

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
 Data File : VX047257.D
 Acq On : 07 Aug 2025 13:06
 Operator : JC/MD
 Sample : Q2790-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 250806078-01 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\82X072125W.M
 Title : SW846 8260

Signal : TIC: VX047257.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	10	12	26	rVB2	76676	162943	2.95%	0.501%
2	1.276	26	31	68	rBV	2290692	5518462	100.00%	16.983%
3	1.569	75	79	89	rVV	77069	124899	2.26%	0.384%
4	2.148	170	174	184	rVB3	43418	104788	1.90%	0.322%
5	2.386	204	213	231	rBV	1101478	2412002	43.71%	7.423%
6	2.532	231	237	258	rVB	339539	832156	15.08%	2.561%
7	2.959	296	307	328	rBV2	707165	2144658	38.86%	6.600%
8	4.562	555	570	604	rBV	1550675	5138975	93.12%	15.815%
9	5.007	630	643	676	rBV3	516110	2297794	41.64%	7.071%
10	5.397	695	707	724	rBV5	109525	348051	6.31%	1.071%
11	5.562	724	734	758	rVB	237909	743699	13.48%	2.289%
12	5.964	790	800	809	rBV2	140593	394266	7.14%	1.213%
13	6.080	809	819	839	rVV2	247022	881751	15.98%	2.714%
14	6.769	923	932	954	rBV	381893	979996	17.76%	3.016%
15	7.458	1032	1045	1066	rBV	204880	555179	10.06%	1.709%
16	7.909	1113	1119	1134	rBV	42323	99346	1.80%	0.306%
17	8.574	1220	1228	1235	rBV	86258	164183	2.98%	0.505%
18	8.653	1235	1241	1248	rVV	610665	1019660	18.48%	3.138%
19	8.720	1248	1252	1262	rVV	145128	245712	4.45%	0.756%
20	9.378	1354	1360	1368	rBV	123749	195423	3.54%	0.601%
21	10.055	1461	1471	1483	rBV	863744	1285652	23.30%	3.957%
22	10.195	1489	1494	1501	rBV	233211	324406	5.88%	0.998%
23	10.299	1504	1511	1518	rVB	206344	287073	5.20%	0.883%
24	10.640	1563	1567	1574	rBV	126042	172545	3.13%	0.531%
25	10.768	1581	1588	1597	rBV	49159	84780	1.54%	0.261%
26	11.079	1634	1639	1645	rBV	682983	880307	15.95%	2.709%
27	11.378	1682	1688	1694	rVV3	31399	56844	1.03%	0.175%
28	11.750	1745	1749	1754	rVB	87646	104650	1.90%	0.322%
29	11.884	1761	1771	1778	rVB3	59218	92696	1.68%	0.285%
30	12.018	1787	1793	1801	rBV	1015806	1422506	25.78%	4.378%
31	12.097	1801	1806	1811	rVB3	103371	164353	2.98%	0.506%
32	12.219	1821	1826	1827	rBV	60768	73998	1.34%	0.228%
33	12.238	1827	1829	1838	rVV	67531	103574	1.88%	0.319%
34	12.420	1854	1859	1863	rBV2	53357	69153	1.25%	0.213%
35	12.579	1881	1885	1889	rVB	114125	143981	2.61%	0.443%
36	12.762	1911	1915	1920	rVB3	51083	72037	1.31%	0.222%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M

Title : SW846 8260

37	12.902	1932	1938	1945	rBV	396717	546905	9.91%	1.683%
38	12.963	1945	1948	1957	rVB5	37263	67708	1.23%	0.208%
39	13.335	2005	2009	2013	rVB	68315	89003	1.61%	0.274%
40	13.475	2028	2032	2033	rBV3	49087	55669	1.01%	0.171%
41	13.506	2033	2037	2045	rVV	473021	688249	12.47%	2.118%
42	13.585	2045	2050	2059	rVV3	257992	416055	7.54%	1.280%
43	13.725	2069	2073	2076	rVV2	61688	85582	1.55%	0.263%
44	13.774	2076	2081	2088	rVB	520950	640238	11.60%	1.970%
45	13.914	2100	2104	2117	rVB10	20937	56734	1.03%	0.175%
46	14.097	2127	2134	2144	rBV3	40161	81086	1.47%	0.250%
47	14.633	2214	2222	2231	rBV	39633	64405	1.17%	0.198%

