

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
 Data File : VN086980.D
 Acq On : 12 Jun 2025 16:17
 Operator : JC\MD
 Sample : Q2302-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 250611078-02-VOA

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: VN086980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.059	13	18	43	rVB	249939	705246	7.11%	1.506%
2	2.324	57	63	75	rBV	115225	210958	2.13%	0.450%
3	2.877	150	157	172	rVB2	87656	209703	2.11%	0.448%
4	4.441	410	423	449	rBV	244815	831435	8.38%	1.775%
5	5.541	592	610	644	rBV	2587851	9547190	96.22%	20.384%
6	7.447	919	934	951	rBV	3233240	9921821	100.00%	21.184%
7	7.847	985	1002	1023	rBV	1359864	3637945	36.67%	7.767%
8	8.177	1048	1058	1062	rBV	168409	388718	3.92%	0.830%
9	8.229	1062	1067	1078	rVB	270413	630807	6.36%	1.347%
10	8.588	1112	1128	1137	rBV4	207956	802814	8.09%	1.714%
11	8.671	1137	1142	1153	rVB3	150072	357605	3.60%	0.764%
12	8.971	1184	1193	1205	rBV	85882	195555	1.97%	0.418%
13	9.106	1207	1216	1230	rVB	455608	933807	9.41%	1.994%
14	10.447	1433	1444	1457	rBV3	37619	109814	1.11%	0.234%
15	10.570	1457	1465	1471	rVV	728923	1367593	13.78%	2.920%
16	10.635	1471	1476	1488	rVV2	264093	646468	6.52%	1.380%
17	11.170	1559	1567	1581	rVV	292631	561095	5.66%	1.198%
18	11.865	1677	1685	1695	rVV	608320	1261571	12.72%	2.694%
19	11.965	1695	1702	1711	rVV	323040	595946	6.01%	1.272%
20	12.070	1711	1720	1740	rVB	242437	527778	5.32%	1.127%
21	12.400	1769	1776	1787	rVB	163303	299941	3.02%	0.640%
22	12.694	1819	1826	1833	rBV2	49838	103423	1.04%	0.221%
23	12.847	1845	1852	1862	rVB	481147	860436	8.67%	1.837%
24	13.482	1953	1960	1971	rBV	103986	217096	2.19%	0.464%
25	13.606	1976	1981	1987	rBV2	75471	120674	1.22%	0.258%
26	13.729	1996	2002	2007	rBV	325965	510110	5.14%	1.089%
27	13.794	2007	2013	2019	rVV	626484	1196787	12.06%	2.555%
28	13.853	2019	2023	2034	rVB	378236	655910	6.61%	1.400%
29	13.994	2042	2047	2061	rVB2	49014	117070	1.18%	0.250%
30	14.253	2085	2091	2095	rBV2	187300	358409	3.61%	0.765%
31	14.294	2095	2098	2113	rVV	203487	412476	4.16%	0.881%
32	14.453	2116	2125	2133	rVB7	59755	162173	1.63%	0.346%
33	14.670	2150	2162	2170	rBV	1156424	2129874	21.47%	4.547%
34	14.947	2203	2209	2215	rBV6	57061	117903	1.19%	0.252%
35	15.100	2229	2235	2243	rVV	198660	361731	3.65%	0.772%
36	15.282	2257	2266	2267	rBV3	163685	395989	3.99%	0.845%

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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

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Title : SW846 8260

37	15.323	2267	2273	2278	rBV	1708231	3283254	33.09%	7.010%
38	15.517	2300	2306	2317	rBV	344022	725639	7.31%	1.549%
39	15.635	2320	2326	2334	rVB	387604	774422	7.81%	1.653%
40	16.005	2382	2389	2401	rVB	257209	590147	5.95%	1.260%

