

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050625\
 Data File : VN086522.D
 Acq On : 06 May 2025 18:12
 Operator : JC\MD
 Sample : Q1966-03 100X
 Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SILICA-GEL

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\82N041525W.M
 Title : SW846 8260

Signal : TIC: VN086522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.512	84	95	99	rBV3	16987	43919	1.77%	0.320%
2	3.242	214	219	230	rVB3	16550	39735	1.61%	0.289%
3	5.341	567	576	584	rVB4	8361	26292	1.06%	0.191%
4	6.677	791	803	814	rBV3	15895	57218	2.31%	0.416%
5	8.165	1048	1056	1060	rBV	162109	378269	15.28%	2.753%
6	8.218	1060	1065	1078	rVB	327663	753710	30.45%	5.485%
7	8.577	1119	1126	1137	rBV2	189747	471099	19.03%	3.428%
8	9.100	1207	1215	1226	rVB	485376	1019980	41.20%	7.423%
9	9.594	1295	1299	1305	rVB2	25996	48094	1.94%	0.350%
10	10.565	1457	1464	1470	rBV	787976	1454395	58.75%	10.584%
11	10.623	1470	1474	1481	rVB	116996	227176	9.18%	1.653%
12	10.735	1491	1493	1499	rVB4	31448	48971	1.98%	0.356%
13	11.865	1679	1685	1692	rVB	687616	1222372	49.38%	8.896%
14	12.065	1713	1719	1726	rBV	215273	518931	20.96%	3.777%
15	12.465	1773	1787	1801	rVB3	506740	2475577	100.00%	18.016%
16	12.847	1847	1852	1857	rBV	502204	776355	31.36%	5.650%
17	13.788	2007	2012	2020	rVB	771146	1358150	54.86%	9.884%
18	14.012	2040	2050	2059	rVB6	486686	1705608	68.90%	12.413%
19	14.764	2174	2178	2184	rVB3	71960	118031	4.77%	0.859%
20	15.635	2315	2326	2332	rBV5	66690	236275	9.54%	1.720%
21	16.158	2411	2415	2421	rVB2	75798	140588	5.68%	1.023%
22	16.476	2461	2469	2477	rBV2	116163	332123	13.42%	2.417%
23	16.705	2501	2508	2514	rBV3	63335	158479	6.40%	1.153%
24	16.776	2514	2520	2522	rBV3	70312	129480	5.23%	0.942%

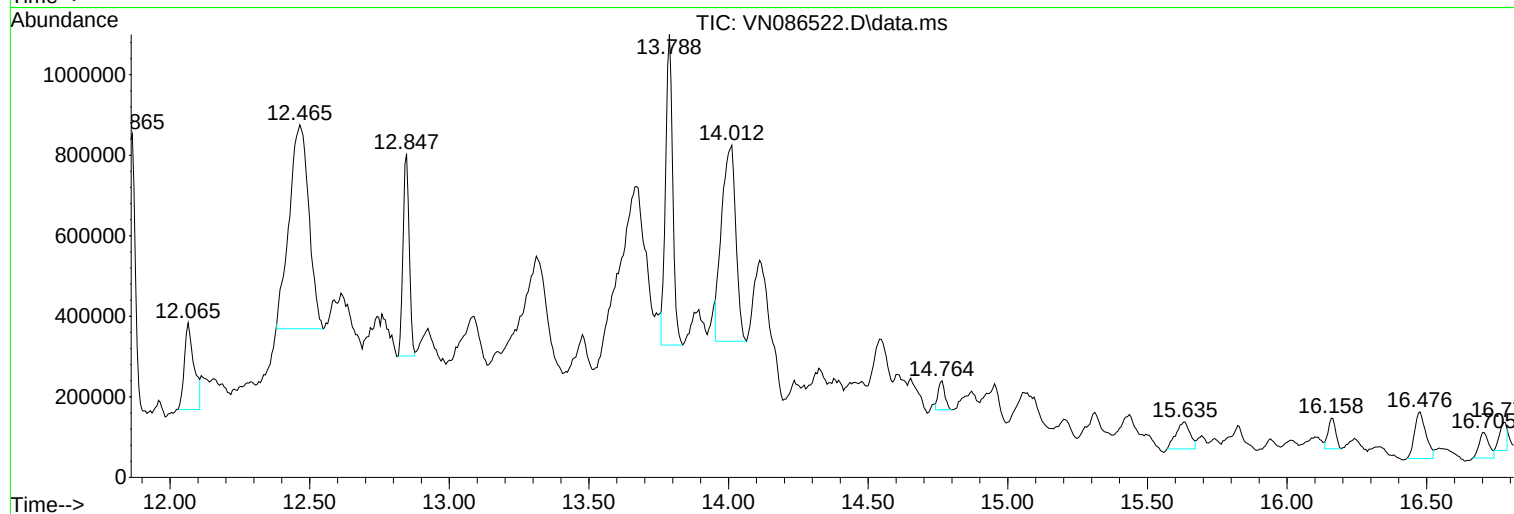
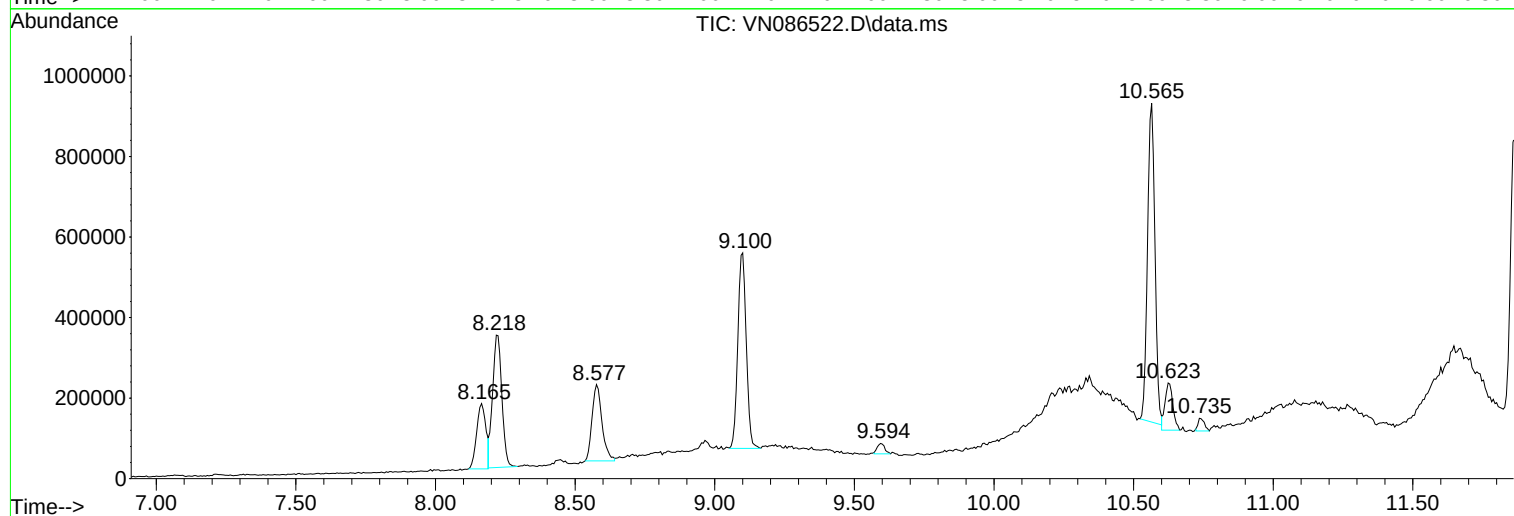
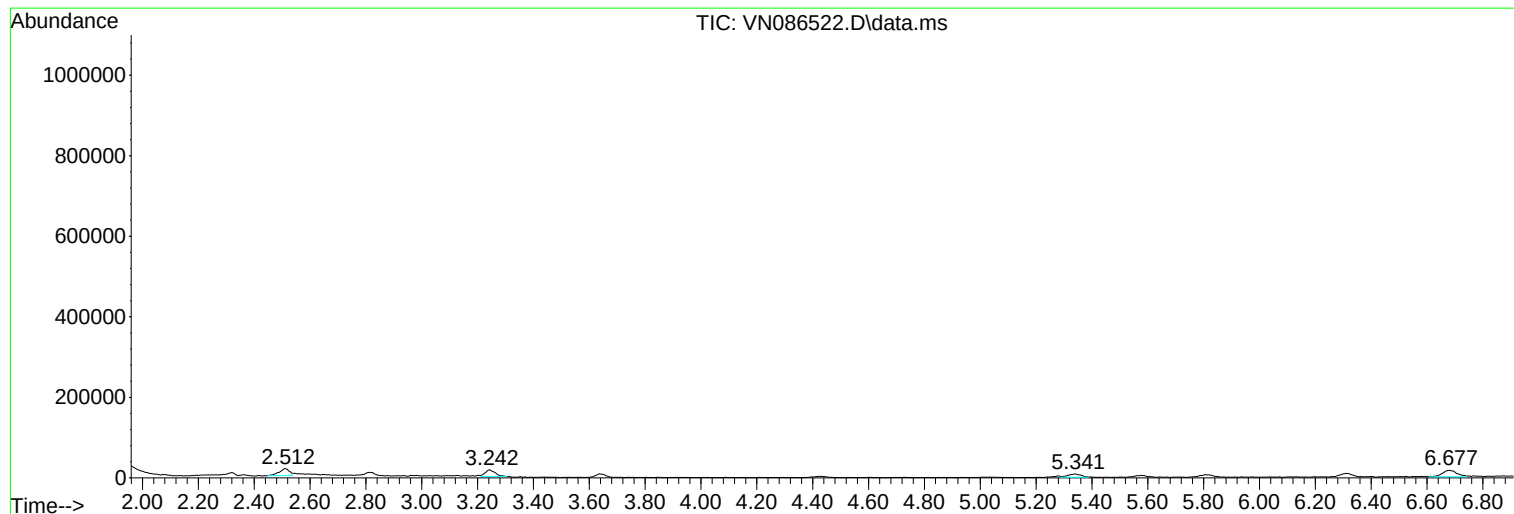
