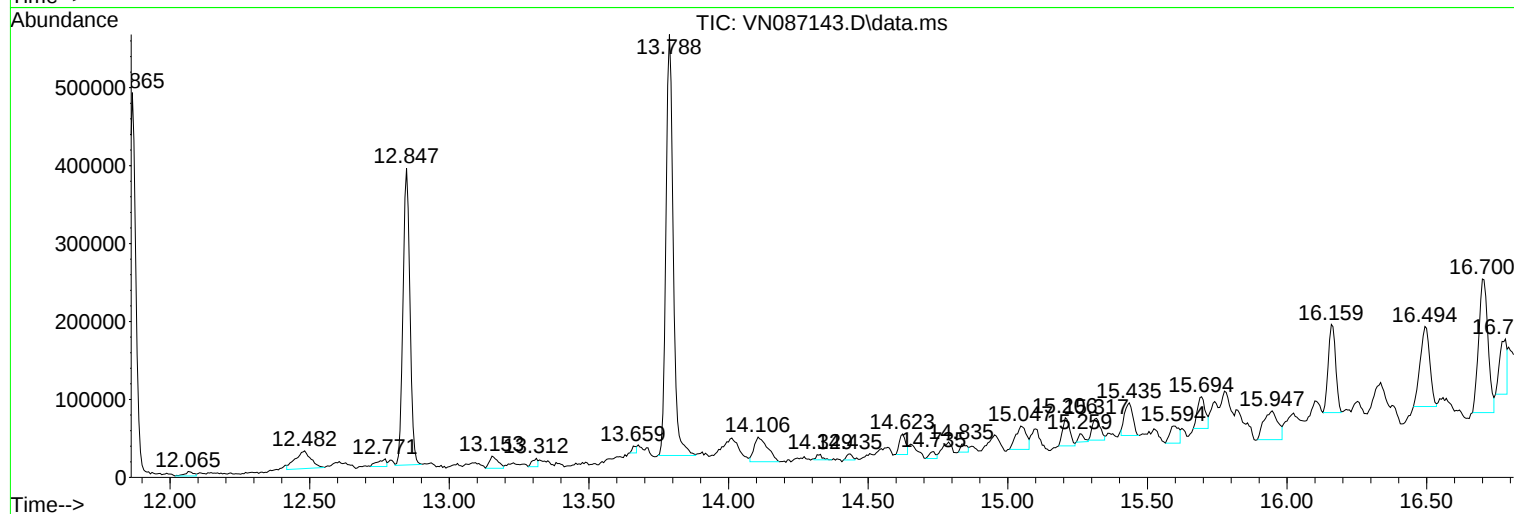
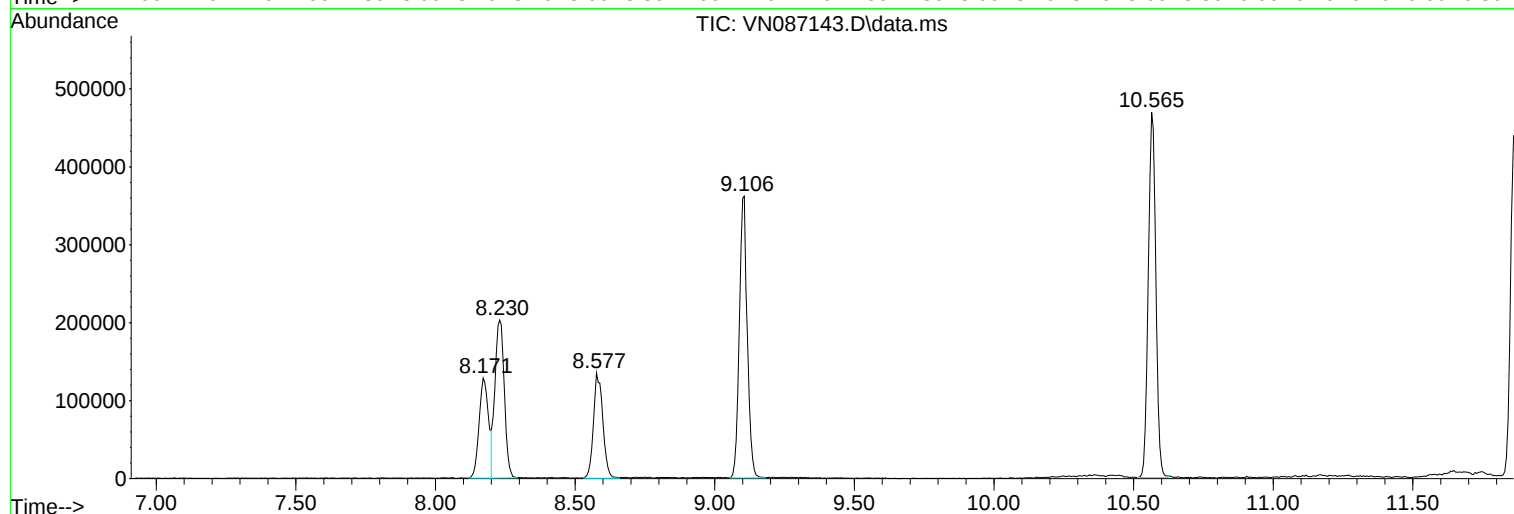
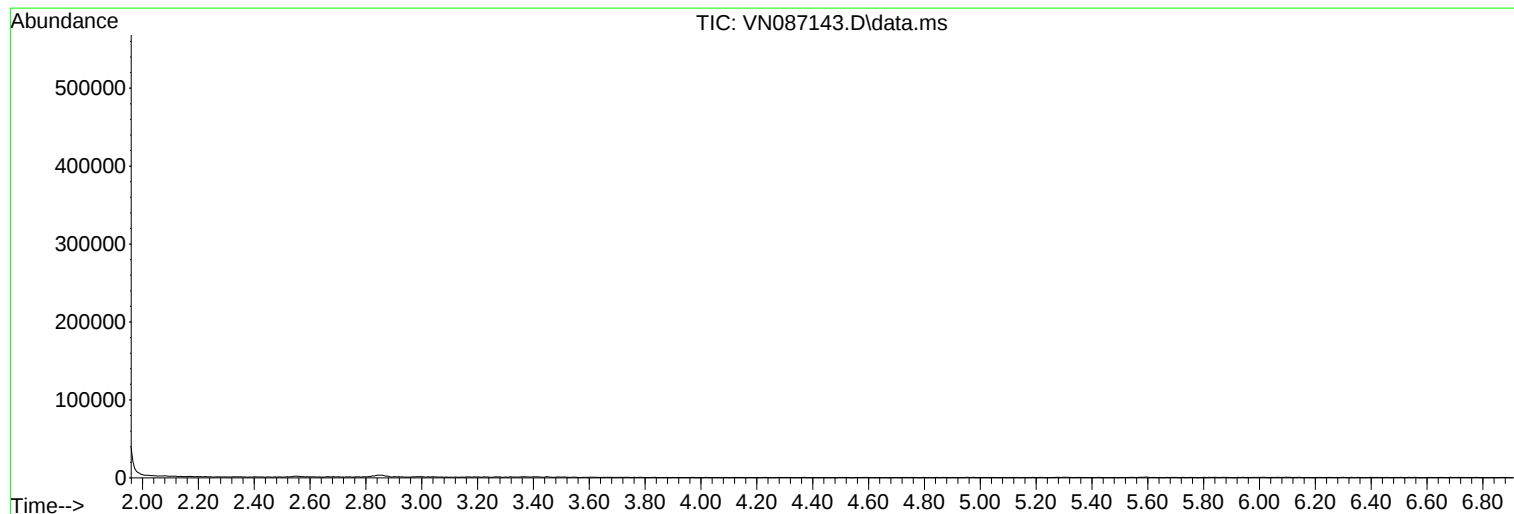
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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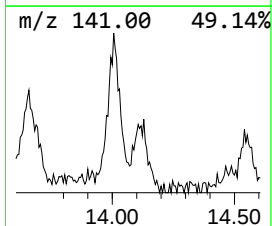
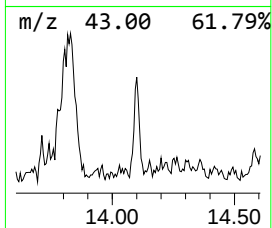
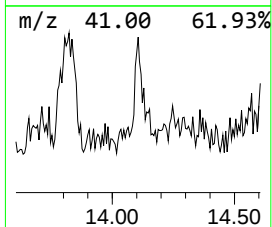
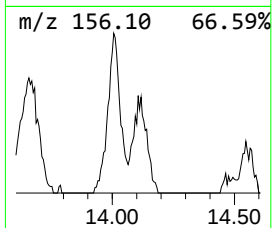
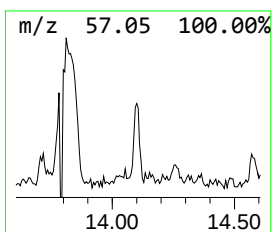
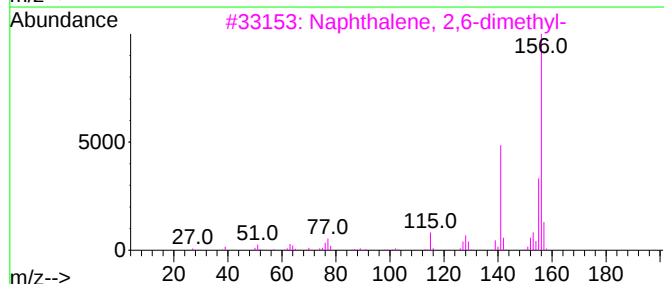
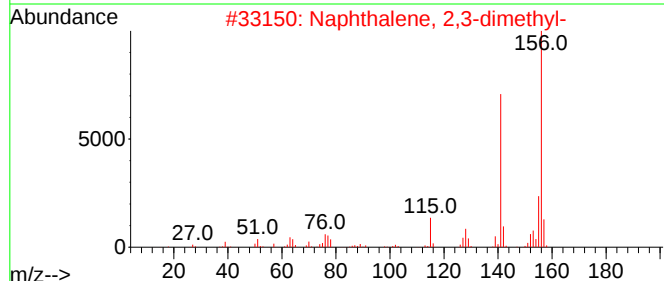
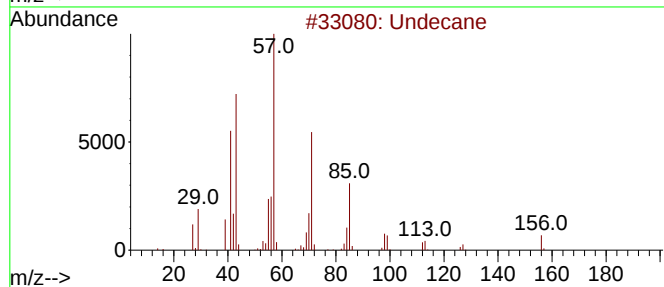
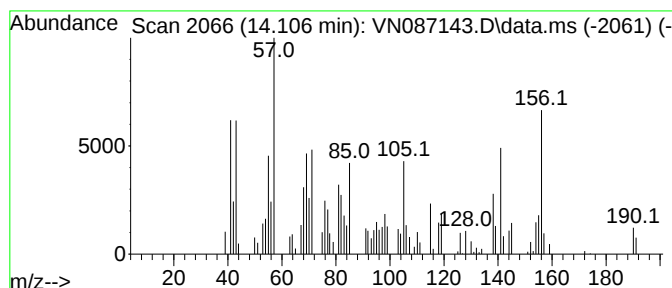
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	5.36 ug/l	104739	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	50