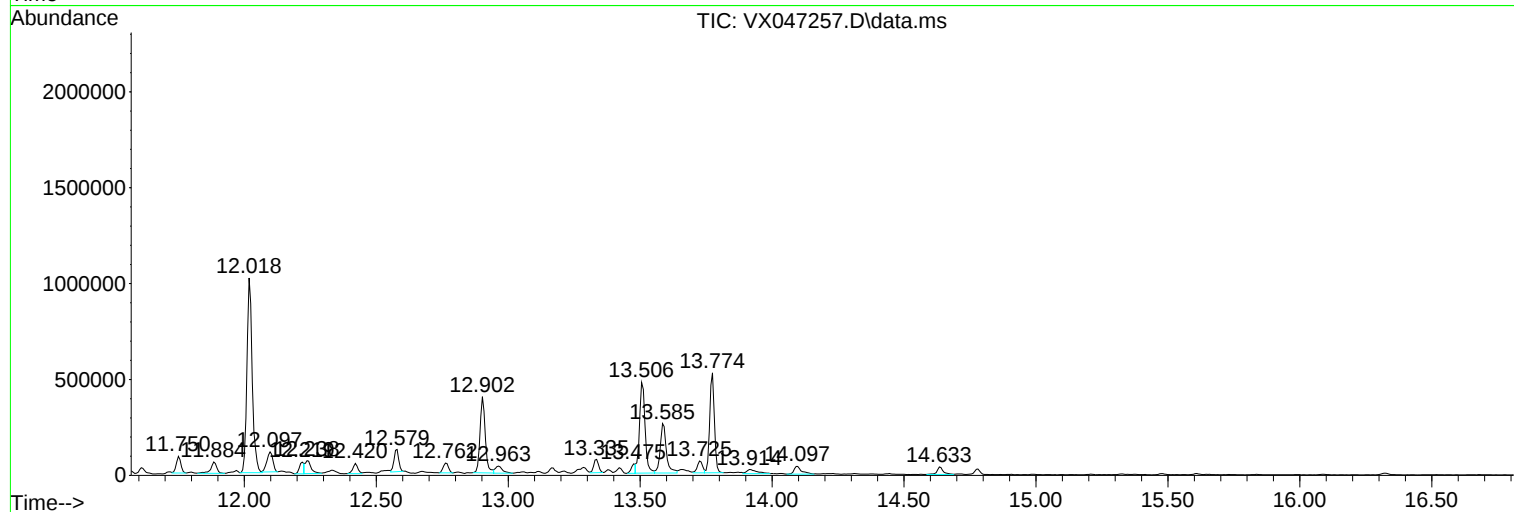
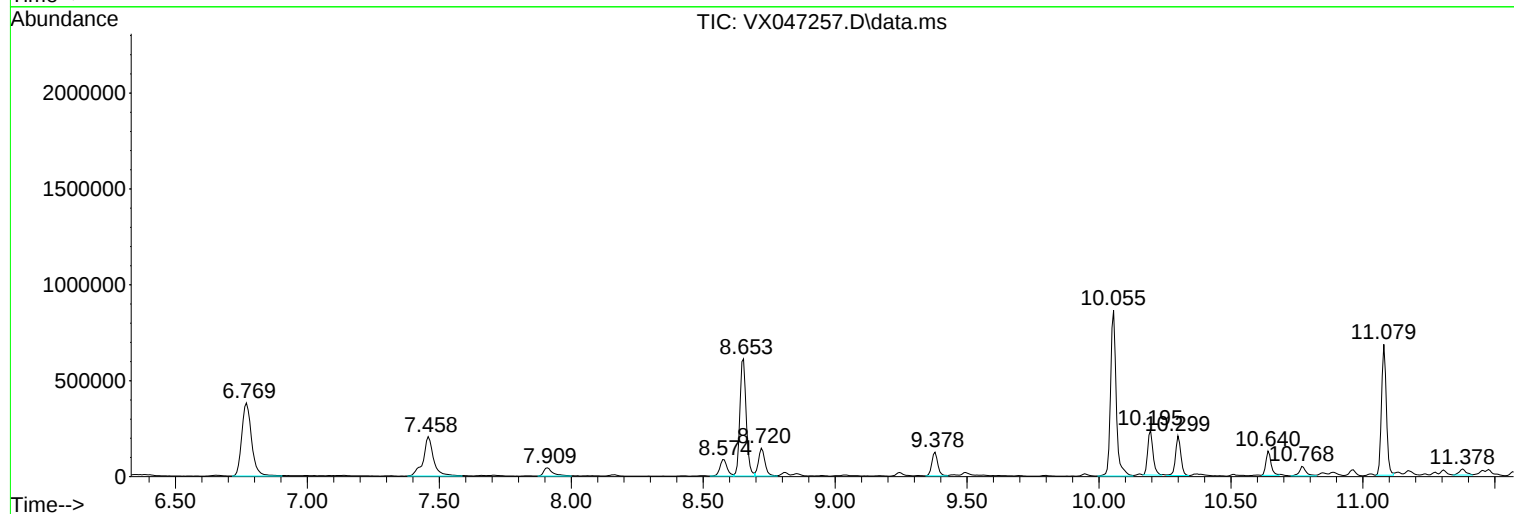
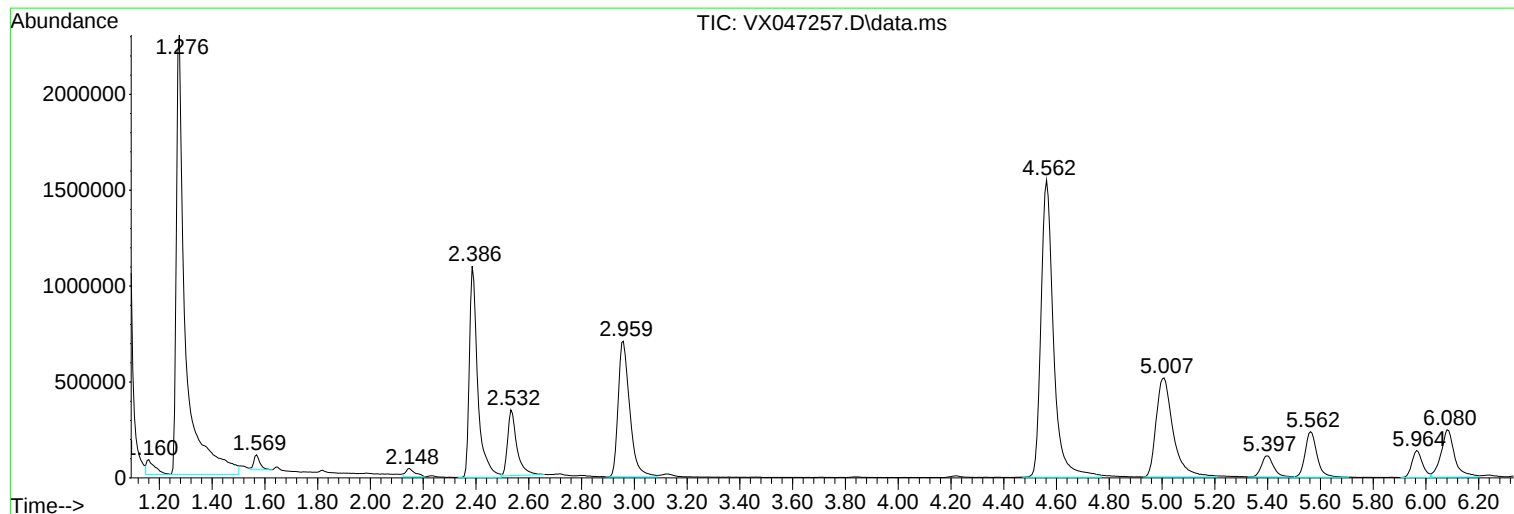
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