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Instrument :
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ClientSampleId :
SILICA-GEL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



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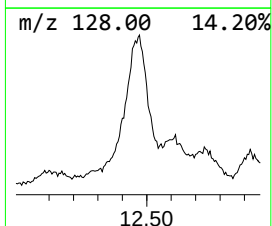
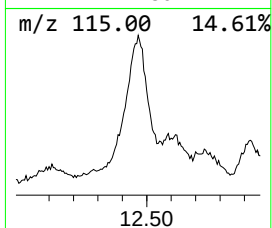
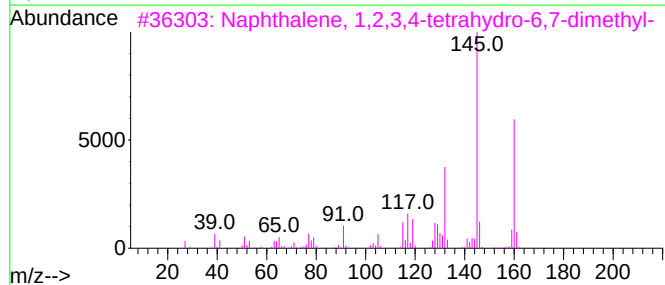
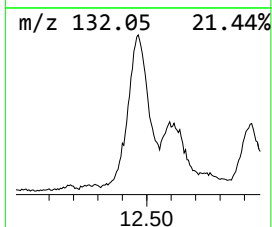
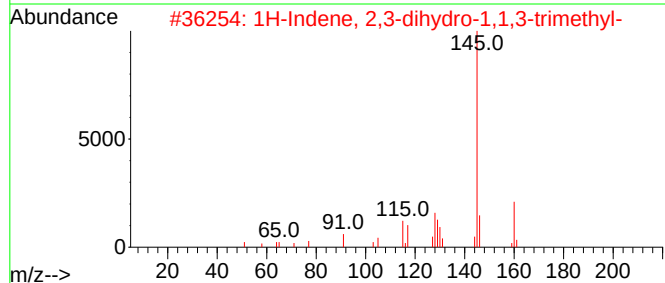
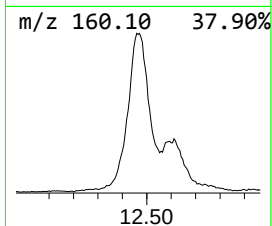
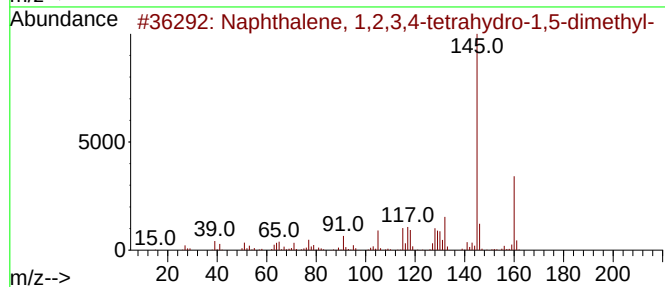
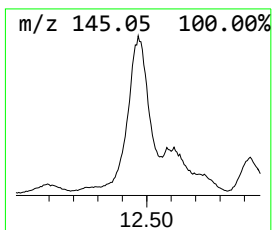
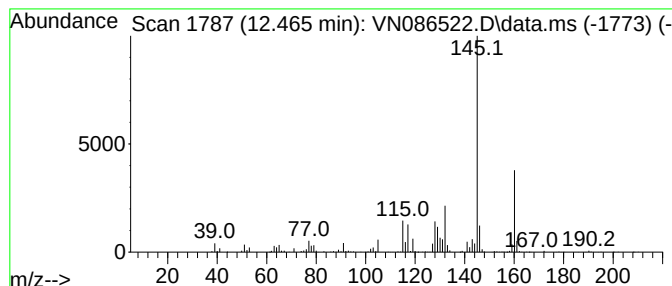
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.465	101.26 ug/l	2475580	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	94
2			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	93
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	91