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	50
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	50
4			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	50
5			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	50



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ClientSampleId :
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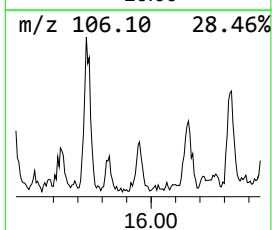
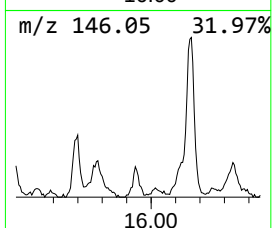
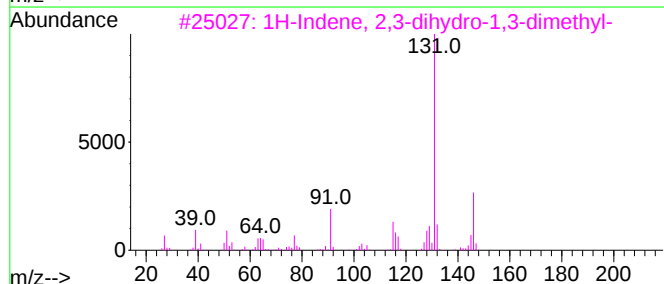
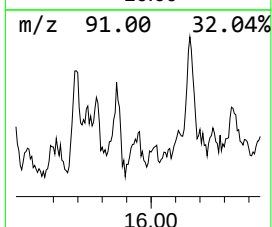
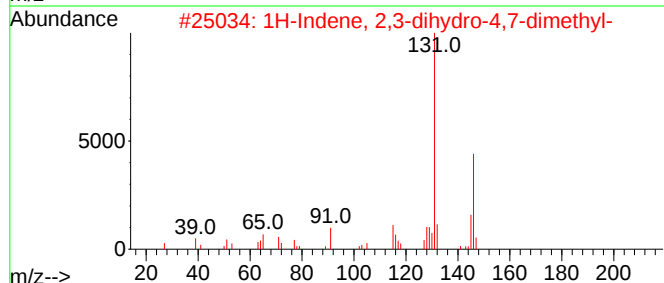
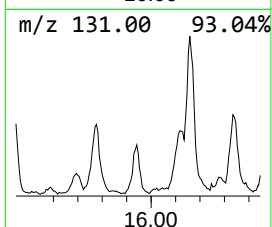
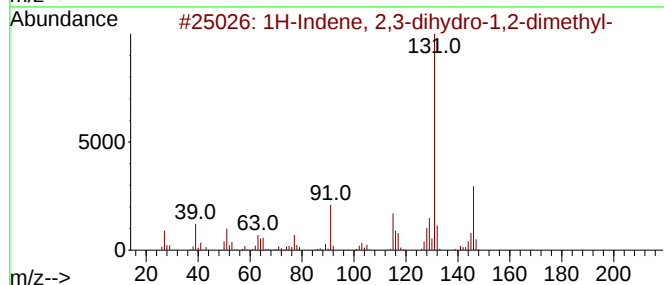
