

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
 Data File : VX046951.D
 Acq On : 10 Jul 2025 17:34
 Operator : JC/MD
 Sample : Q2554-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 250709071-01 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_X\Method\82X070225W.M
 Title : SW846 8260

Signal : TIC: VX046951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.136	5	8	26	rVB	565304	1053689	12.22%	2.158%
2	1.270	27	30	42	rVB	533071	639129	7.41%	1.309%
3	1.374	42	47	52	rBV3	41805	109811	1.27%	0.225%
4	1.569	74	79	87	rBV	224303	365686	4.24%	0.749%
5	2.148	170	174	184	rVB2	48806	125956	1.46%	0.258%
6	2.386	206	213	220	rBV	1521858	2861222	33.17%	5.859%
7	2.532	231	237	252	rBV	329692	674737	7.82%	1.382%
8	2.953	297	306	328	rBV	1182578	3452377	40.03%	7.069%
9	4.562	553	570	612	rBV2	2578747	8625375	100.00%	17.662%
10	5.001	630	642	682	rBV3	862960	3239610	37.56%	6.634%
11	5.397	696	707	722	rBV2	250536	779991	9.04%	1.597%
12	5.562	724	734	755	rVB2	403968	1253084	14.53%	2.566%
13	5.964	790	800	808	rBV2	282562	793489	9.20%	1.625%
14	6.080	808	819	837	rVV3	392644	1424613	16.52%	2.917%
15	6.769	923	932	952	rVV	686410	1765719	20.47%	3.616%
16	8.574	1221	1228	1234	rBV	69329	135661	1.57%	0.278%
17	8.647	1234	1240	1247	rVV	1521191	2480604	28.76%	5.079%
18	8.720	1247	1252	1261	rVV	247133	425023	4.93%	0.870%
19	8.805	1261	1266	1270	rVV2	50543	88974	1.03%	0.182%
20	9.378	1353	1360	1368	rBV	236584	381393	4.42%	0.781%
21	10.055	1461	1471	1483	rBV	1633783	2426574	28.13%	4.969%
22	10.195	1490	1494	1504	rVV	337466	514874	5.97%	1.054%
23	10.299	1504	1511	1518	rVV	348195	498918	5.78%	1.022%
24	10.640	1563	1567	1573	rBV	210680	281201	3.26%	0.576%
25	10.768	1580	1588	1596	rBV	60488	117833	1.37%	0.241%
26	10.957	1613	1619	1625	rVB	75958	125441	1.45%	0.257%
27	11.079	1633	1639	1645	rBV	1370972	1784416	20.69%	3.654%
28	11.378	1682	1688	1694	rBV3	51866	100729	1.17%	0.206%
29	11.457	1694	1701	1703	rBV2	60493	92891	1.08%	0.190%
30	11.610	1722	1726	1735	rVB	59403	94665	1.10%	0.194%
31	11.750	1745	1749	1753	rVB	139947	162871	1.89%	0.334%
32	11.884	1767	1771	1779	rVB2	123833	163252	1.89%	0.334%
33	12.018	1787	1793	1800	rBV2	1880462	2638492	30.59%	5.403%
34	12.097	1800	1806	1811	rBV2	212633	336114	3.90%	0.688%
35	12.213	1821	1825	1828	rBV	311163	426424	4.94%	0.873%
36	12.420	1853	1859	1863	rBV3	73590	111057	1.29%	0.227%

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

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37	12.542	1872	1879	1881	rBV5	40658	93174	1.08%	0.191%
38	12.573	1881	1884	1889	rVB	197413	252493	2.93%	0.517%
39	12.762	1910	1915	1920	rVB2	145938	209004	2.42%	0.428%
40	12.902	1931	1938	1944	rBV	873309	1156720	13.41%	2.369%
41	12.963	1944	1948	1958	rVB3	103901	180037	2.09%	0.369%
42	13.286	1995	2001	2005	rVV4	89248	139075	1.61%	0.285%
43	13.335	2005	2009	2014	rVV	222863	309403	3.59%	0.634%
44	13.420	2019	2023	2027	rVB2	81114	109927	1.27%	0.225%
45	13.475	2027	2032	2033	rBV2	171246	236884	2.75%	0.485%
46	13.506	2033	2037	2045	rVV	1310504	1842654	21.36%	3.773%
47	13.585	2045	2050	2059	rVV3	677182	1060017	12.29%	2.171%
48	13.658	2059	2062	2069	rVV3	54529	105505	1.22%	0.216%
49	13.725	2069	2073	2077	rVV2	262111	349919	4.06%	0.717%
50	13.774	2077	2081	2089	rVB	1248162	1559506	18.08%	3.193%
51	13.920	2100	2105	2112	rBV5	51835	105630	1.22%	0.216%
52	14.097	2128	2134	2145	rBV2	137560	248579	2.88%	0.509%
53	14.633	2219	2222	2231	rVB	138826	195609	2.27%	0.401%
54	14.780	2239	2246	2252	rVB2	92141	130670	1.51%	0.268%