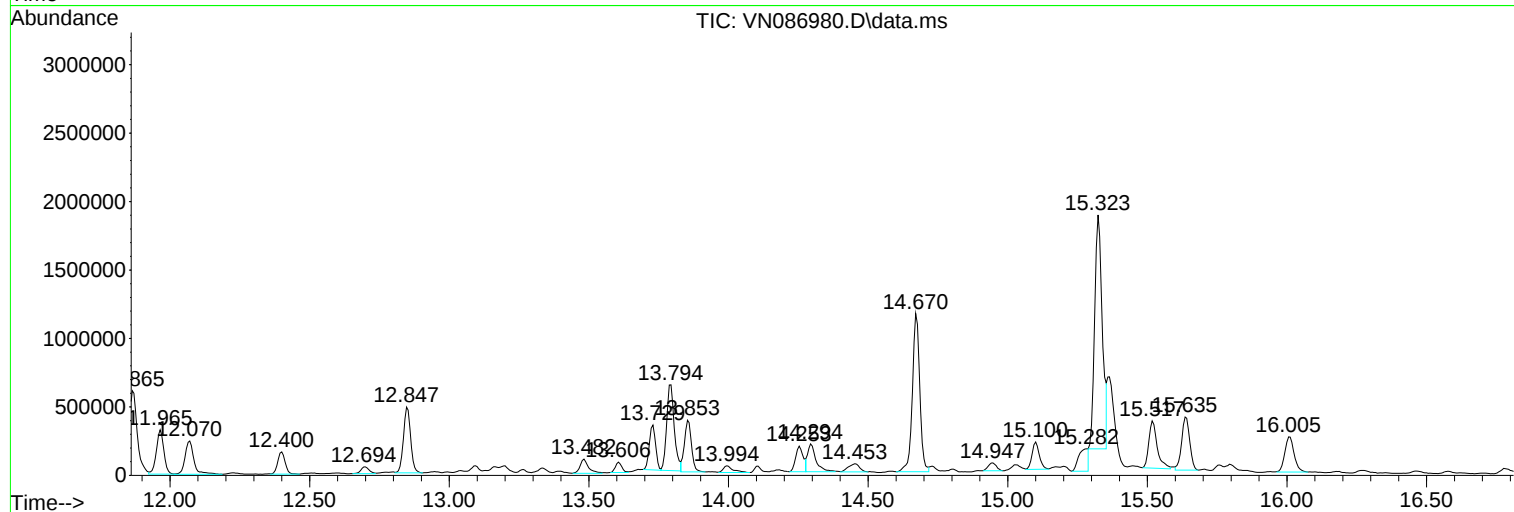
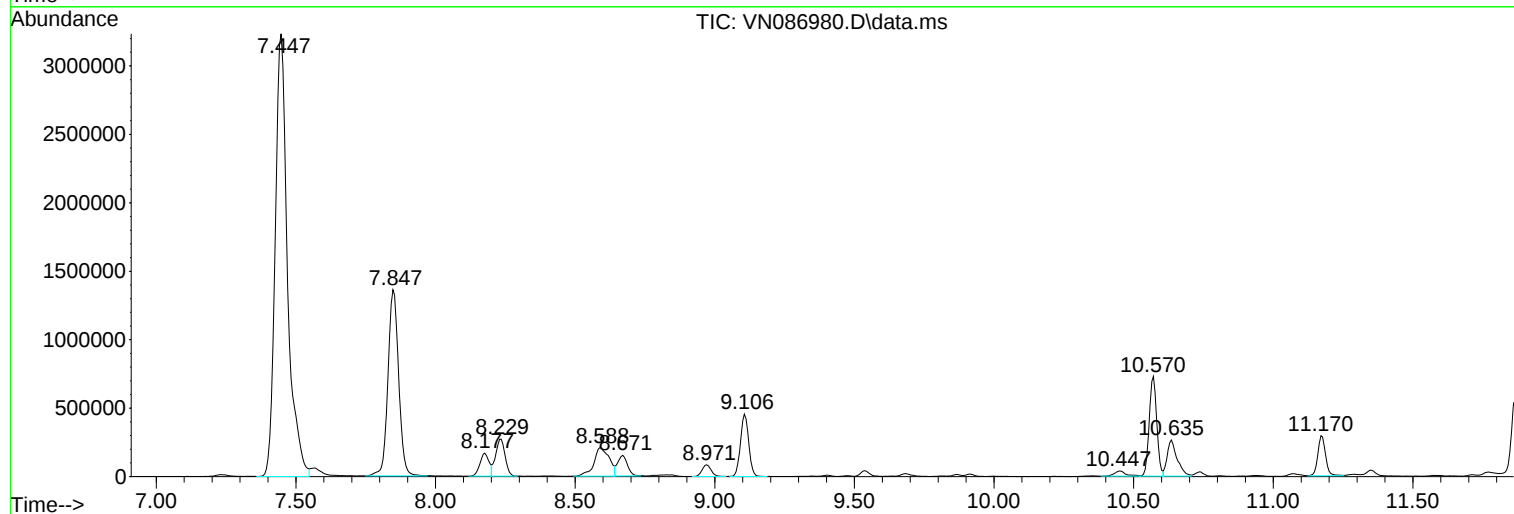
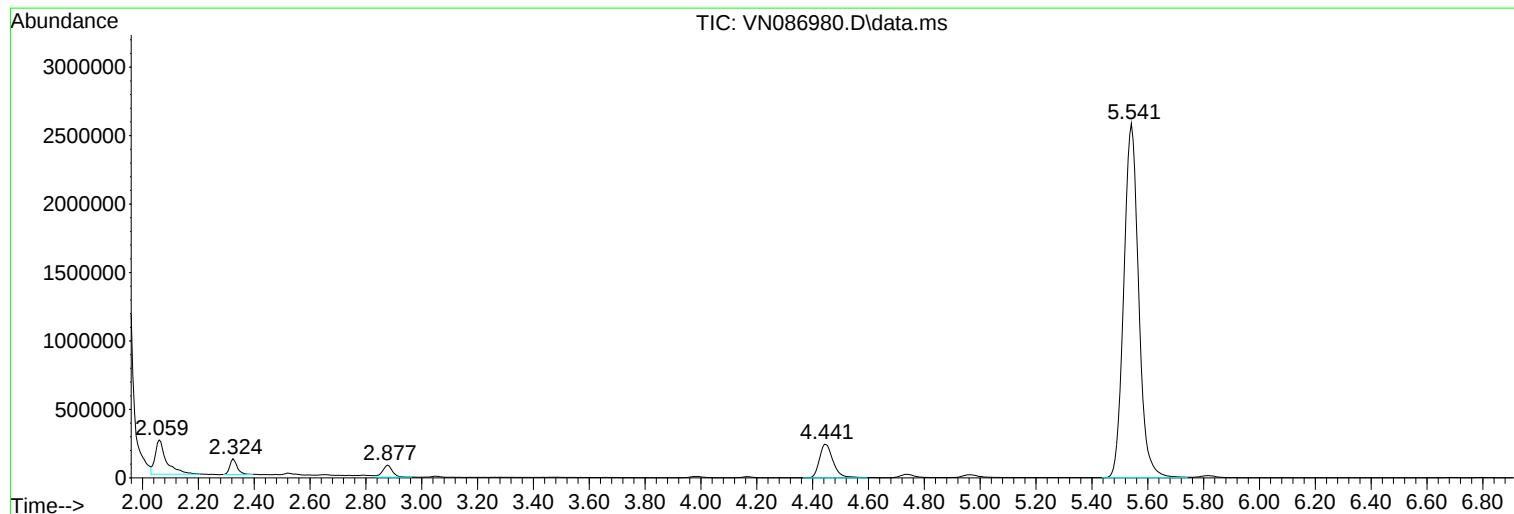
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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MSVOA_N
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250611078-02-VOA