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	91
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	91



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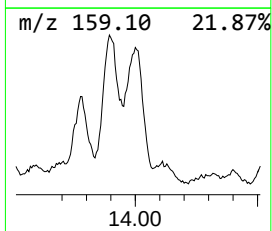
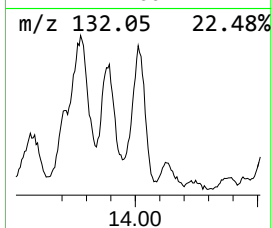
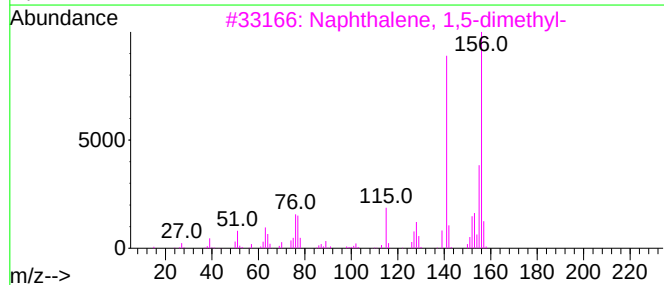
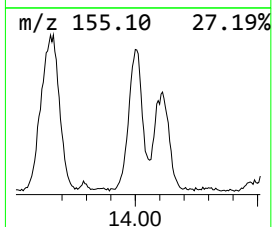
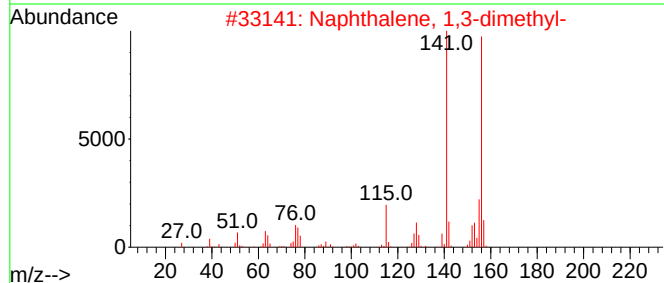
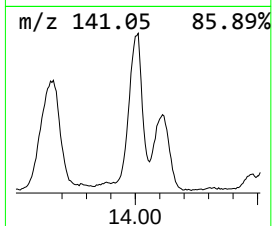
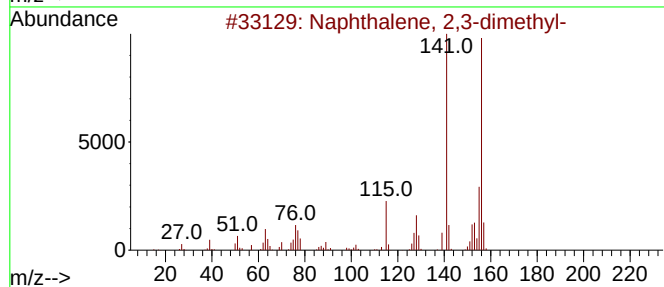
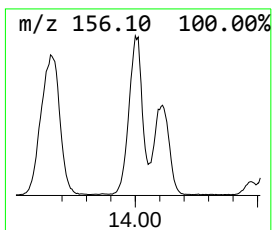
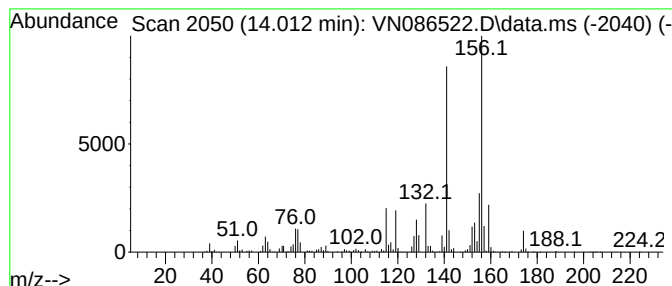
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.012	62.79 ug/l	1705610	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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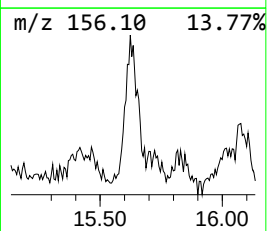
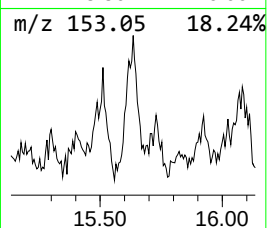
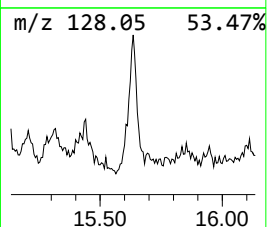
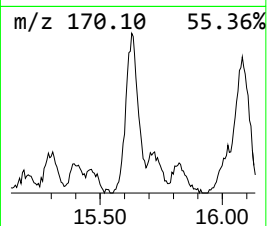
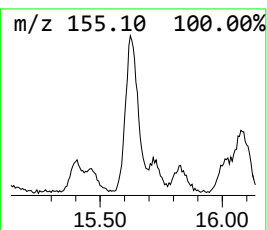