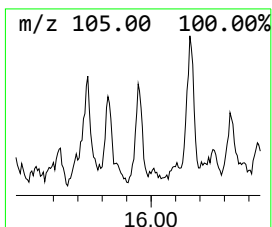
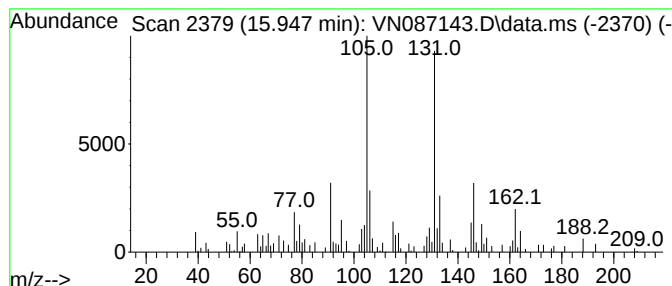
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	6.71 ug/l	131106	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	90		
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90		
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	89		
4	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	55		
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	55		



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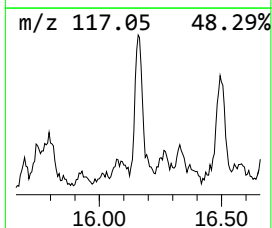
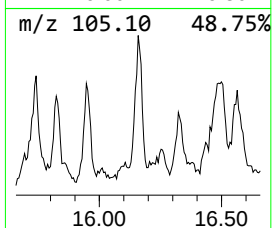
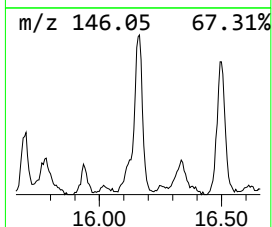
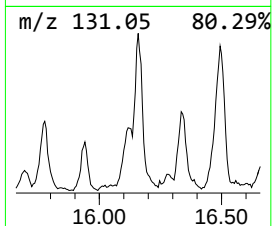
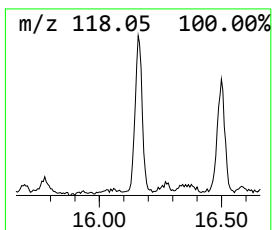