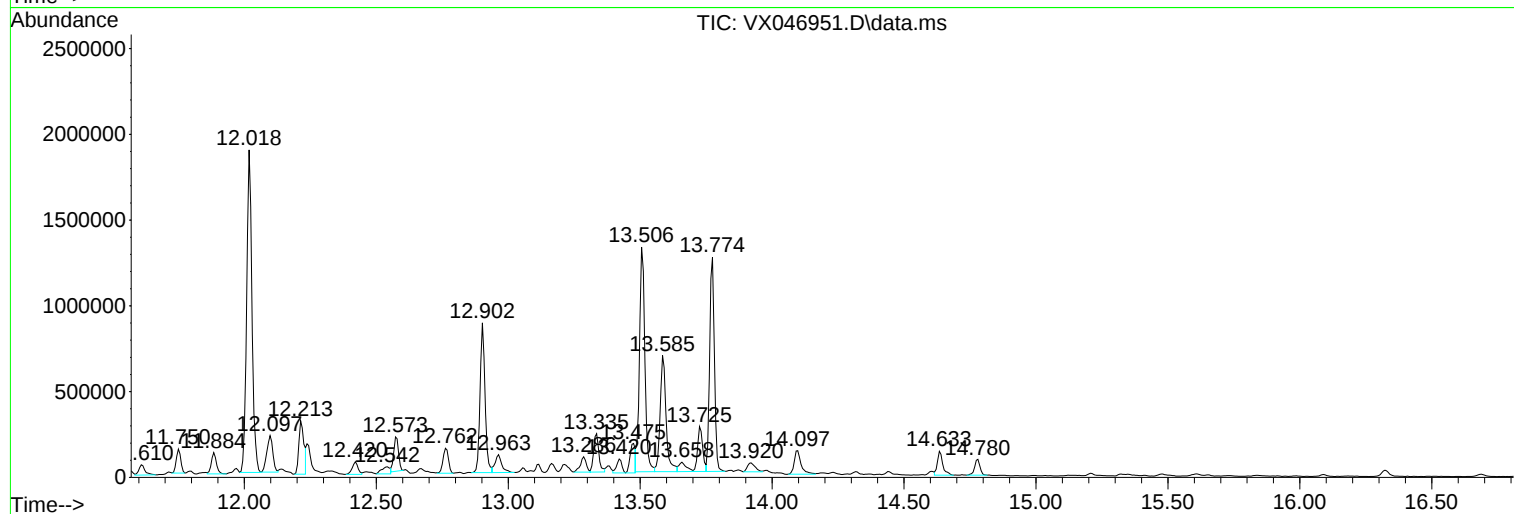
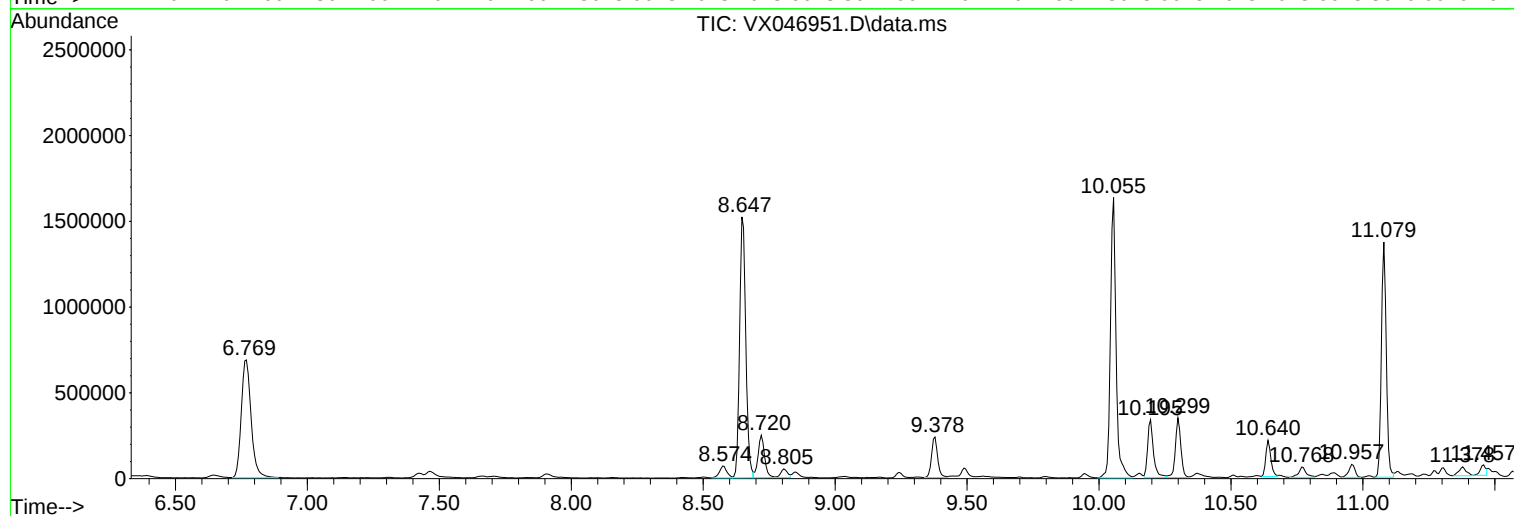
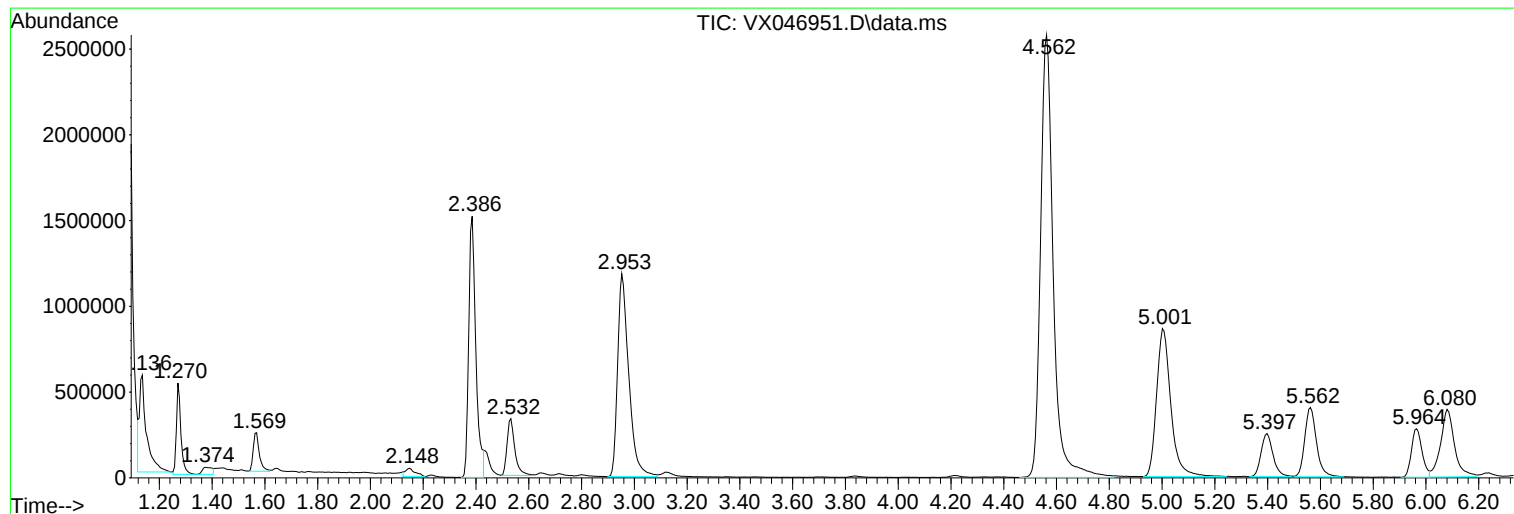
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Quant Title : SW846 8260