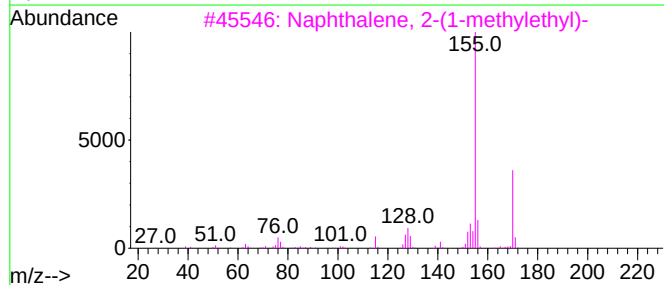
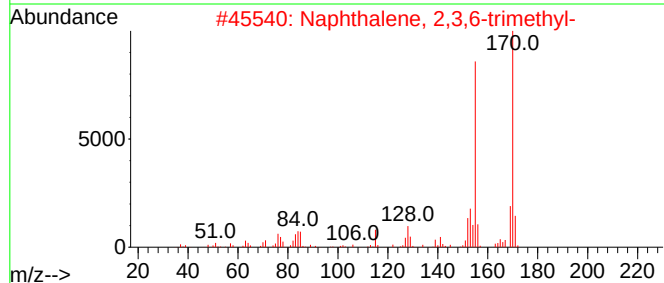
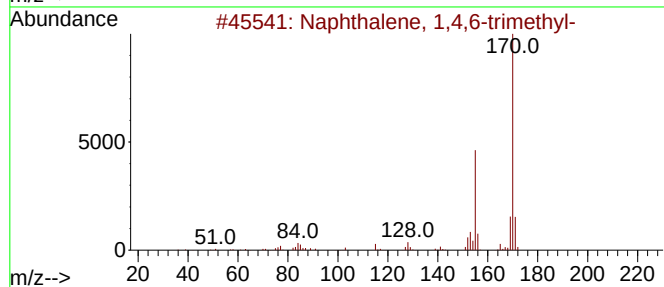
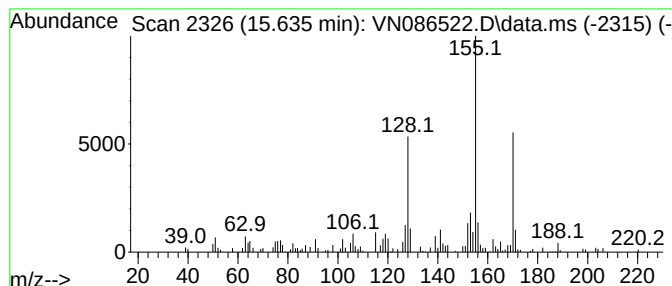
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,4,6-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.635	8.70 ug/l	236275	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	87
2			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	87
3			Naphthalene, 2-(1-methylethyl)-	170	C13H14	002027-17-0	81
4			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	74
5			Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	68



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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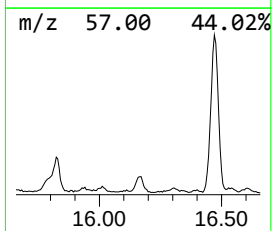
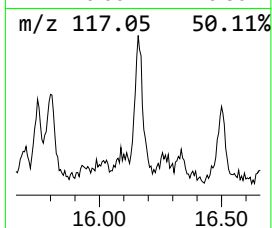
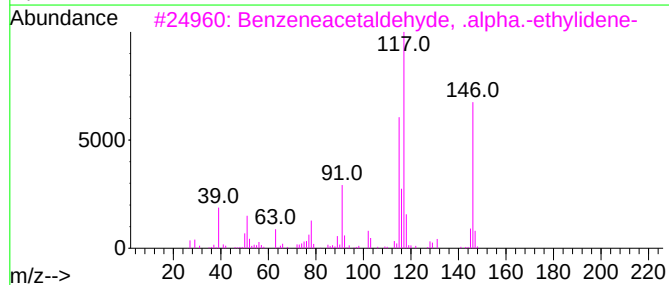
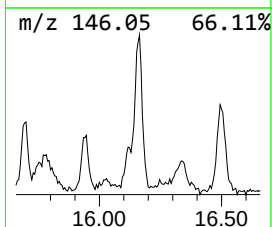
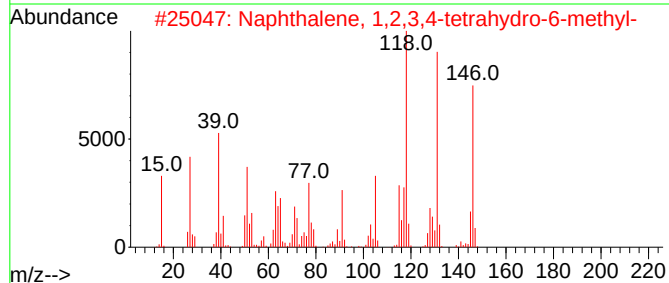