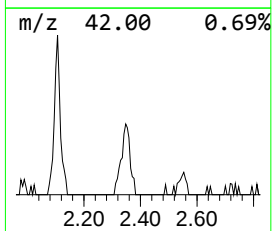
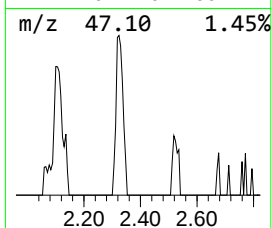
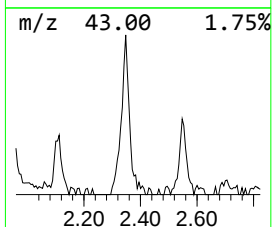
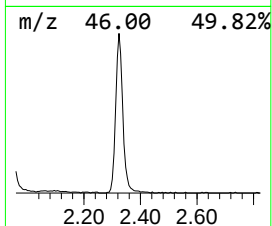
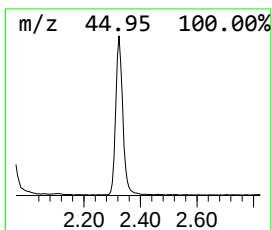
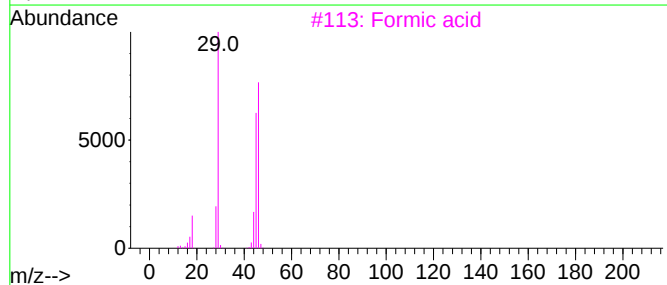
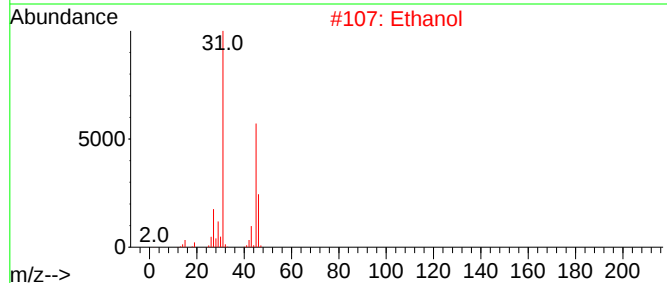
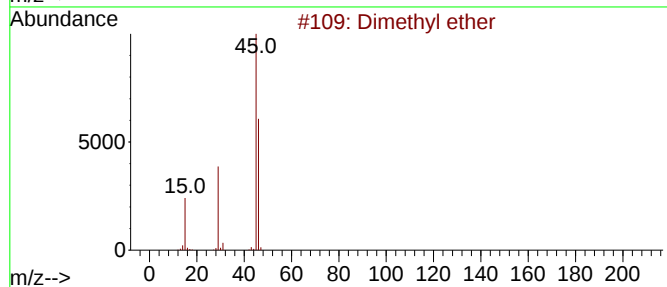
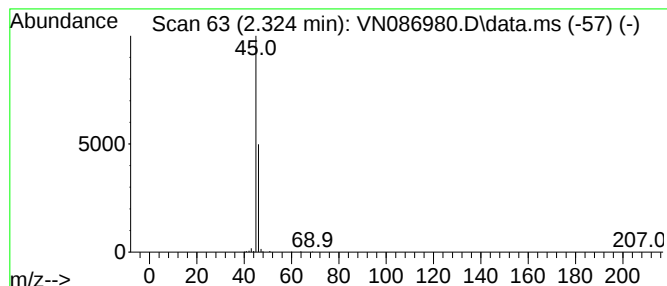
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 Dimethyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.324	16.72 ug/l	210958	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
250611078-02-VOA