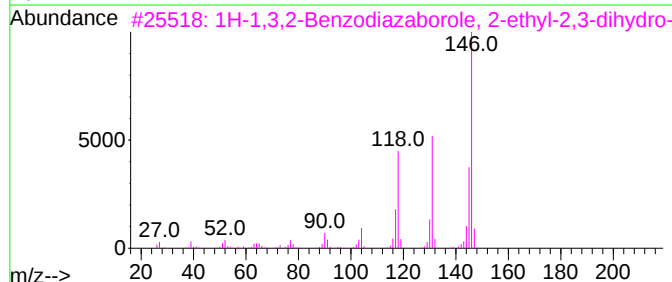
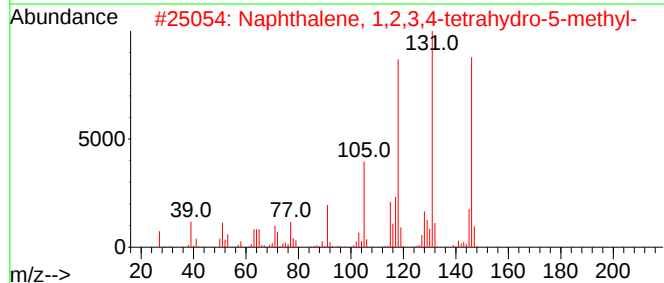
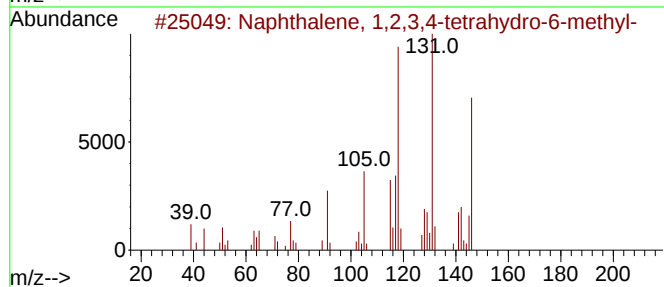
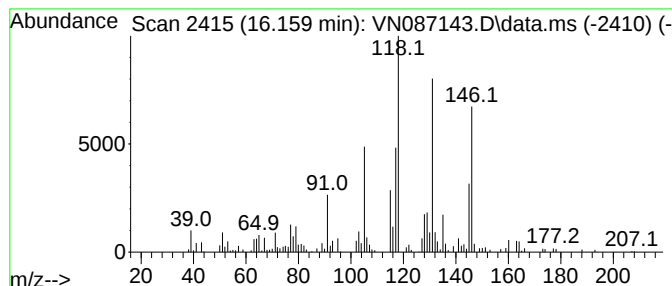
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Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.159	10.68 ug/l	208722	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	87
4			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	72
5			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	72



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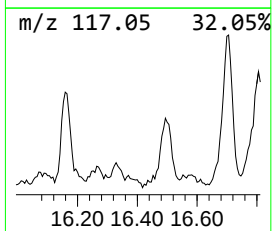
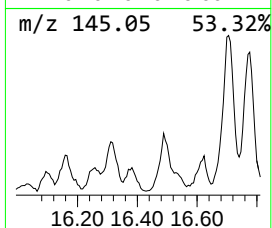
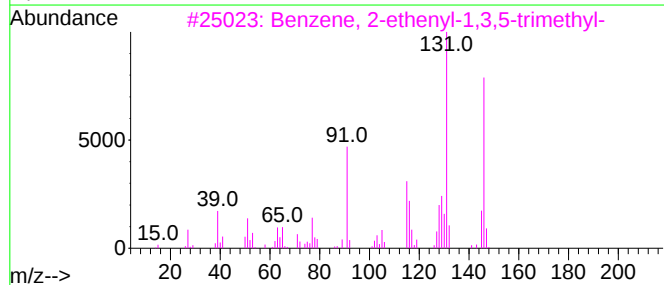
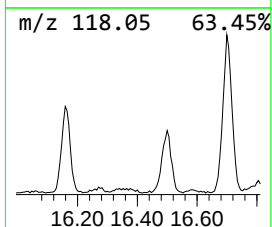