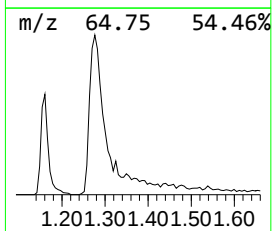
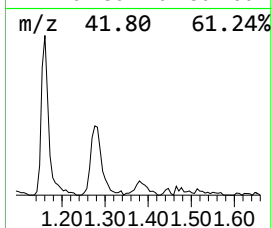
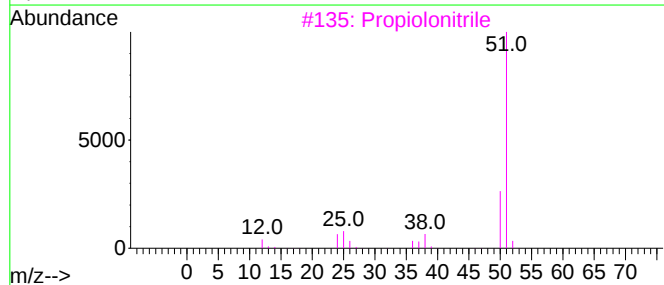
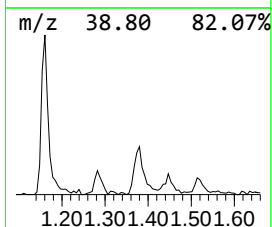
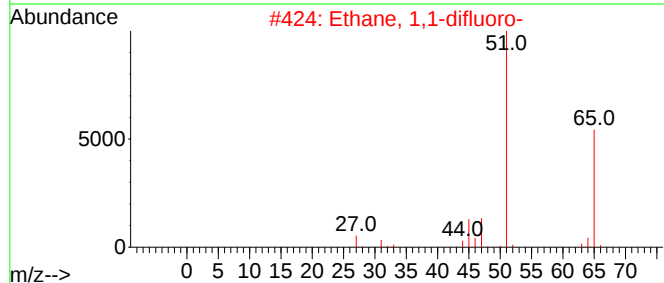
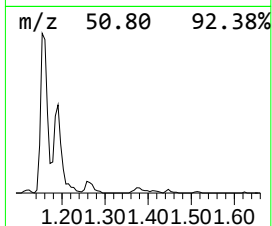
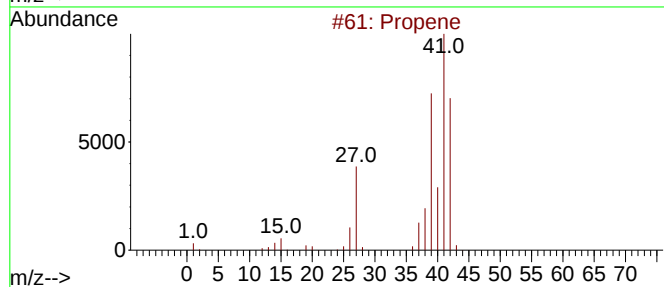
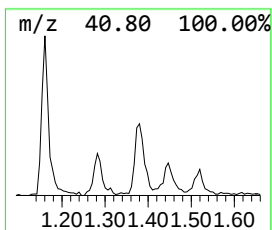
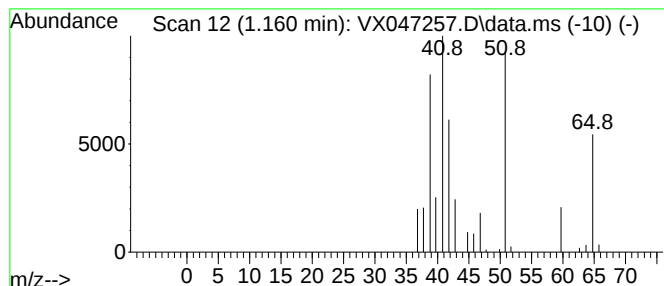
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.160 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.160	10.95 ug/l	162943	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	35
2			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	25
3			Propiolonitrile	51	C3HN	001070-71-9	4
4			Cyclopropane	42	C3H6	000075-19-4	2
5			Cyclopropene	40	C3H4	002781-85-3	2



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

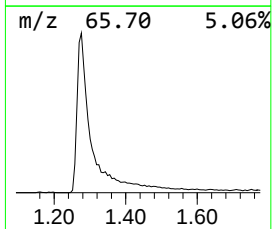
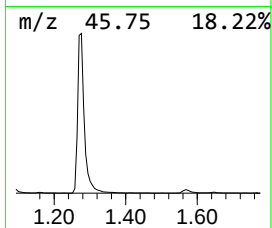
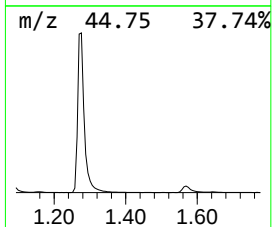
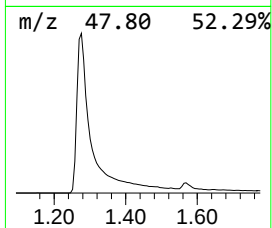
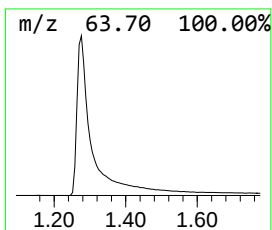
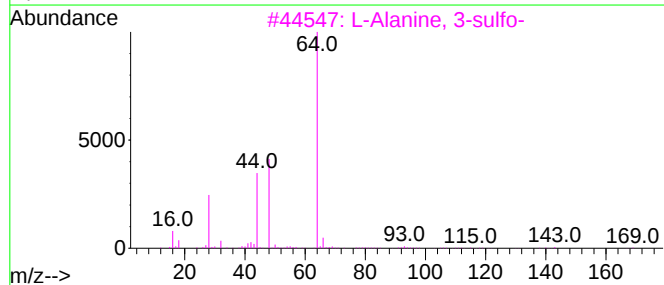
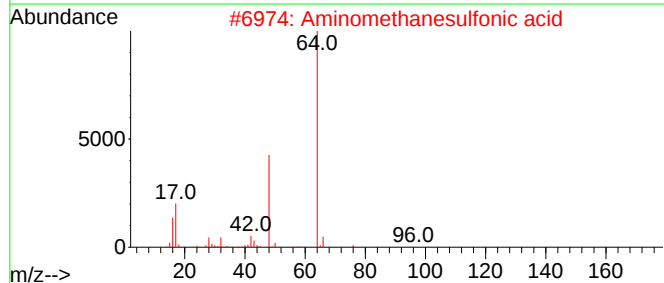
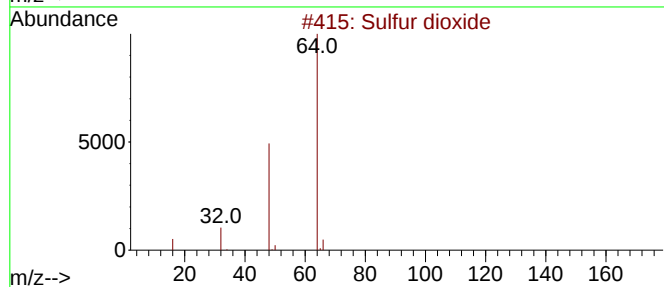
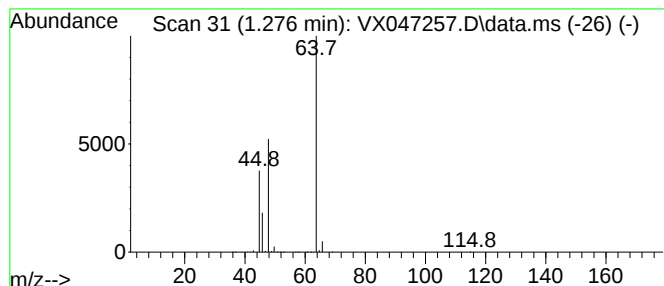
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.276	371.01 ug/l	5518460	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfur dioxide	64	O2S	007446-09-5	78
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5		Ethanol, 2-fluoro-	64	C2H5FO	000371-62-0	5