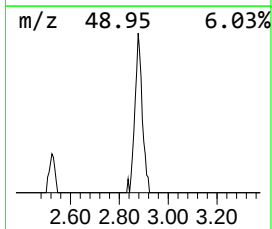
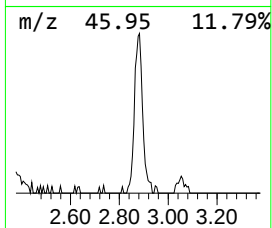
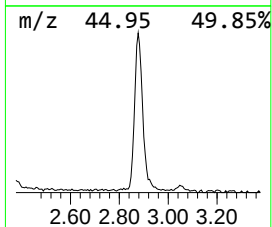
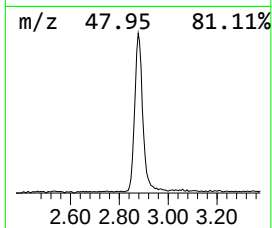
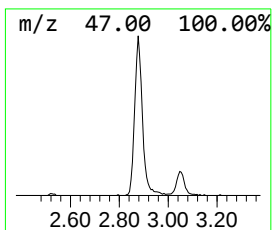
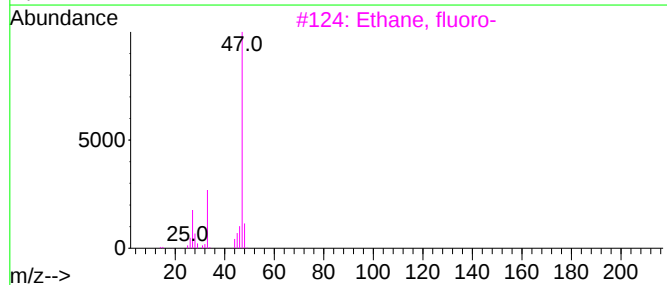
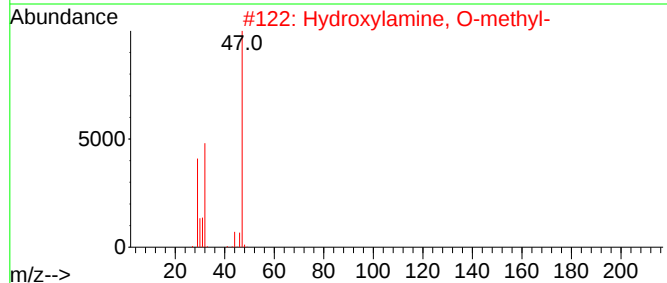
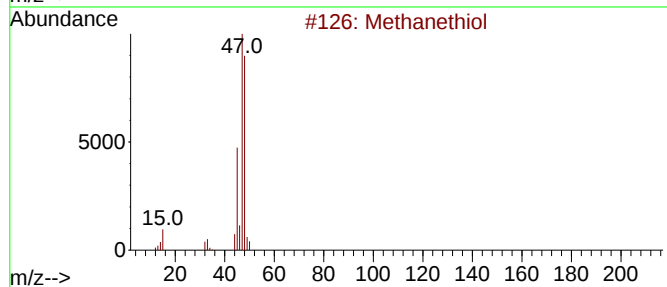
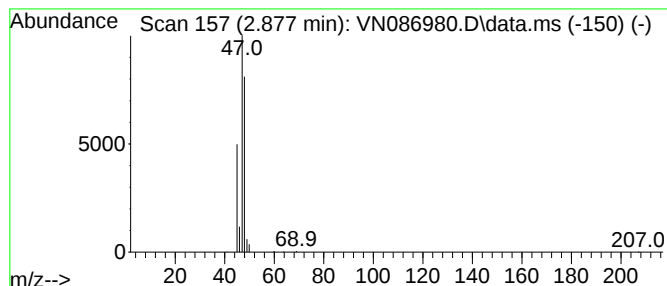
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 3 Methanethiol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.877	16.62 ug/l	209703	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4
3			Ethane, fluoro-	48	C2H5F	000353-36-6	4
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Tetraborane(10)	54	B4H10	018283-93-7	2



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Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

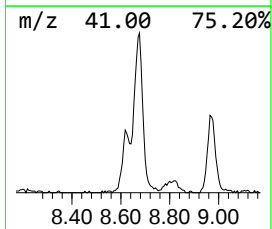
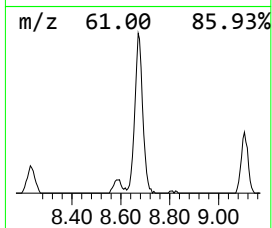
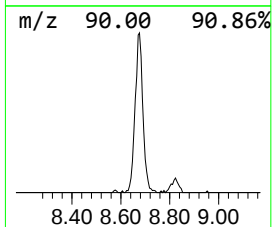
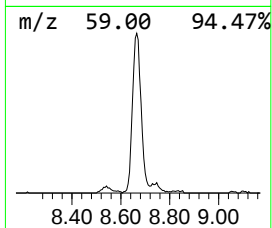
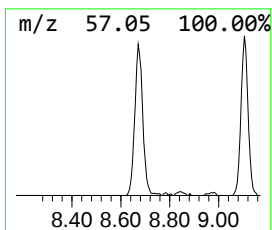
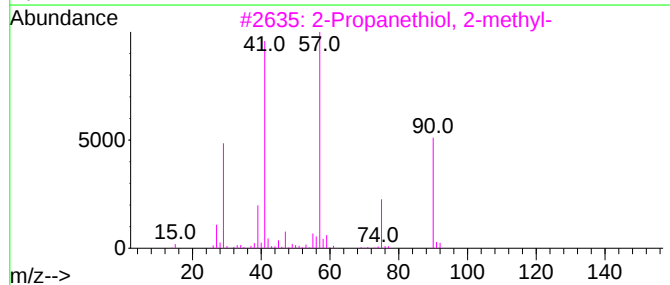
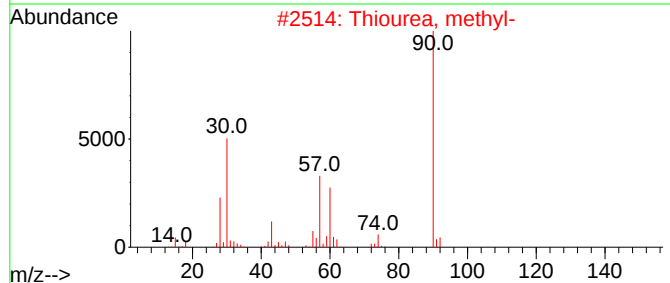
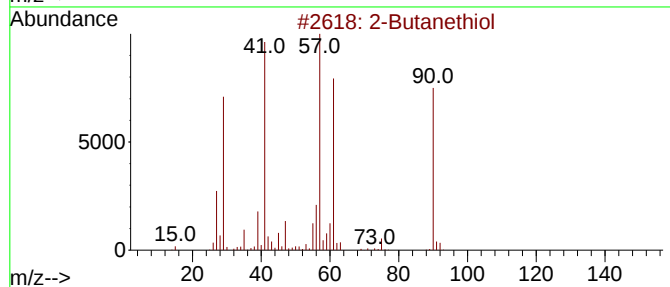
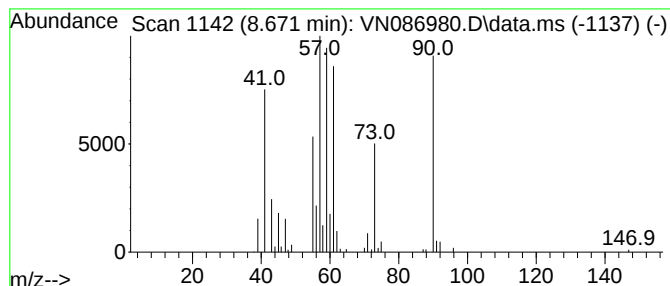
Instrument :
MSVOA_N
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250611078-02-VOA