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



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MSVOA_X
ClientSampleId :
250709071-01 VOA

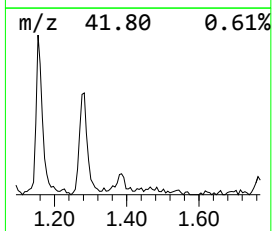
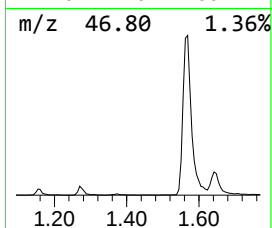
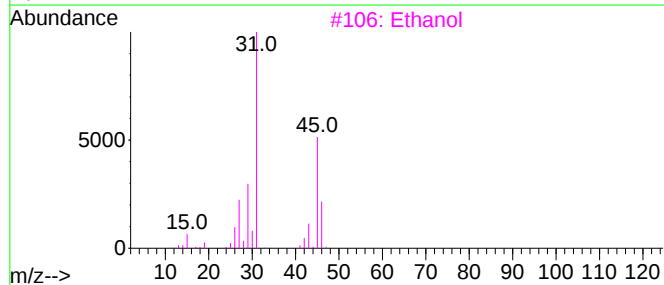
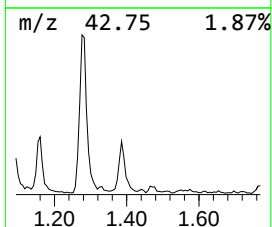
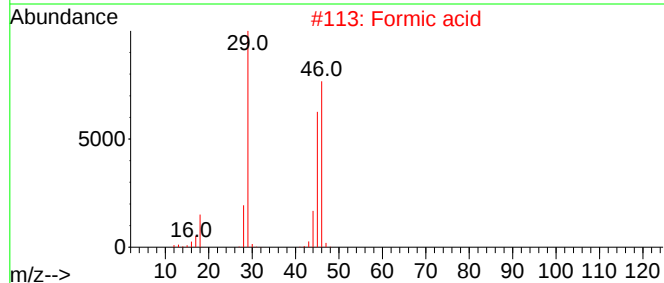
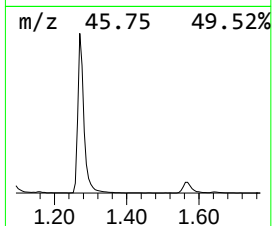
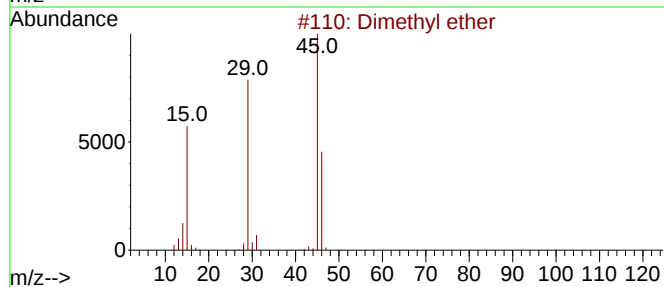
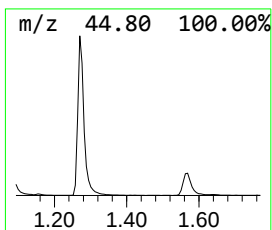
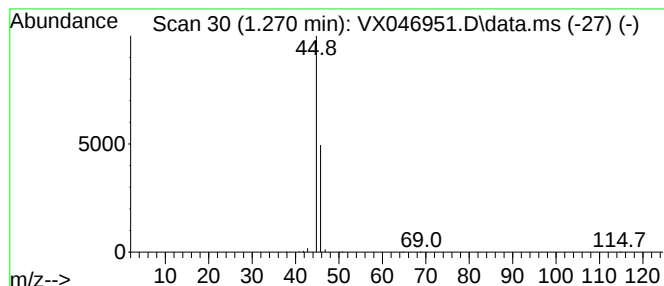
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 2 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	25.50 ug/l	639129	Pentafluorobenzene	5.562

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



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Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