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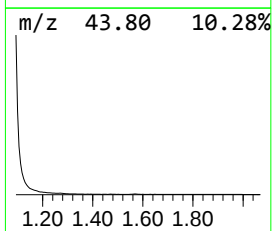
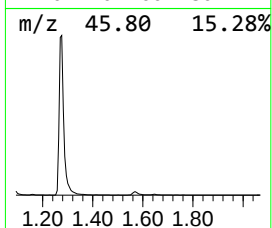
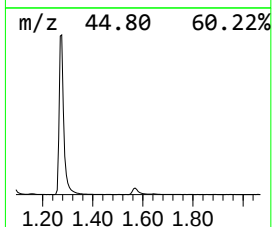
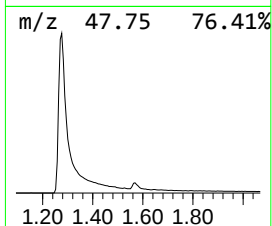
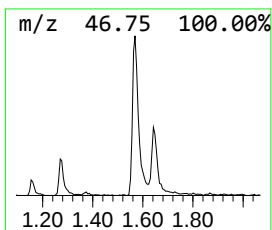
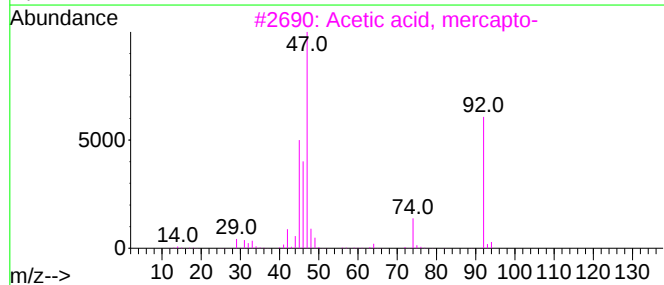
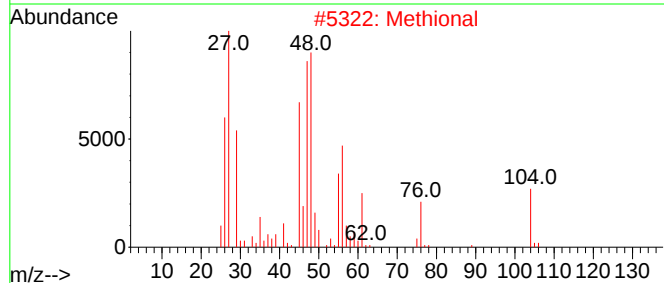
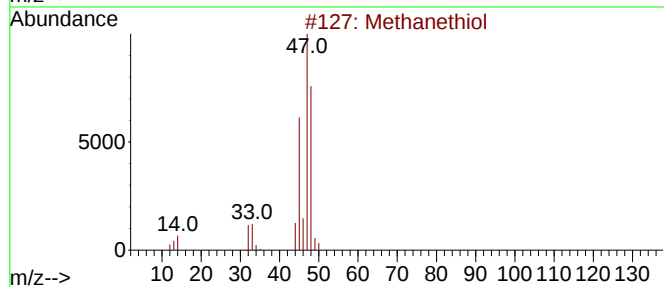
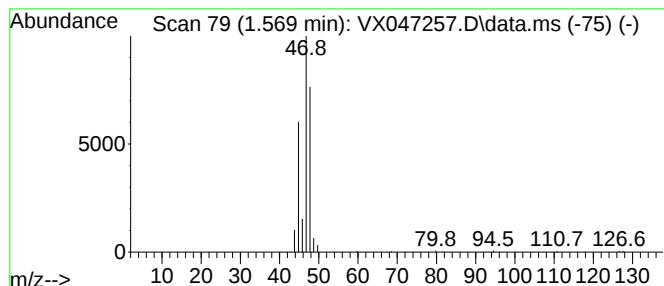
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.569	8.40 ug/l	124899	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			Methional	104	C4H8OS	003268-49-3	64
3			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	4
5			Ethanol	46	C2H6O	000064-17-5	4



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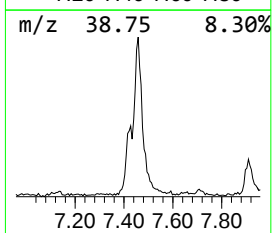
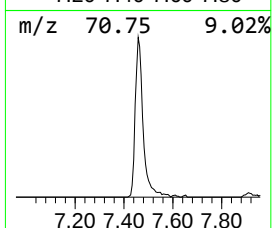
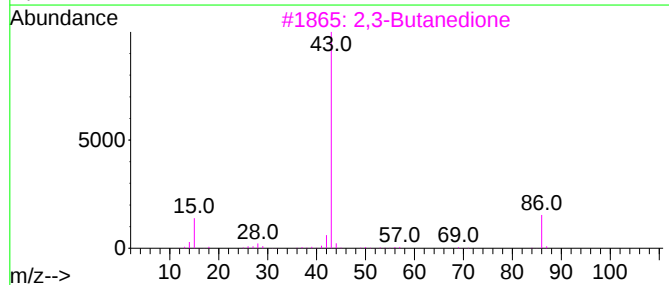
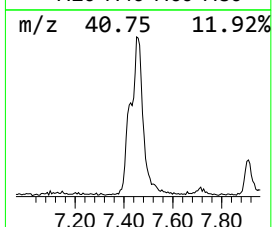
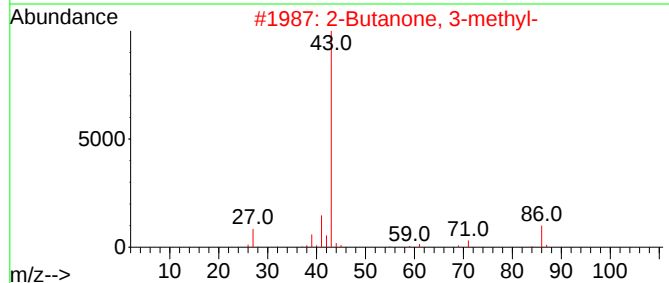
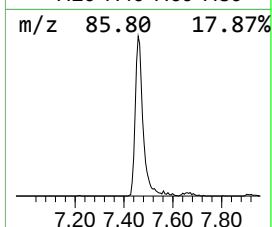
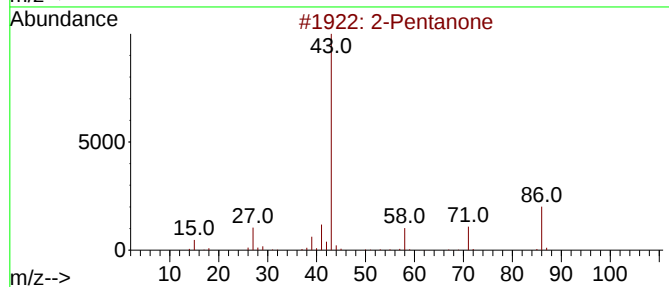
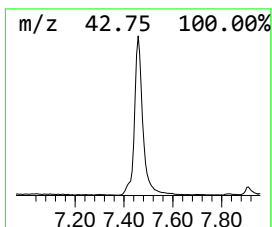
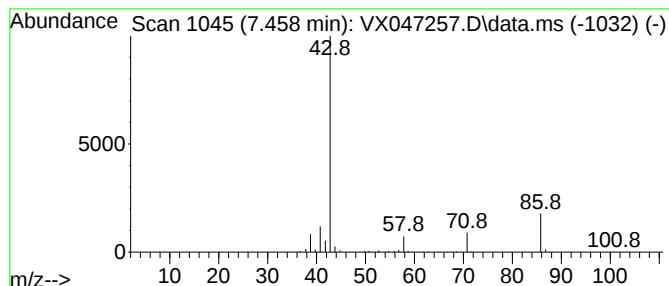
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	28.33 ug/l	555179	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	90
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3			2,3-Butanedione	86	C4H6O2	000431-03-8	47
4			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	33
5			Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	9