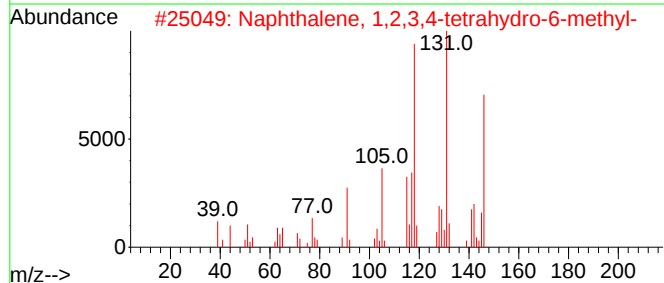
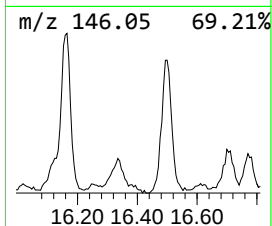
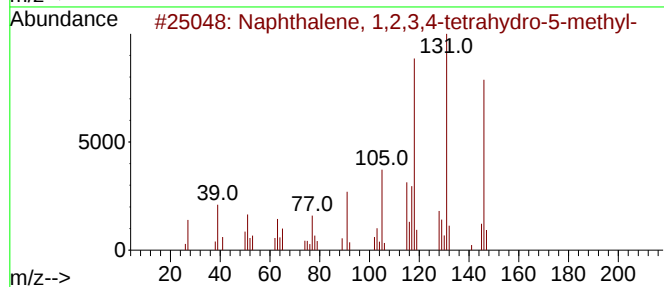
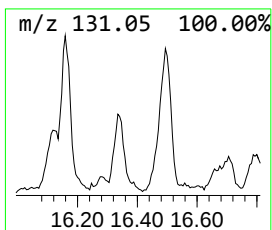
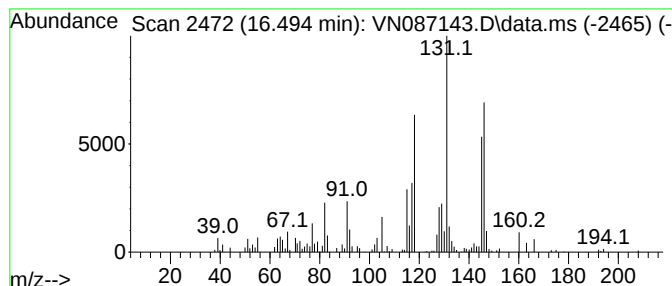
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2,3,4-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.494	12.54 ug/l	245055	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	83
4			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	62
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	58



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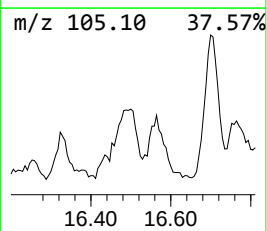
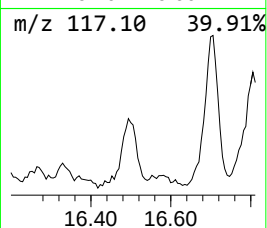
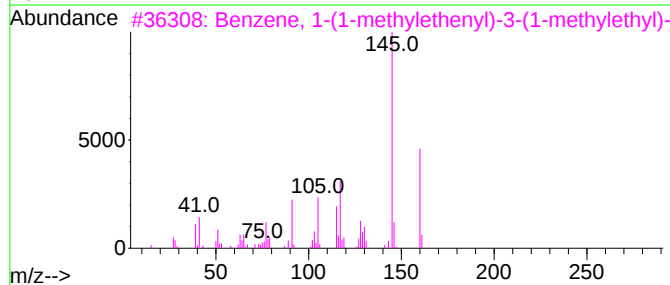