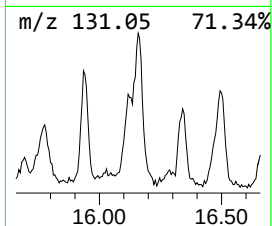
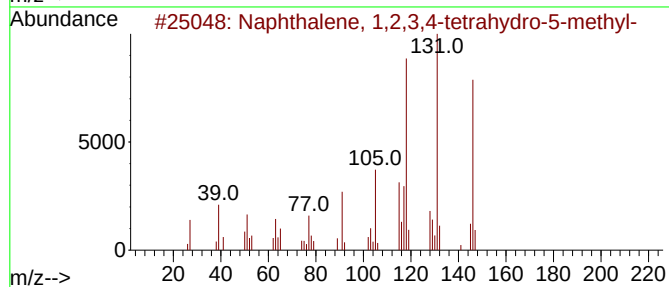
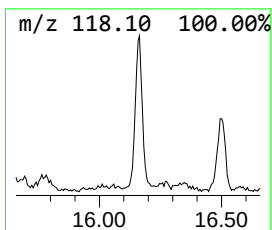
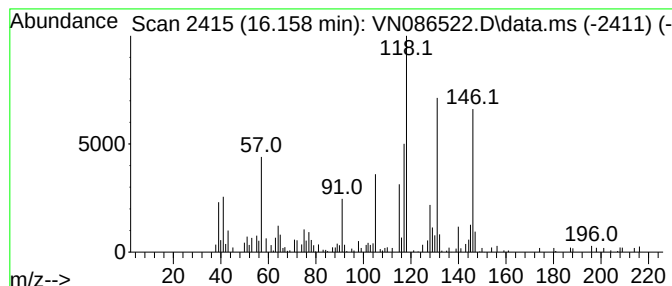
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.158	5.18 ug/l	140588	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	87
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	68
3			Benzeneacetaldehyde, .alpha.-eth...	146	C10H10O	004411-89-6	46
4			1-Methylindan-2-one	146	C10H10O	035587-60-1	45
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	43



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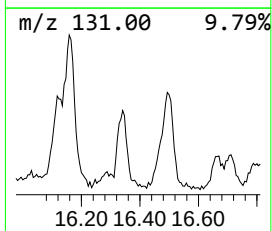
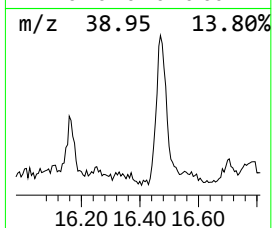
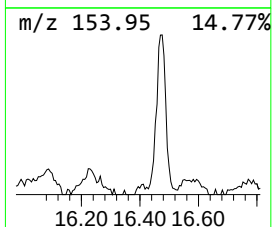
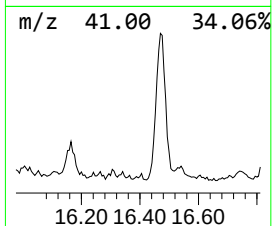
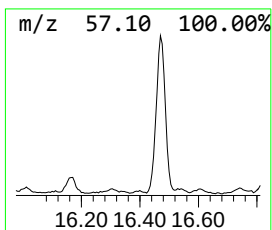
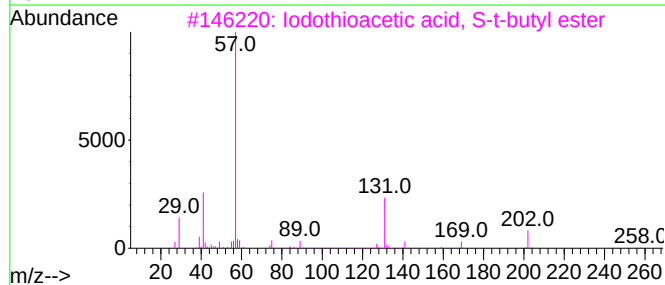
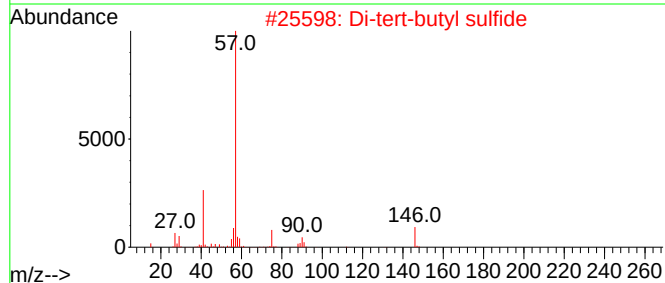
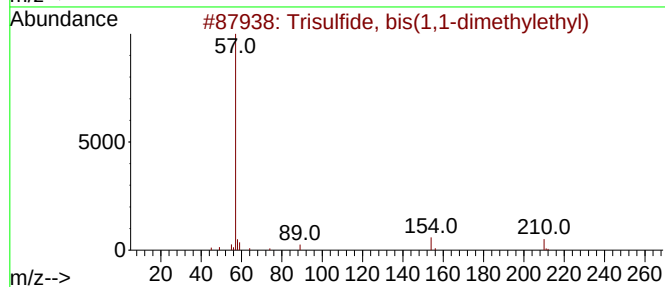