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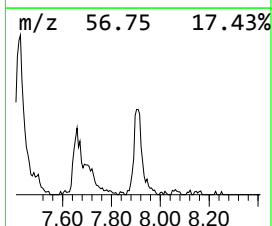
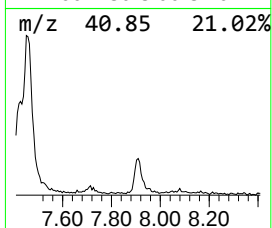
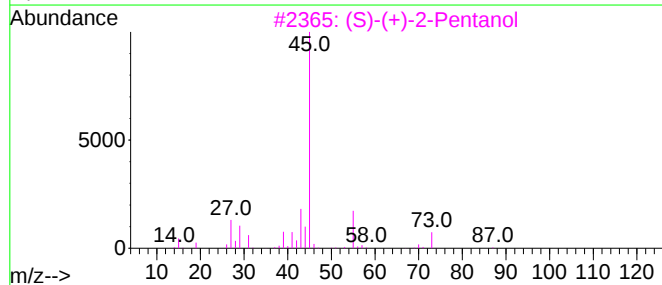
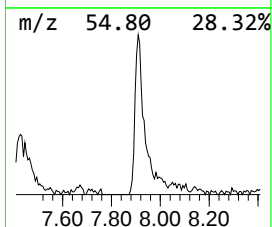
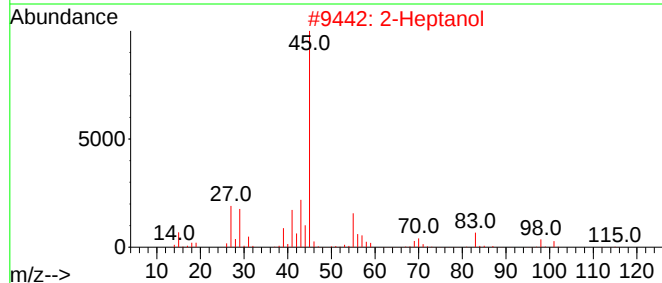
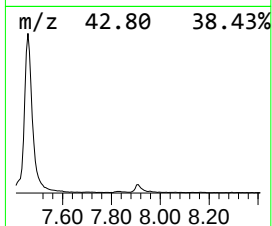
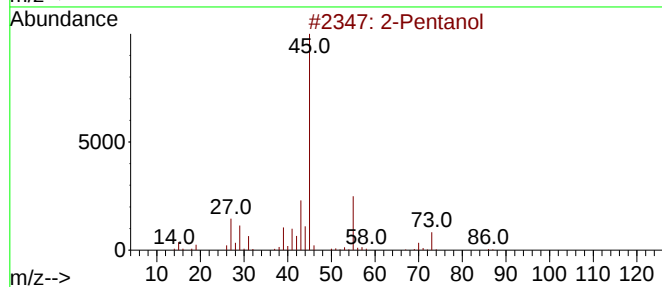
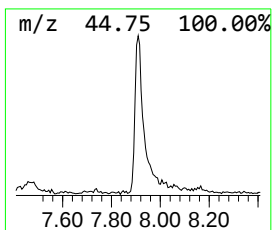
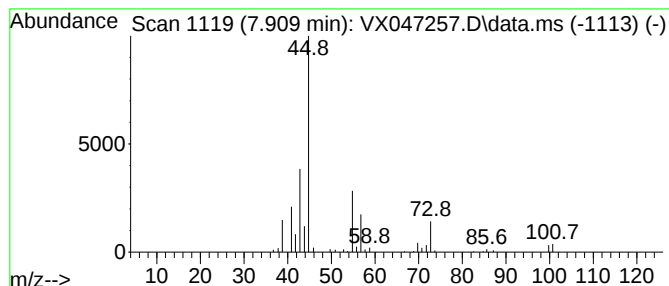
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Quant Title : SW846 8260

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

Peak Number 5 2-Pentanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.909	5.07 ug/l	99346	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol	88	C5H12O	006032-29-7	72
2			2-Heptanol	116	C7H16O	000543-49-7	45
3			(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	40
4			2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	39
5			Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