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 2-Butanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.671	19.15 ug/l	357605	1,4-Difluorobenzene	9.106	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanethiol	90	C4H10S	000513-53-1	76
2	Thiourea, methyl-	90	C2H6N2S	000598-52-7	43
3	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	38
4	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
5	2,3-Dimercaptopropan-1-ol	124	C3H8OS2	000059-52-9	36



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Instrument :
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ClientSampleId :
250611078-02-VOA

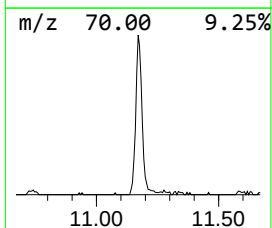
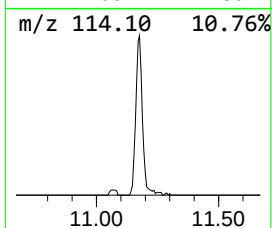
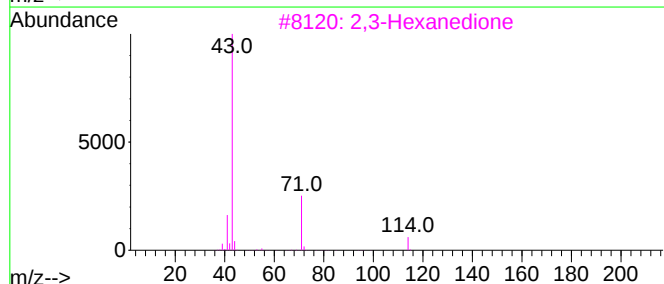
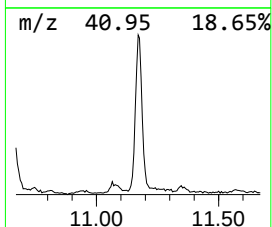
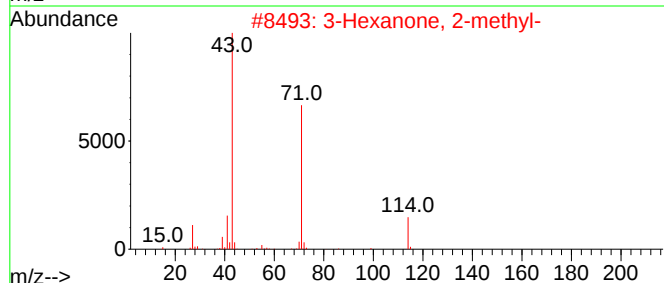
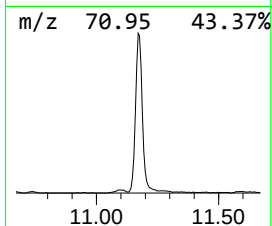
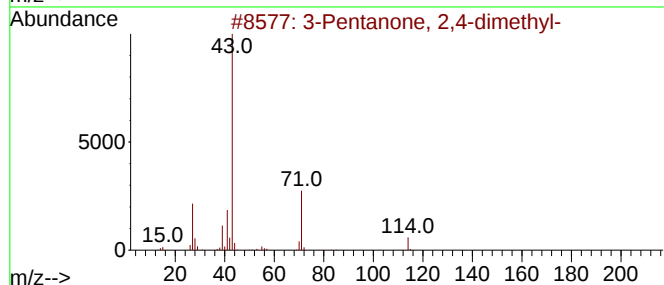
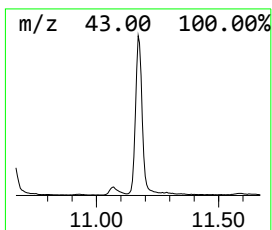
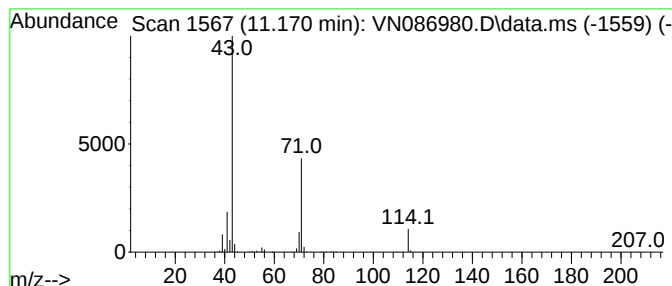
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Quant Title : SW846 8260

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

Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	22.24 ug/l	561095	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	72
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4			4-Heptanone	114	C7H14O	000123-19-3	53
5			Pyrrolidine	71	C4H9N	000123-75-1	53