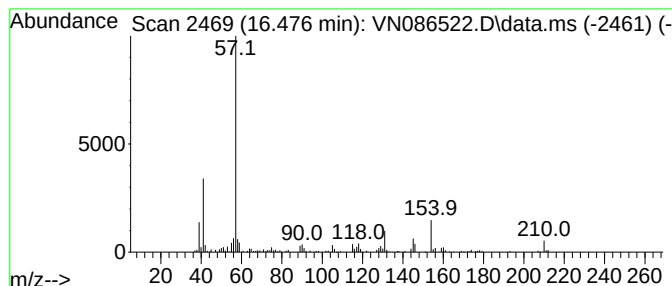
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown16.476 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	12.23 ug/l	332123	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	41
2			Di-tert-butyl sulfide	146	C8H18S	000107-47-1	35
3			Iodothioacetic acid, S-t-butyl e...	258	C6H11IOS	1010192-69-7	25
4			Boc-ON	246	C13H14N2O3	058632-95-4	16
5			Carbonic acid, bis(2-methylpropy...	174	C9H18O3	000539-92-4	16



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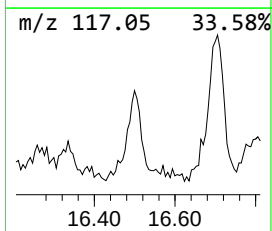
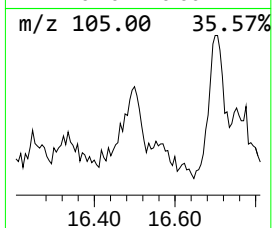
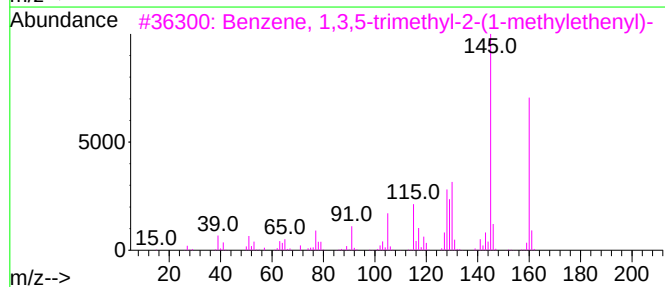
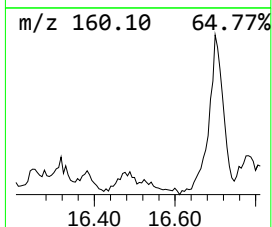
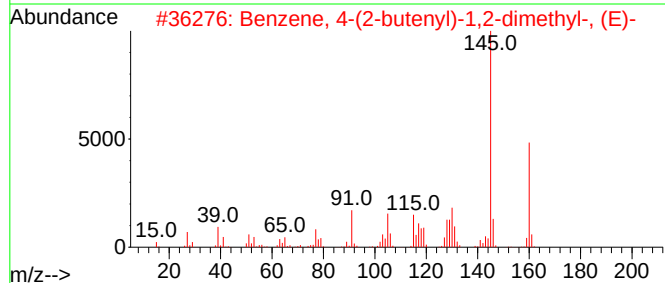
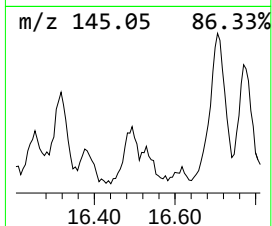
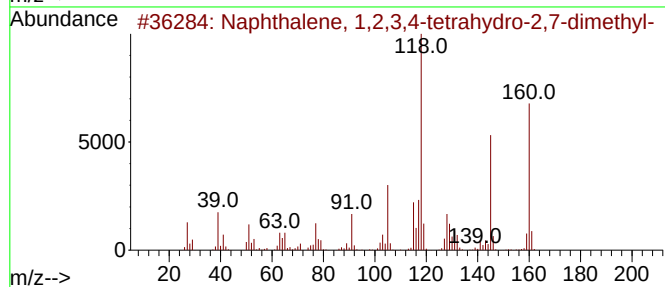
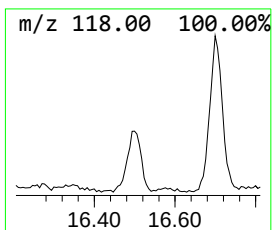
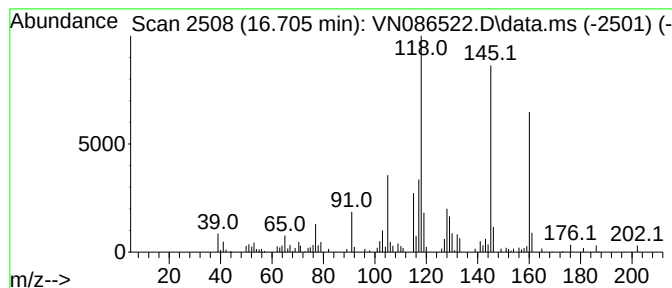
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	5.83 ug/l	158479	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	94
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	83
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	78
4			2,5-Dimethylbenzyl cyanide	145	C10H11N	016213-85-7	76
5			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050625\
Data File : VN086522.D
Acq On : 06 May 2025 18:12
Operator : JC\MD
Sample : Q1966-03 100X
Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SILICA-GEL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
Naphthalene, 1,...	12.465	101.3	ug/l	2475580	3	11.865	1222370	50.0
Naphthalene, 2,...	14.012	62.8	ug/l	1705610	4	13.788	1358150	50.0
Naphthalene, 1,...	15.635	8.7	ug/l	236275	4	13.788	1358150	50.0
Naphthalene, 1,...	16.158	5.2	ug/l	140588	4	13.788	1358150	50.0
unknown16.476	16.476	12.2	ug/l	332123	4	13.788	1358150	50.0
Naphthalene, 1,...	16.706	5.8	ug/l	158479	4	13.788	1358150	50.0