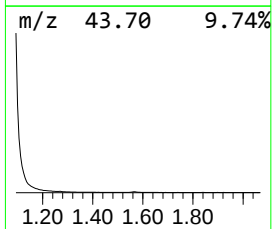
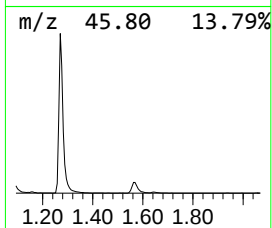
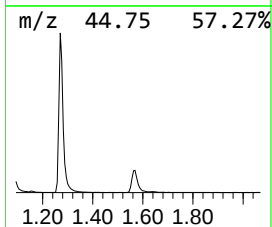
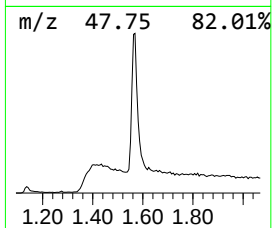
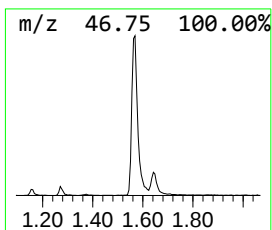
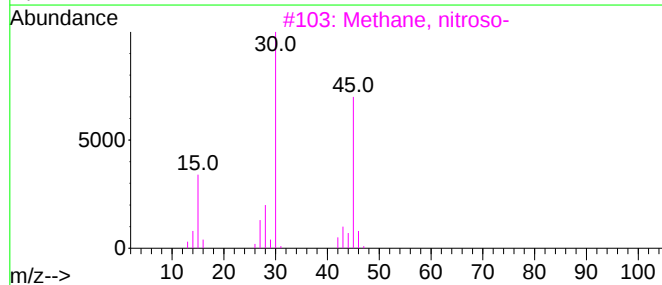
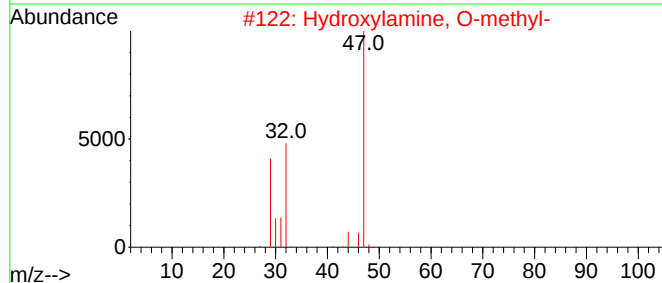
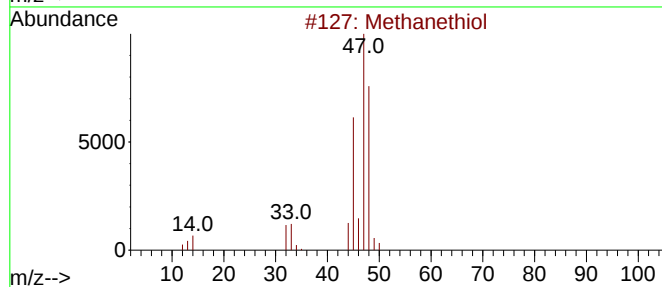
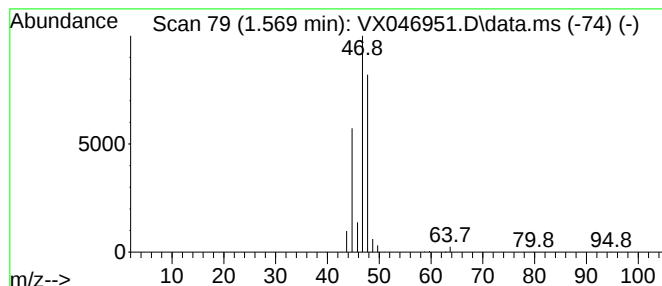
Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 3 Methanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.569	14.59 ug/l	365686	Pentafluorobenzene	5.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
3	Methane, nitroso-	45	CH3NO	000865-40-7	5
4	Formamide	45	CH3NO	000075-12-7	4
5	Nitrous acid	47	HNO2	007782-77-6	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

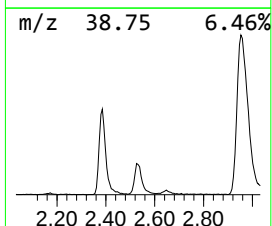
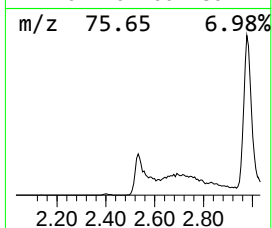
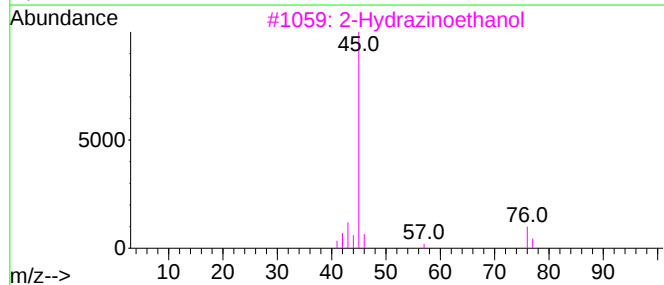
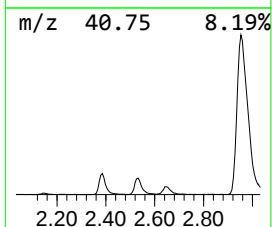
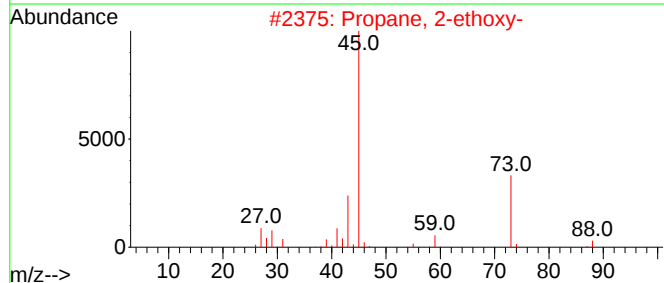
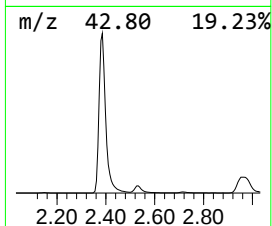
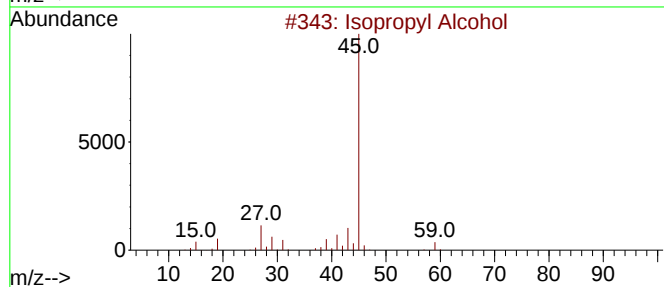
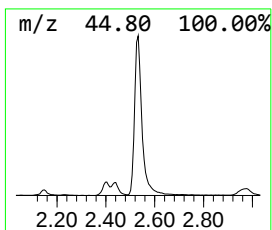
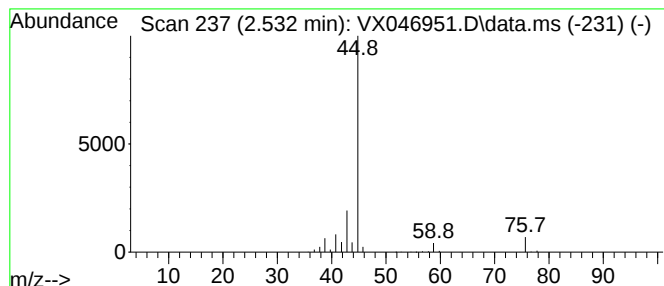
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	26.92 ug/l	674737	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3			2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
4			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
5			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