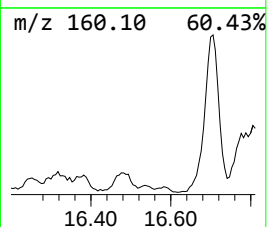
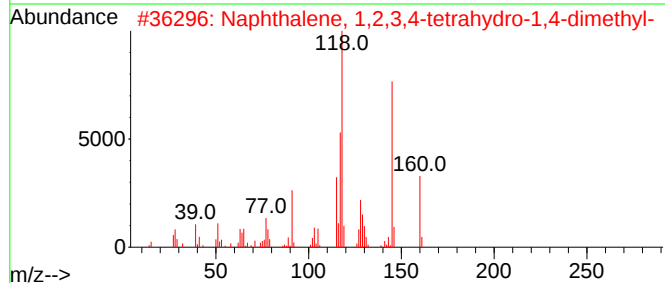
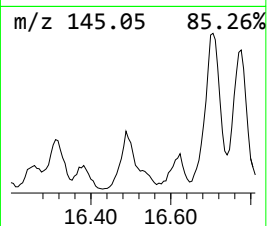
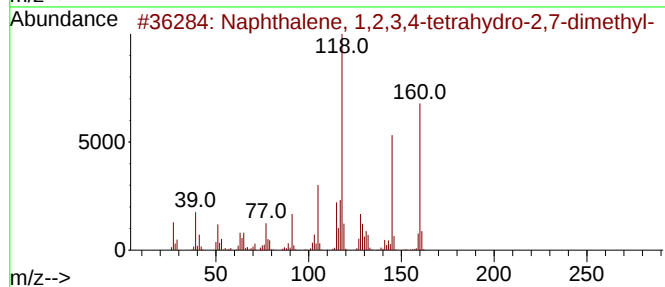
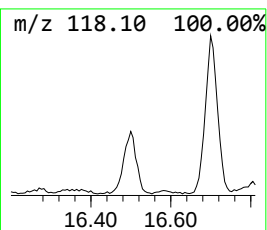
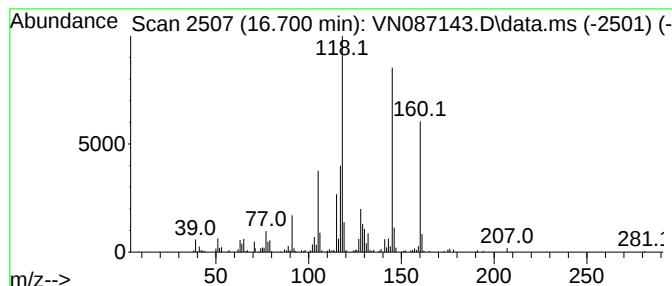
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.700	20.44 ug/l	399492	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	74
3			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	70
4			2,5-Dimethylbenzyl cyanide	145	C10H11N	016213-85-7	62
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062025\
Data File : VN087143.D
Acq On : 20 Jun 2025 16:31
Operator : JC\MD
Sample : Q2355-03 20X