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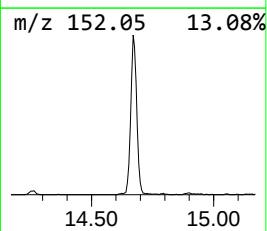
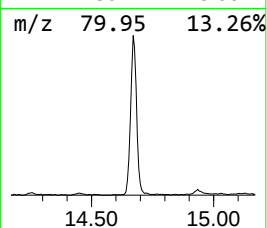
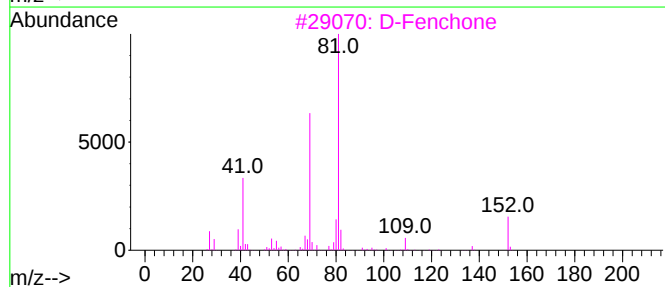
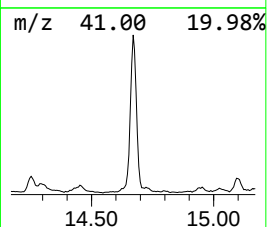
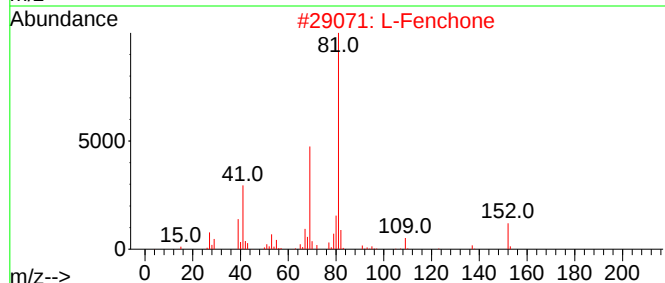
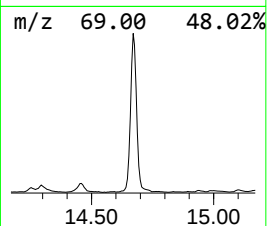
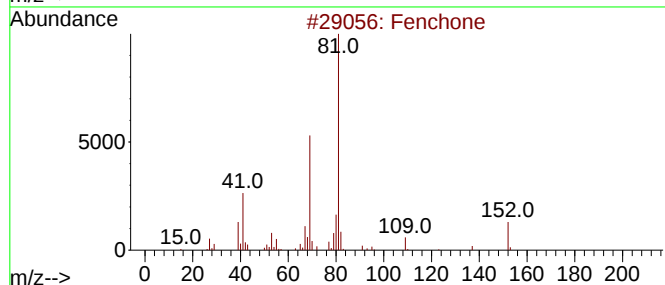
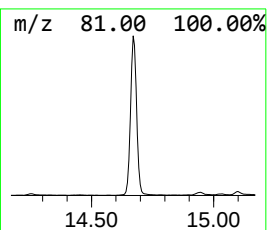
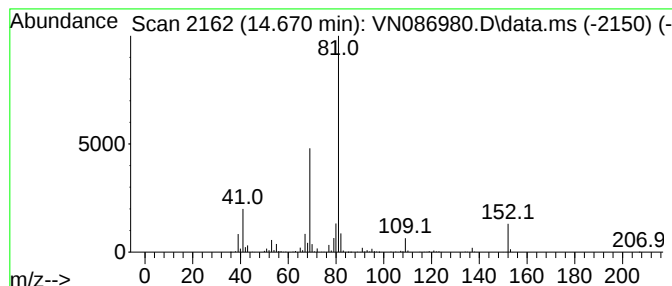
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Quant Title : SW846 8260

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

Peak Number 7 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	88.98 ug/l	2129870	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			2-Cycloocten-1-one	124	C8H12O	001728-25-2	64
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086980.D
Acq On : 12 Jun 2025 16:17
Operator : JC\MD
Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
250611078-02-VOA

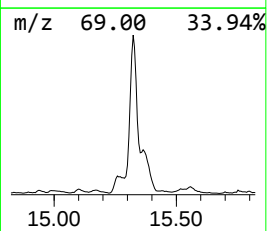
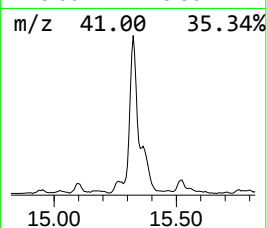
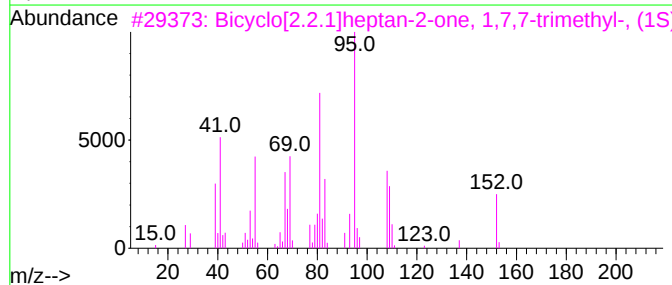
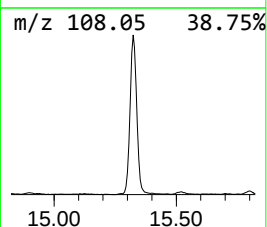
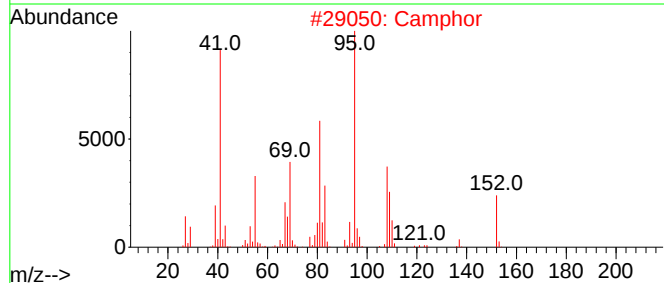
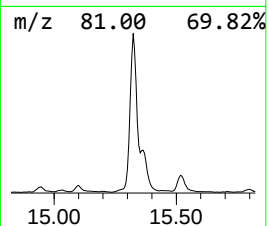
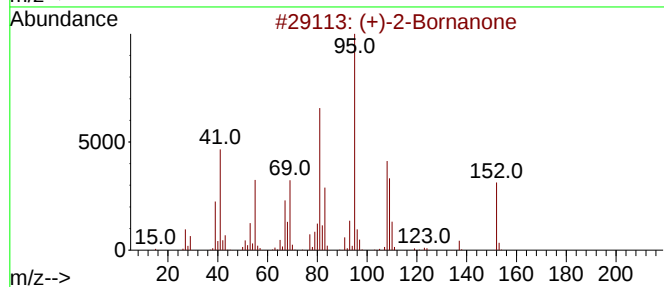
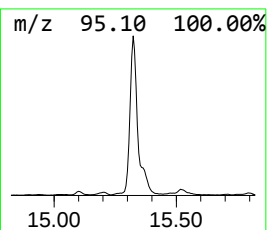
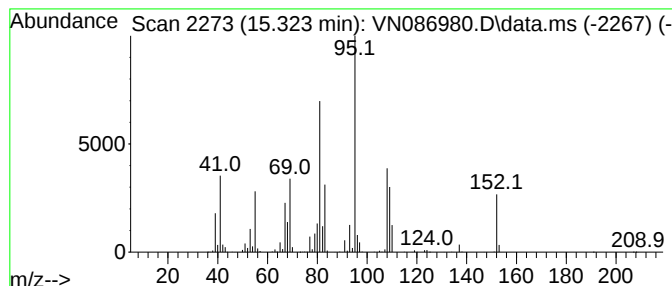
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Quant Title : SW846 8260