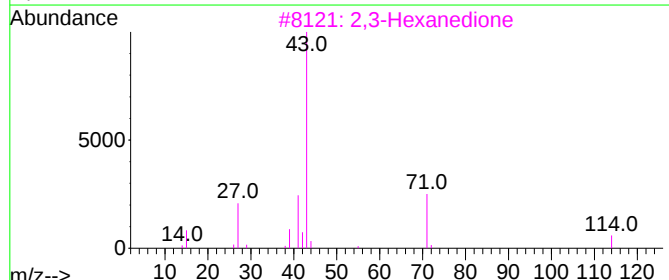
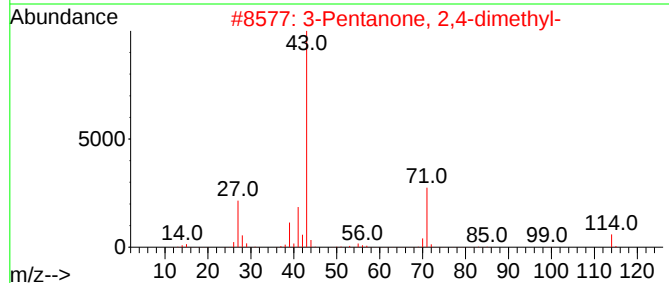
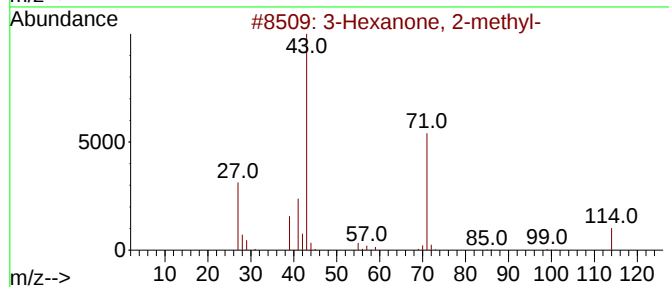
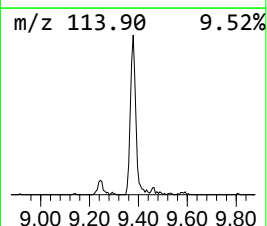
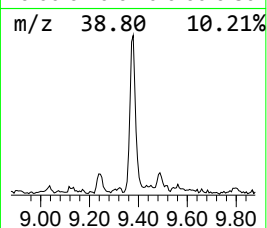
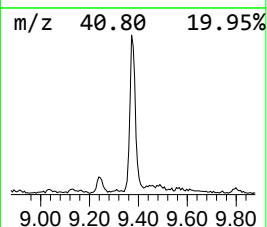
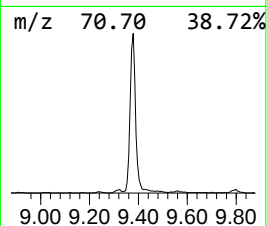
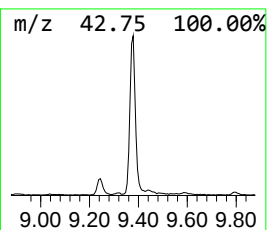
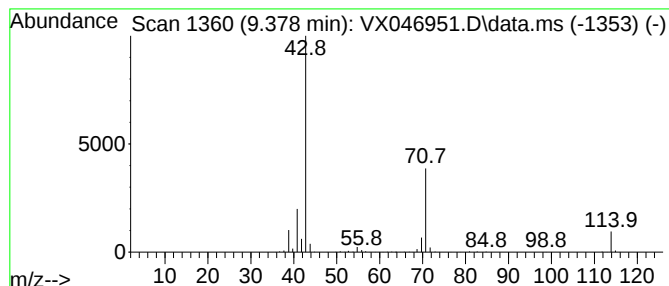
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 5 3-Hexanone, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	7.86 ug/l	381393	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	90
2			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	86
4			4-Heptanone	114	C7H14O	000123-19-3	59
5			Pyrrolidine	71	C4H9N	000123-75-1	59



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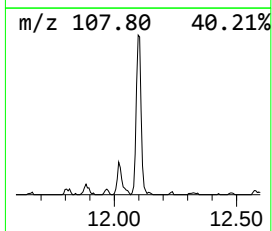
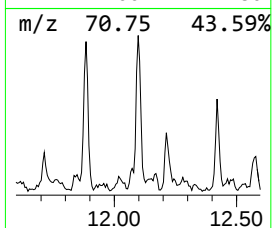
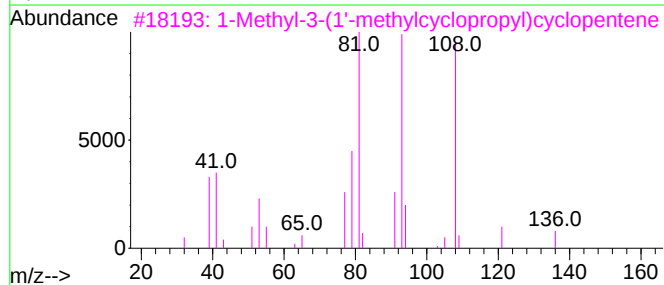
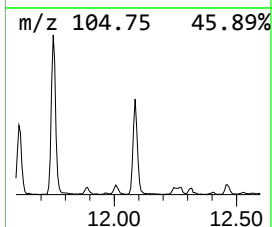
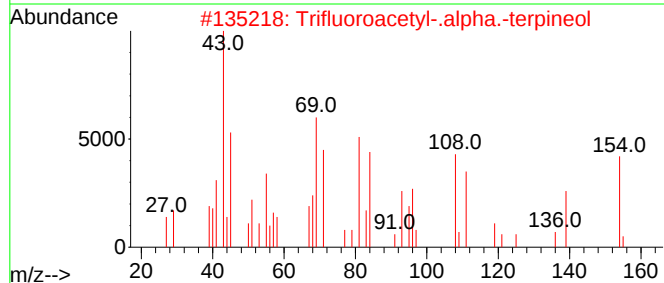
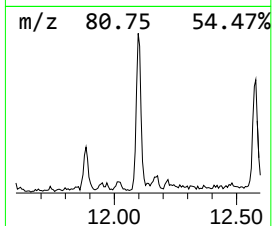
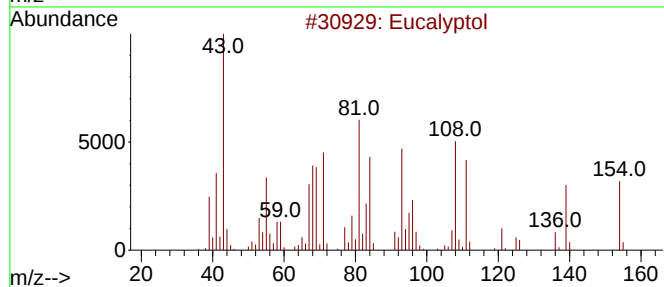
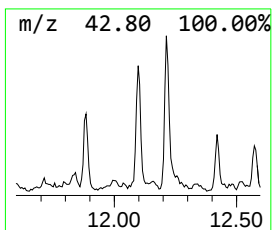
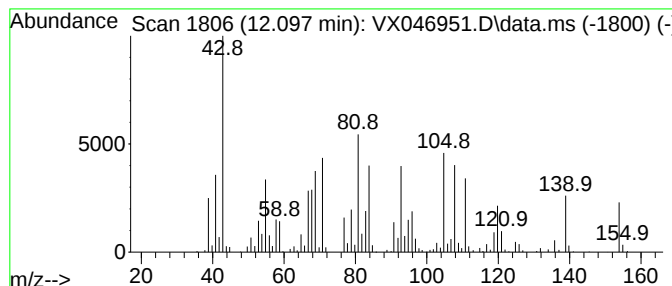
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Quant Title : SW846 8260