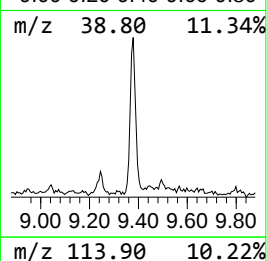
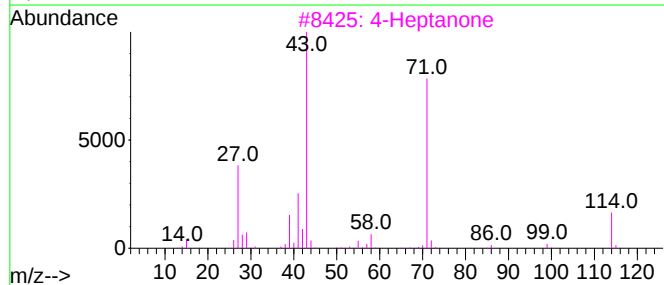
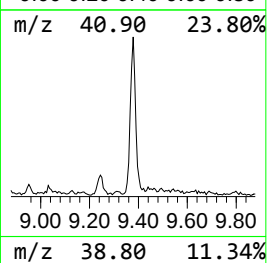
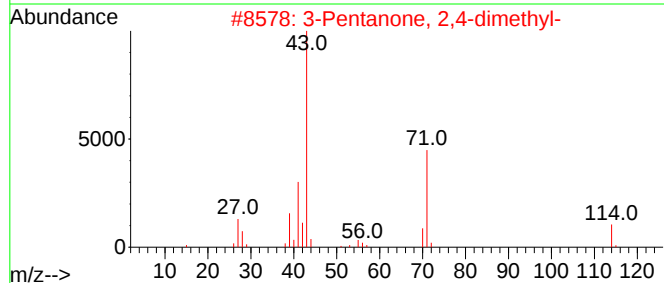
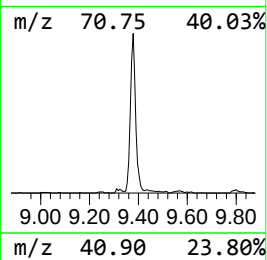
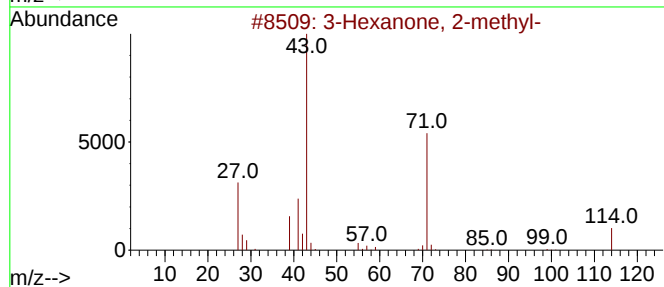
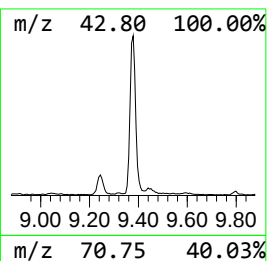
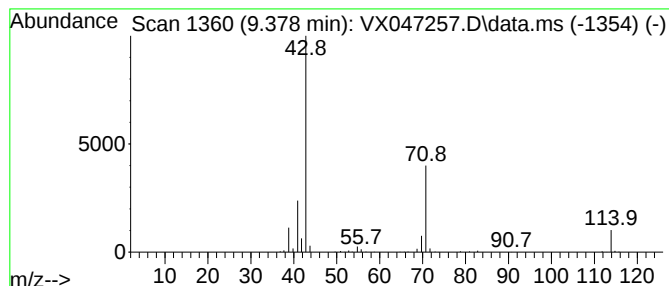
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Quant Title : SW846 8260

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

Peak Number 6 3-Hexanone, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	7.60 ug/l	195423	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
2			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	72
3			4-Heptanone	114	C7H14O	000123-19-3	53
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	45
5			2,3-Hexanedione	114	C6H10O2	003848-24-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

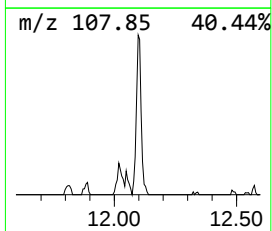
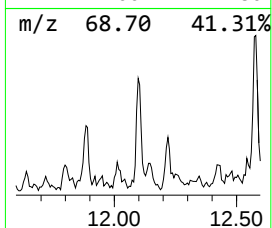
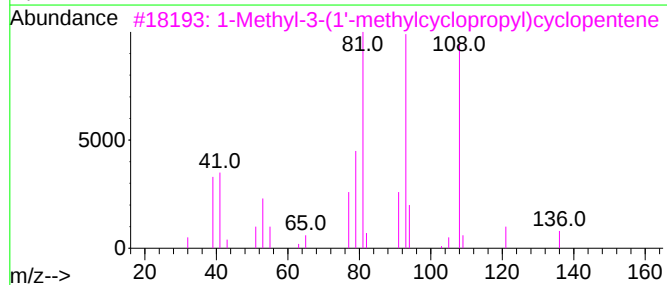
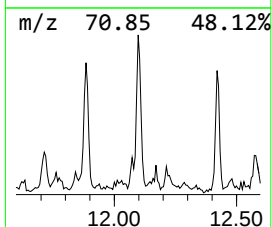
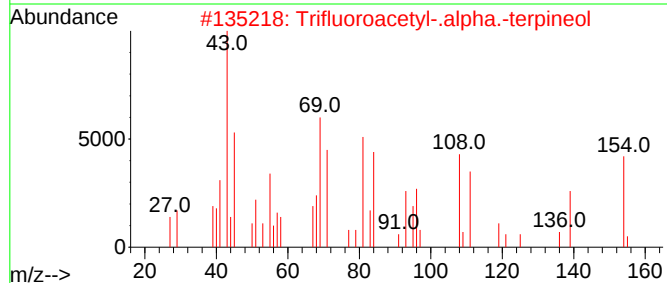
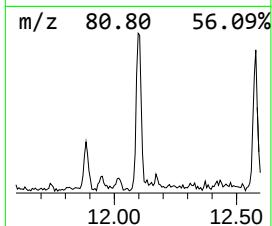
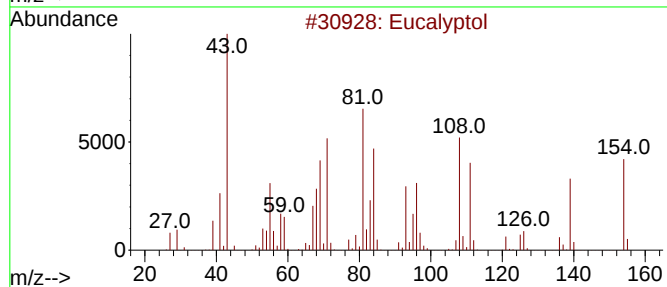
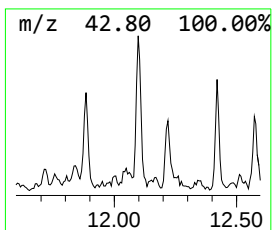
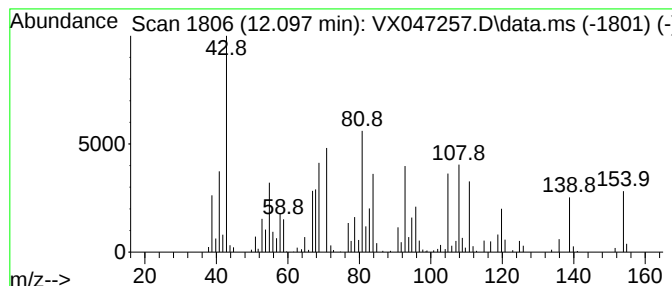
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Quant Title : SW846 8260