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

Peak Number 8 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	137.17 ug/l	3283250	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2			Camphor	152	C10H16O	000076-22-2	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	43
5			1-Adamantanol	152	C10H16O	000768-95-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086980.D
Acq On : 12 Jun 2025 16:17
Operator : JC\MD
Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
250611078-02-VOA

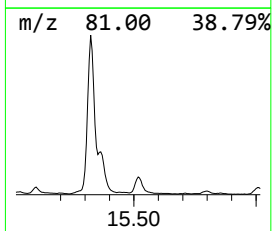
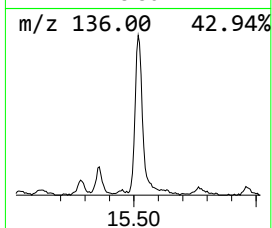
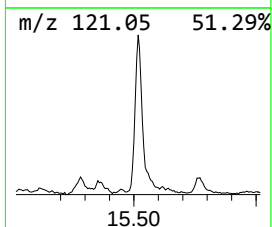
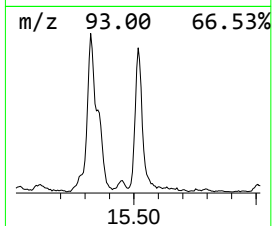
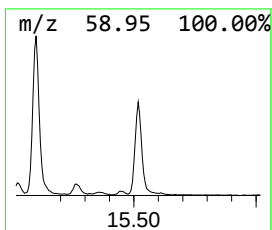
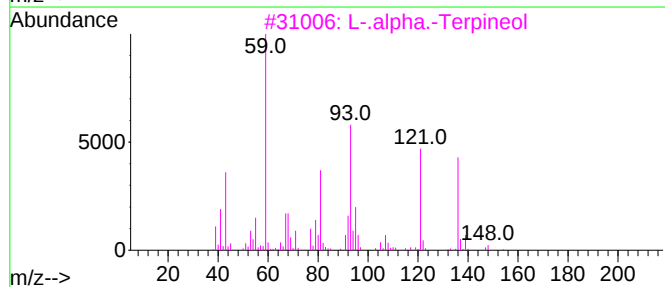
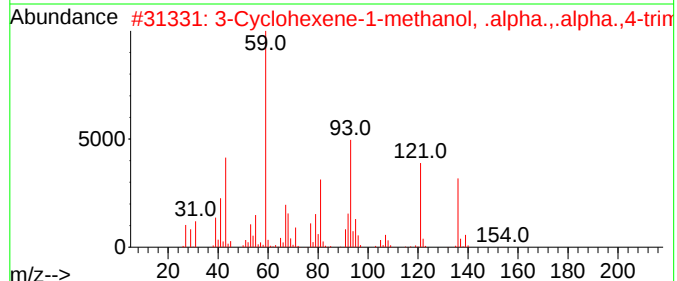
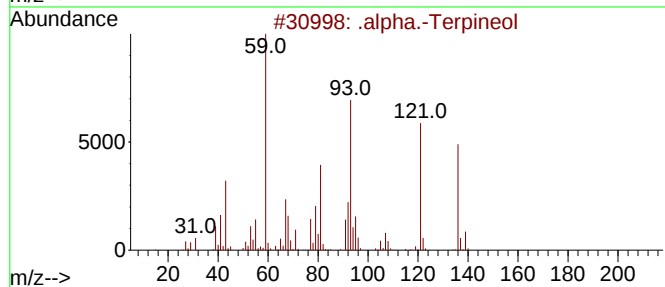
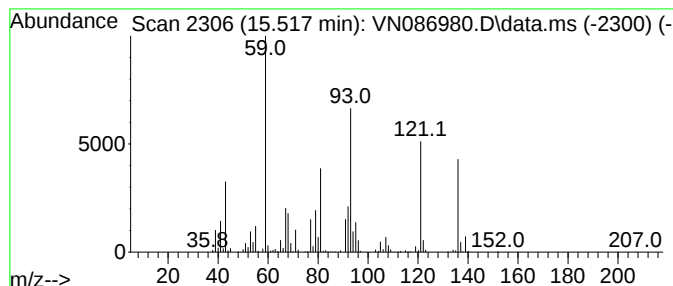
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Quant Title : SW846 8260