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

Peak Number 6 Eucalyptol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	6.37 ug/l	336114	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	38
3			1-Methyl-3-(1'-methylcyclopropyl)...	136	C10H16	103240-53-5	35
4			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	22
5			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

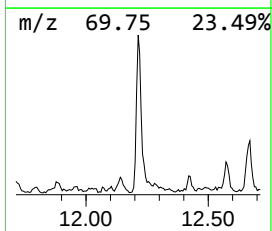
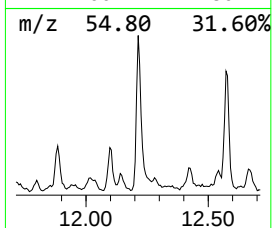
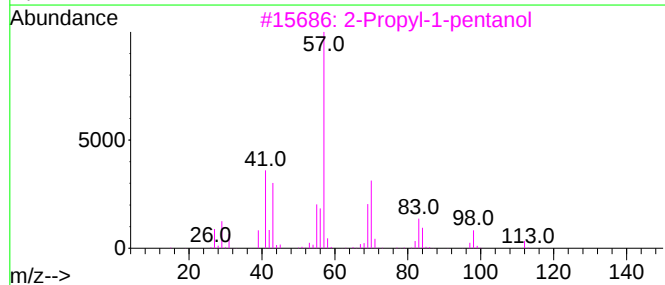
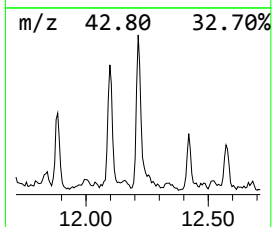
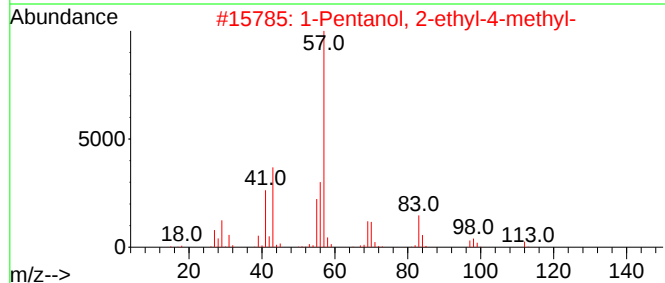
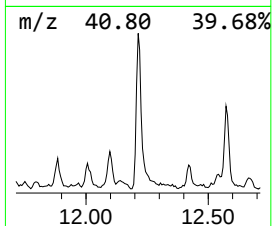
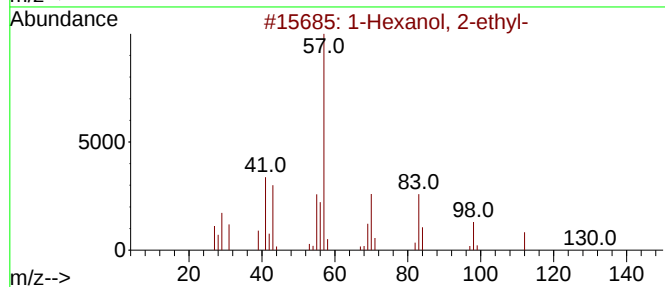
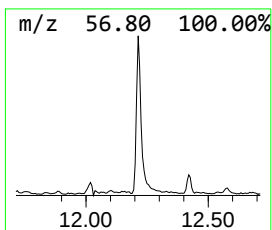
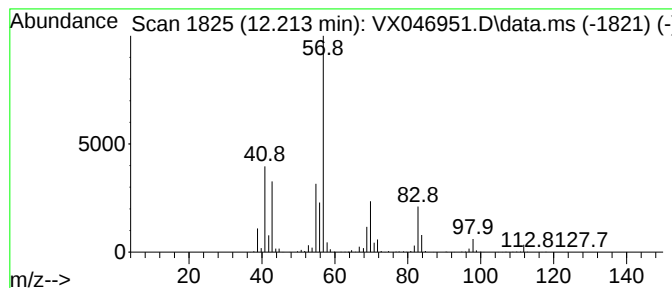
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	8.08 ug/l	426424	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