Misc : 3.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20071

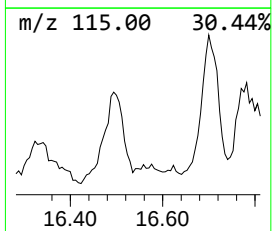
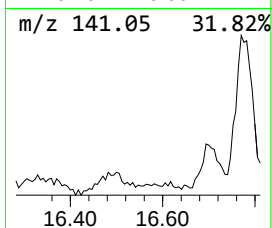
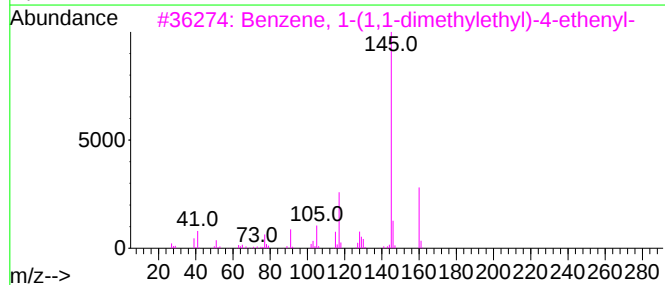
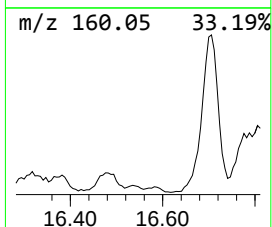
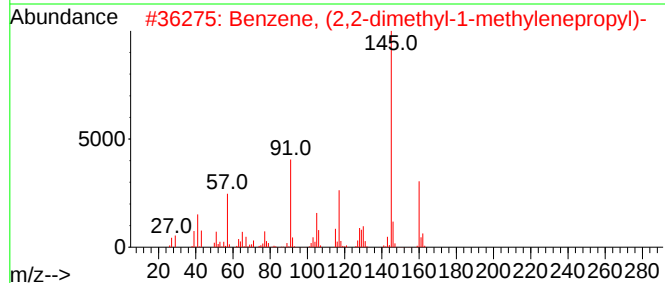
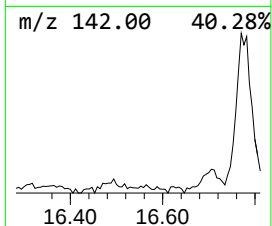
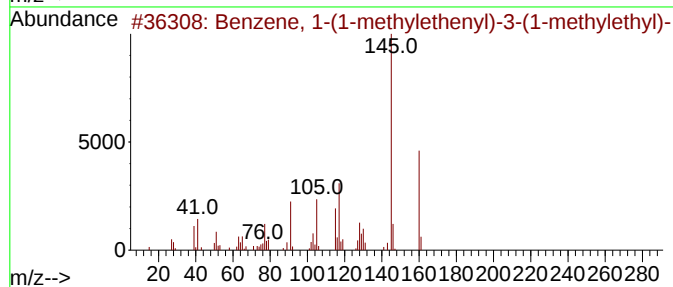
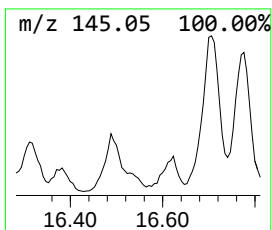
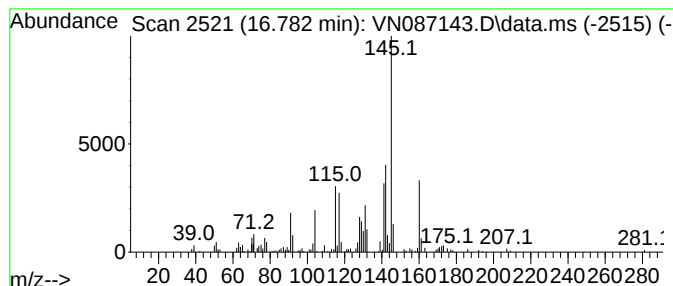
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-(1-methylethenyl)... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	6.64 ug/l	129708	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	55
2			Benzene, (2,2-dimethyl-1-methyle...	160	C12H16	005676-29-9	55
3			Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	50
4			1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	50
5			1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062025\
Data File : VN087143.D
Acq On : 20 Jun 2025 16:31
Operator : JC\MD
Sample : Q2355-03 20X
Misc : 3.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	14.106	5.4	ug/l	104739	4	13.788	977375	50.0
1H-Indene, 2,3-...	15.947	6.7	ug/l	131106	4	13.788	977375	50.0
Naphthalene, 1,...	16.159	10.7	ug/l	208722	4	13.788	977375	50.0
Naphthalene, 1,...	16.494	12.5	ug/l	245055	4	13.788	977375	50.0
Naphthalene, 1,...	16.700	20.4	ug/l	399492	4	13.788	977375	50.0
Benzene, 1-(1-m...	16.782	6.6	ug/l	129708	4	13.788	977375	50.0