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

Peak Number 7 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	5.78 ug/l	164353	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	96
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	64
3			1-Methyl-3-(1'-methylcyclopropyl)...	136	C10H16	103240-53-5	35
4			3-Acetoxy-p-menthan-1-ol	214	C12H22O3	058315-86-9	25
5			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

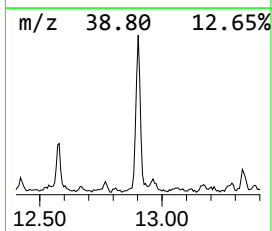
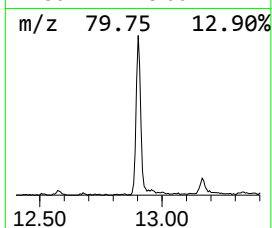
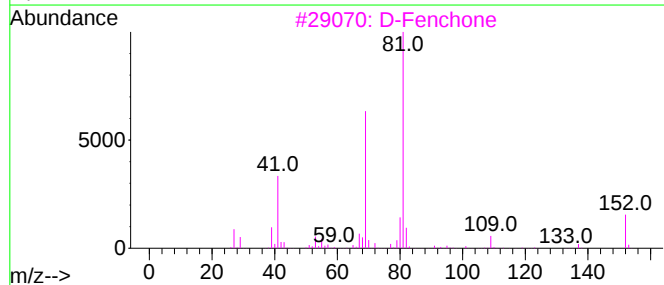
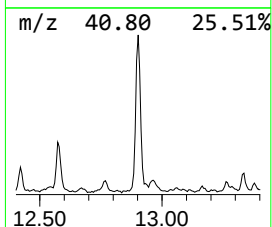
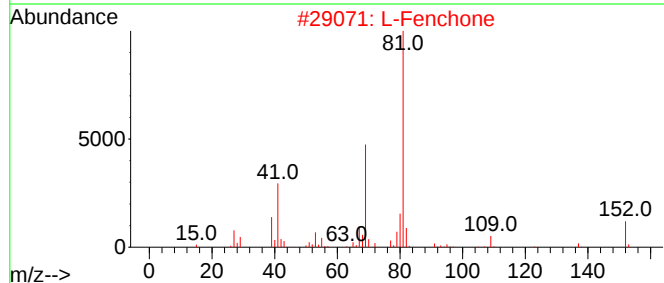
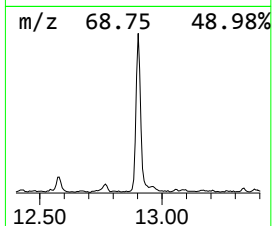
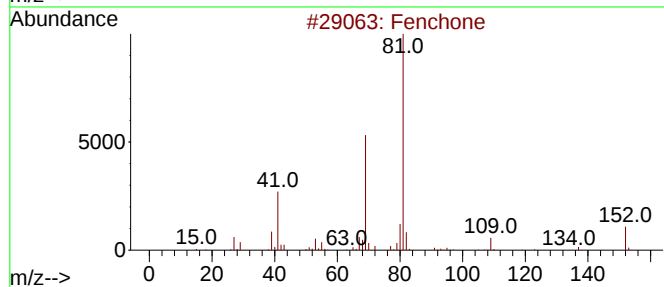
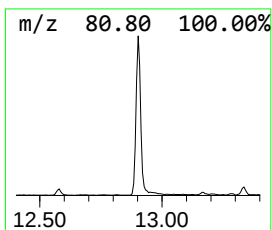
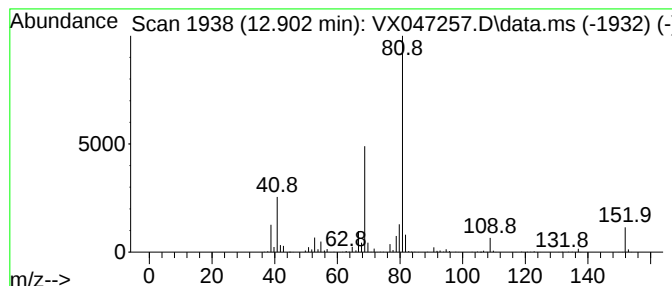
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Quant Title : SW846 8260

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

Peak Number 8 Fenchone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	19.22 ug/l	546905	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	94
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	59
5			Ethanone, 1-(2-methyl-2-cyclopentyl)-	124	C8H12O	001767-84-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

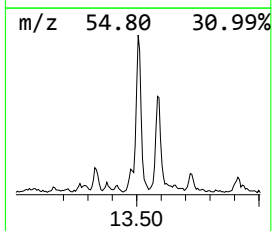
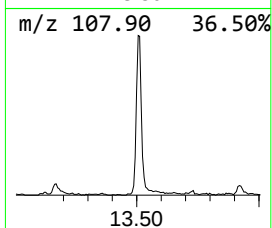
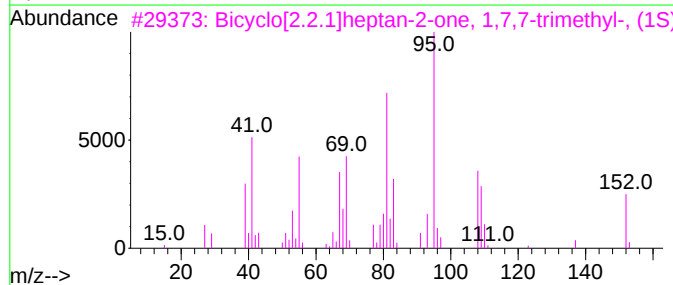
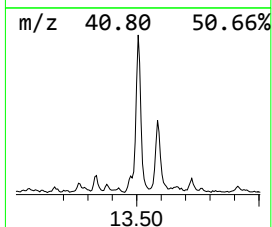
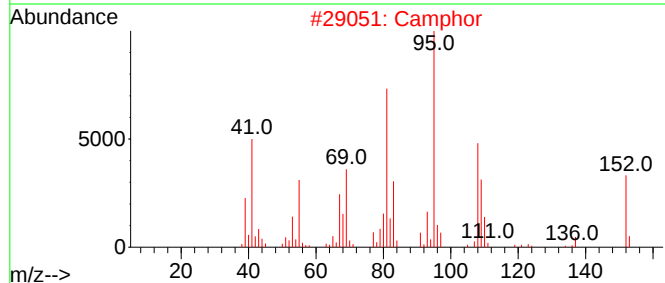
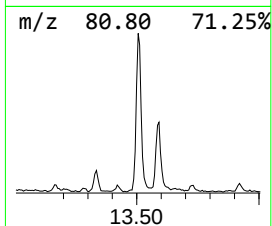
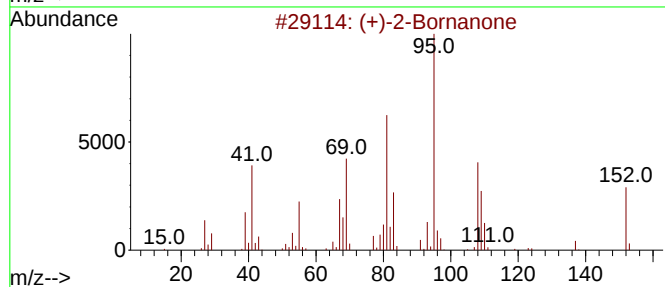
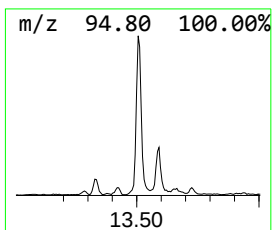
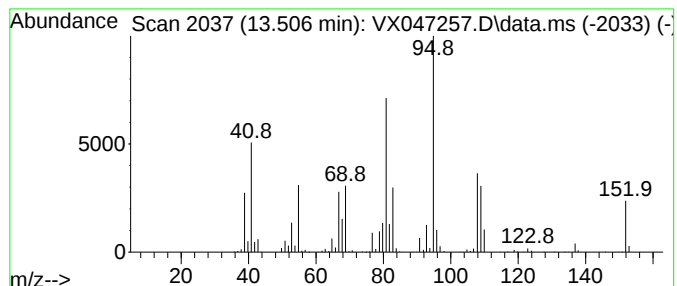
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	24.19 ug/l	688249	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
2			Camphor	152	C10H16O	000076-22-2	94
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	46
5			2-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