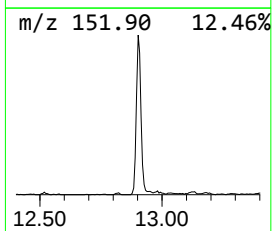
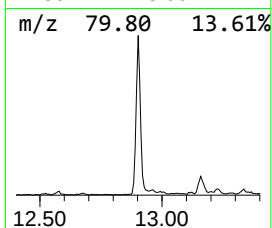
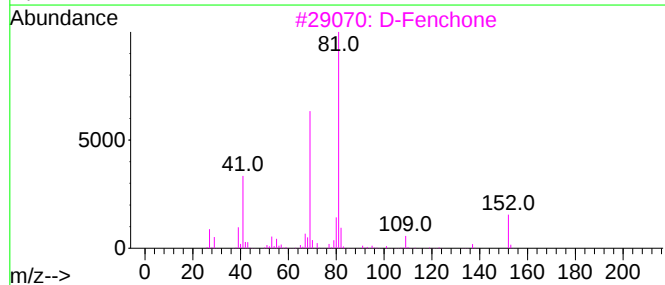
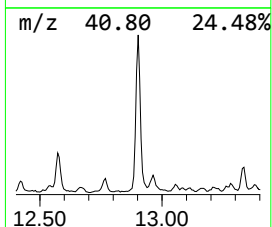
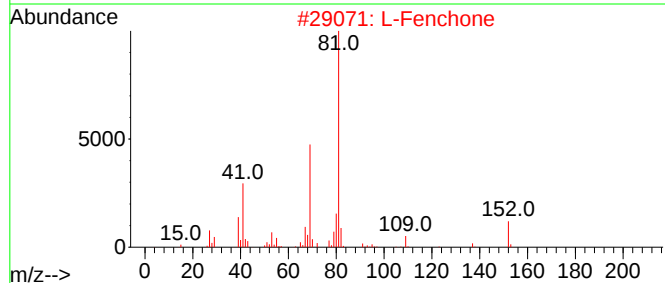
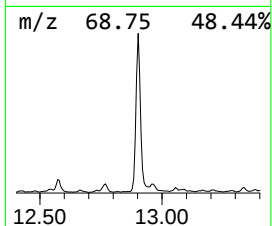
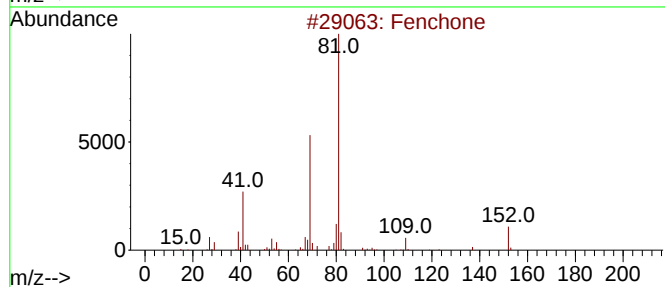
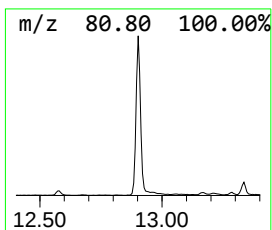
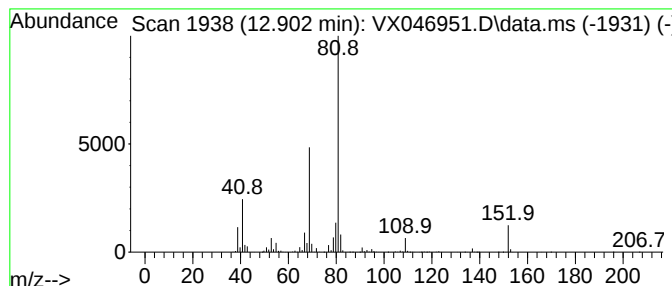
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Quant Title : SW846 8260

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

Peak Number 8 Fenchone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	21.92 ug/l	1156720	1,4-Dichlorobenzene-d4	12.018

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	95
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5			Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

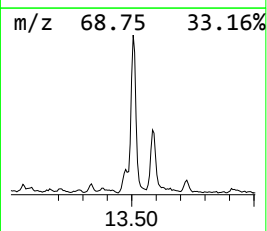
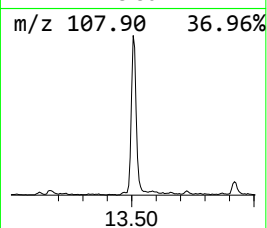
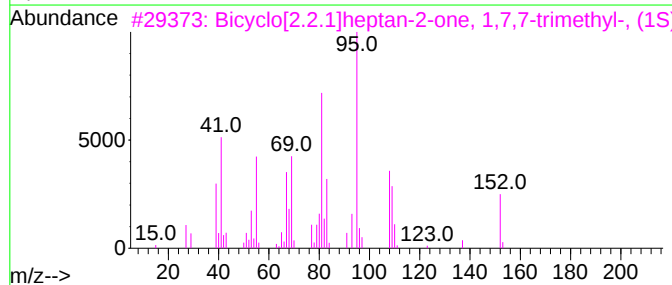
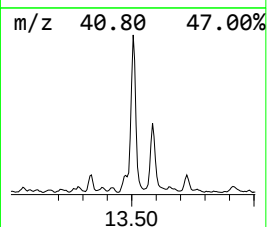
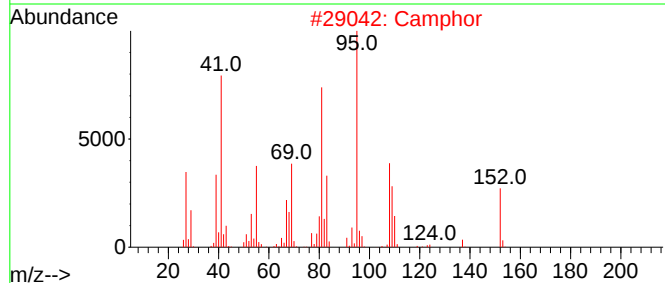
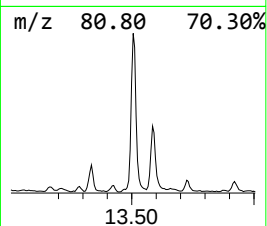
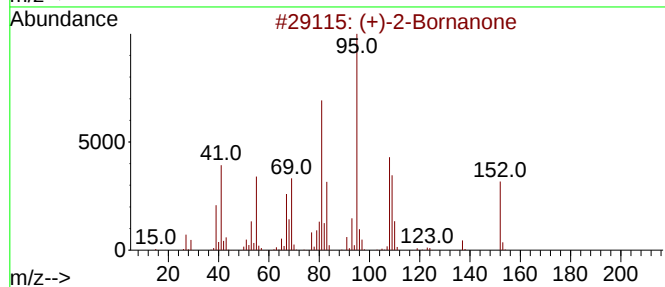
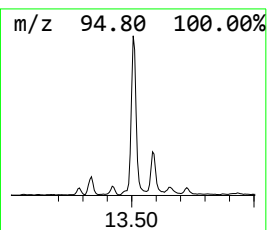
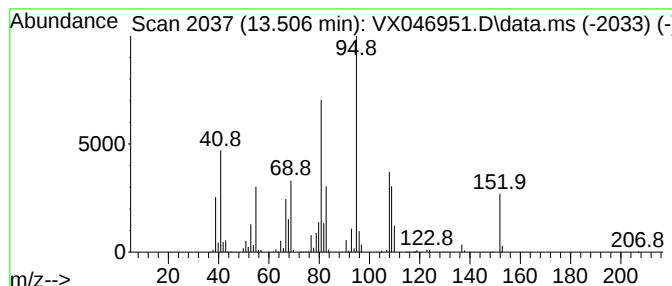
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	34.92 ug/l	1842650	1,4-Dichlorobenzene-d4	12.018