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

Peak Number 9 .alpha.-Terpineol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.517	30.32 ug/l	725639	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	91
2			3-Cyclohexene-1-methanol, .alpha...	154	C10H18O	007785-53-7	91
3			L-.alpha.-Terpineol	154	C10H18O	010482-56-1	64
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	50
5			Cyclohexane, 1-methylene-4-(1-me...	136	C10H16	000499-97-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086980.D
Acq On : 12 Jun 2025 16:17
Operator : JC\MD
Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
250611078-02-VOA

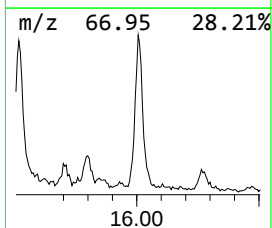
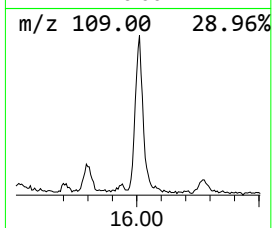
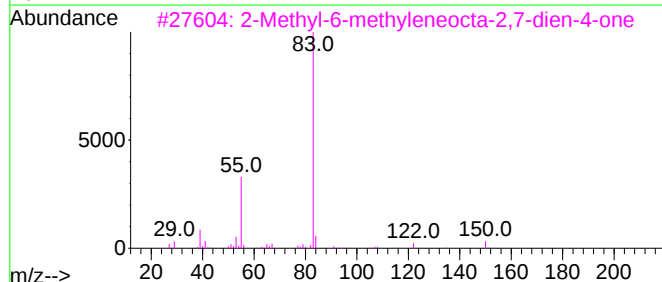
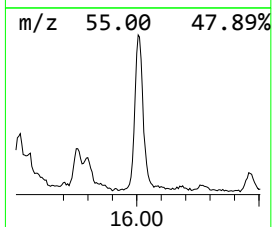
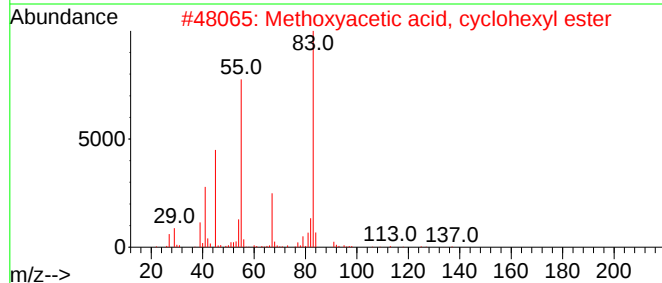
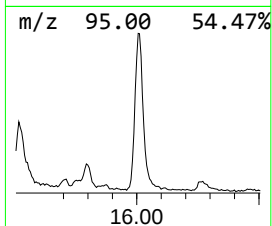
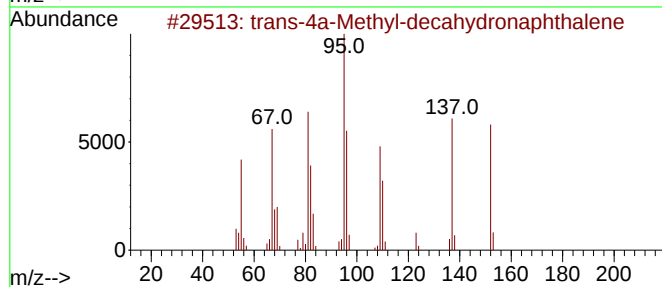
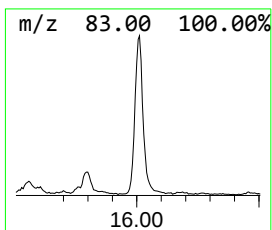
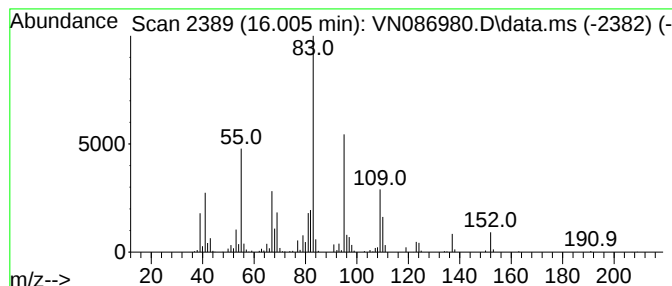
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.005 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.005	24.66 ug/l	590147	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
2			Methoxyacetic acid, cyclohexyl e...	172	C9H16O3	1000282-69-4	38
3			2-Methyl-6-methyleneocta-2,7-die...	150	C10H14O	000539-70-8	30
4			Cyclohexane, azido-	125	C6H11N3	019573-22-9	30
5			Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086980.D
Acq On : 12 Jun 2025 16:17
Operator : JC\MD
Sample : Q2302-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
250611078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.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
Dimethyl ether	2.324	16.7	ug/l	210958	1	8.235	630807	50.0
Methanethiol	2.877	16.6	ug/l	209703	1	8.235	630807	50.0
2-Butanethiol	8.671	19.1	ug/l	357605	2	9.106	933807	50.0
3-Pentanone, 2,...	11.171	22.2	ug/l	561095	3	11.865	1261570	50.0
Fenchone	14.670	89.0	ug/l	2129870	4	13.794	1196790	50.0
(+)-2-Bornanone	15.323	137.2	ug/l	3283250	4	13.794	1196790	50.0
.alpha.-Terpineol	15.517	30.3	ug/l	725639	4	13.794	1196790	50.0
unknown16.005	16.005	24.7	ug/l	590147	4	13.794	1196790	50.0