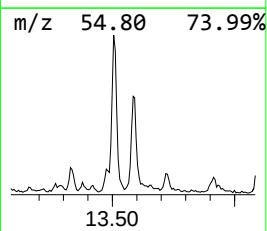
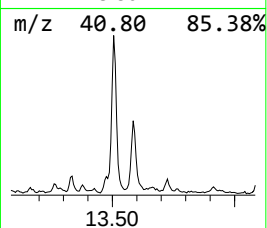
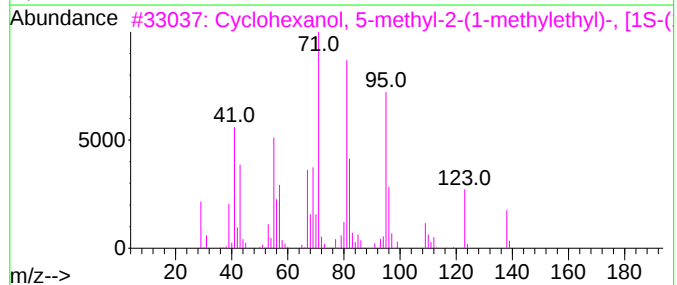
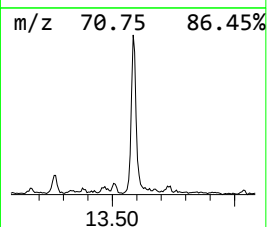
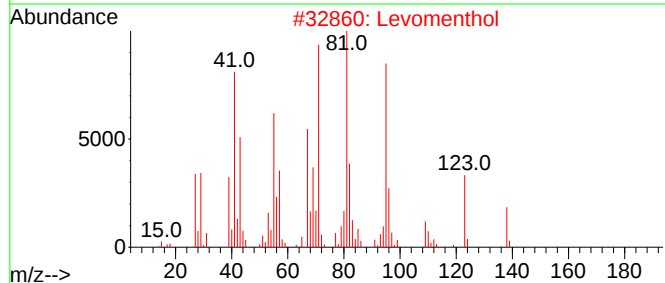
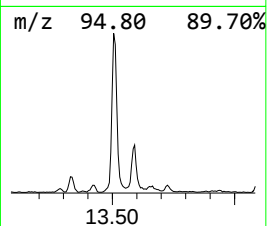
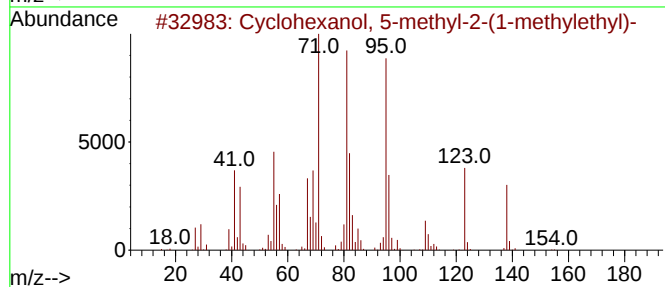
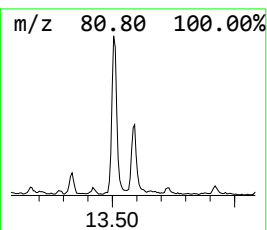
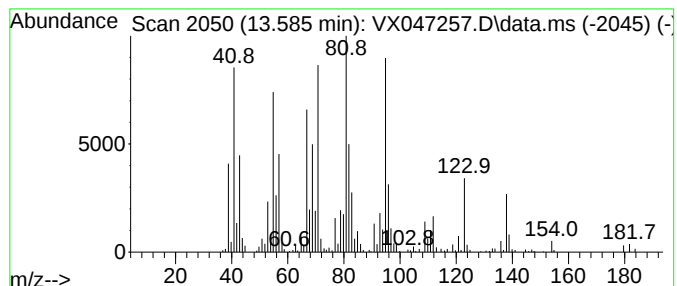
Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.585	14.62 ug/l	416055	1,4-Dichlorobenzene-d4		12.018	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87
2		Levomenthol	156	C10H20O	002216-51-5	87
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	80
4		Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	70
5		Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080725\
Data File : VX047257.D
Acq On : 07 Aug 2025 13:06
Operator : JC/MD
Sample : Q2790-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
250806078-01 VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.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
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Sulfur dioxide	1.276	371.0	ug/l	5518460	1	5.562	743699	50.0
Methanethiol	1.569	8.4	ug/l	124899	1	5.562	743699	50.0
2-Pentanone	7.458	28.3	ug/l	555179	2	6.769	979996	50.0
2-Pentanol	7.909	5.1	ug/l	99346	2	6.769	979996	50.0
3-Hexanone, 2-m...	9.378	7.6	ug/l	195423	3	10.055	1285650	50.0
Eucalyptol	12.097	5.8	ug/l	164353	4	12.018	1422510	50.0
Fenchone	12.902	19.2	ug/l	546905	4	12.018	1422510	50.0
(+)-2-Bornanone	13.506	24.2	ug/l	688249	4	12.018	1422510	50.0
Cyclohexanol, 5...	13.585	14.6	ug/l	416055	4	12.018	1422510	50.0