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	97
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	49
5			1-Adamantanol	152	C10H16O	000768-95-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

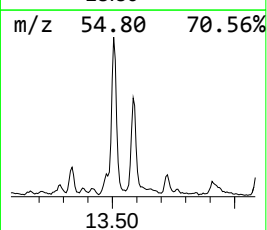
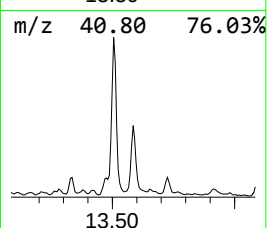
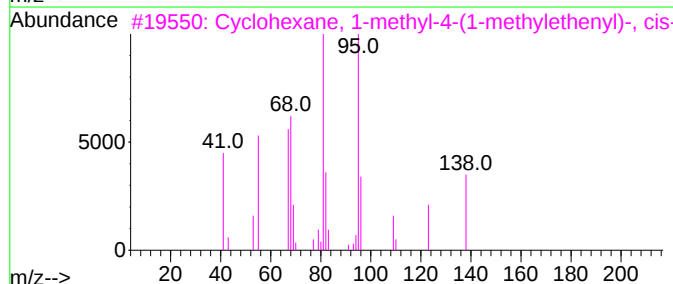
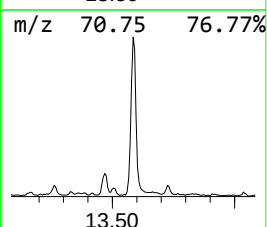
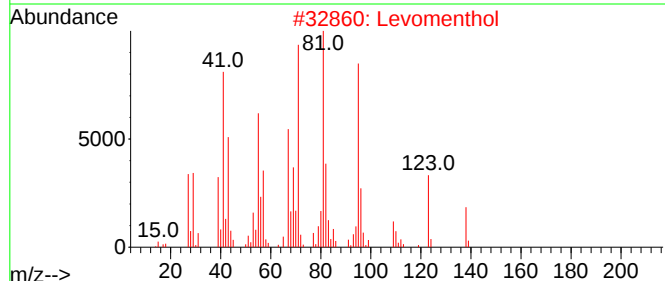
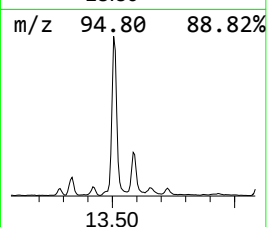
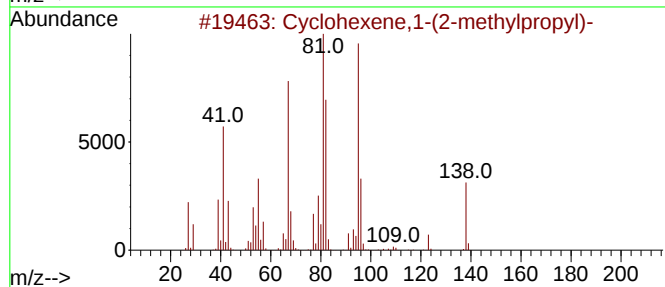
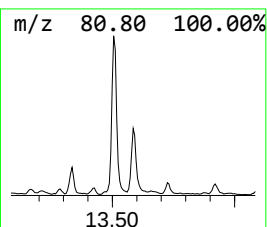
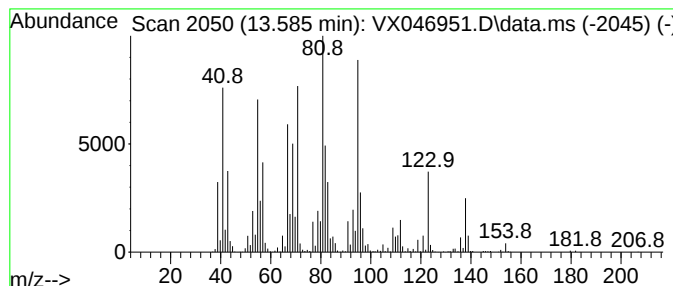
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexene,1-(2-methylprop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.585	20.09 ug/l	1060020	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	96
2			Levomenthol	156	C10H20O	002216-51-5	86
3			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	70
4			d1-Menthol	156	C10H20O	000089-78-1	64
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071025\
Data File : VX046951.D
Acq On : 10 Jul 2025 17:34
Operator : JC/MD
Sample : Q2554-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250709071-01 VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.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	1.270	25.5	ug/l	639129	1	5.562	1253080	50.0
Methanethiol	1.569	14.6	ug/l	365686	1	5.562	1253080	50.0
Isopropyl Alcohol	2.532	26.9	ug/l	674737	1	5.562	1253080	50.0
3-Hexanone, 2-m...	9.378	7.9	ug/l	381393	3	10.055	2426570	50.0
Eucalyptol	12.097	6.4	ug/l	336114	4	12.018	2638490	50.0
1-Hexanol, 2-et...	12.213	8.1	ug/l	426424	4	12.018	2638490	50.0
Fenchone	12.902	21.9	ug/l	1156720	4	12.018	2638490	50.0
(+)-2-Bornanone	13.506	34.9	ug/l	1842650	4	12.018	2638490	50.0
Cyclohexene,1-(...	13.585	20.1	ug/l	1060020	4	12.018	2638490	50.0