

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102023\
 Data File : VX038413.D
 Acq On : 20 Oct 2023 19:22
 Operator : JC/MD
 Sample : 04991-01 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1021-1024

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\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	72	rBV	2442450	2875025	100.00%	32.464%
2	2.050	150	158	176	rBV	380416	628388	21.86%	7.096%
3	2.294	192	198	205	rBV	38967	61631	2.14%	0.696%
4	2.373	205	211	225	rVB	175852	292707	10.18%	3.305%
5	2.526	230	236	246	rBV	17527	35456	1.23%	0.400%
6	3.843	445	452	468	rBV4	12428	35999	1.25%	0.406%
7	4.227	506	515	529	rBV3	41659	112587	3.92%	1.271%
8	5.385	692	705	722	rBV	86105	253032	8.80%	2.857%
9	5.556	722	733	747	rBV	129686	372142	12.94%	4.202%
10	5.952	789	798	812	rVB2	90350	243138	8.46%	2.745%
11	6.763	920	931	946	rBV	213988	520395	18.10%	5.876%
12	7.208	998	1004	1022	rBV	38299	103808	3.61%	1.172%
13	7.458	1039	1045	1060	rBV	15536	32034	1.11%	0.362%
14	8.647	1234	1240	1260	rBV	457642	744935	25.91%	8.412%
15	10.055	1465	1471	1488	rBV	497182	709911	24.69%	8.016%
16	10.585	1553	1558	1565	rBV	19430	35834	1.25%	0.405%
17	11.079	1634	1639	1651	rVB	434903	570616	19.85%	6.443%
18	12.018	1788	1793	1800	rBV	582582	776251	27.00%	8.765%
19	12.219	1822	1826	1829	rBV	18592	31250	1.09%	0.353%
20	12.420	1853	1859	1864	rBV	27378	34596	1.20%	0.391%
21	13.268	1992	1998	2000	rBV	32577	47280	1.64%	0.534%
22	13.292	2000	2002	2007	rVB3	30665	34835	1.21%	0.393%
23	13.420	2019	2023	2032	rVB3	21789	39729	1.38%	0.449%
24	14.036	2120	2124	2127	rVB	31927	31501	1.10%	0.356%
25	14.225	2150	2155	2163	rVB3	28157	49125	1.71%	0.555%
26	14.475	2192	2196	2206	rVB6	18889	37431	1.30%	0.423%
27	14.615	2215	2219	2220	rBV2	27831	30666	1.07%	0.346%
28	14.633	2220	2222	2226	rVB	27631	33567	1.17%	0.379%
29	14.755	2238	2242	2244	rBV	30628	32627	1.13%	0.368%
30	15.487	2355	2362	2368	rBV3	26748	49547	1.72%	0.559%

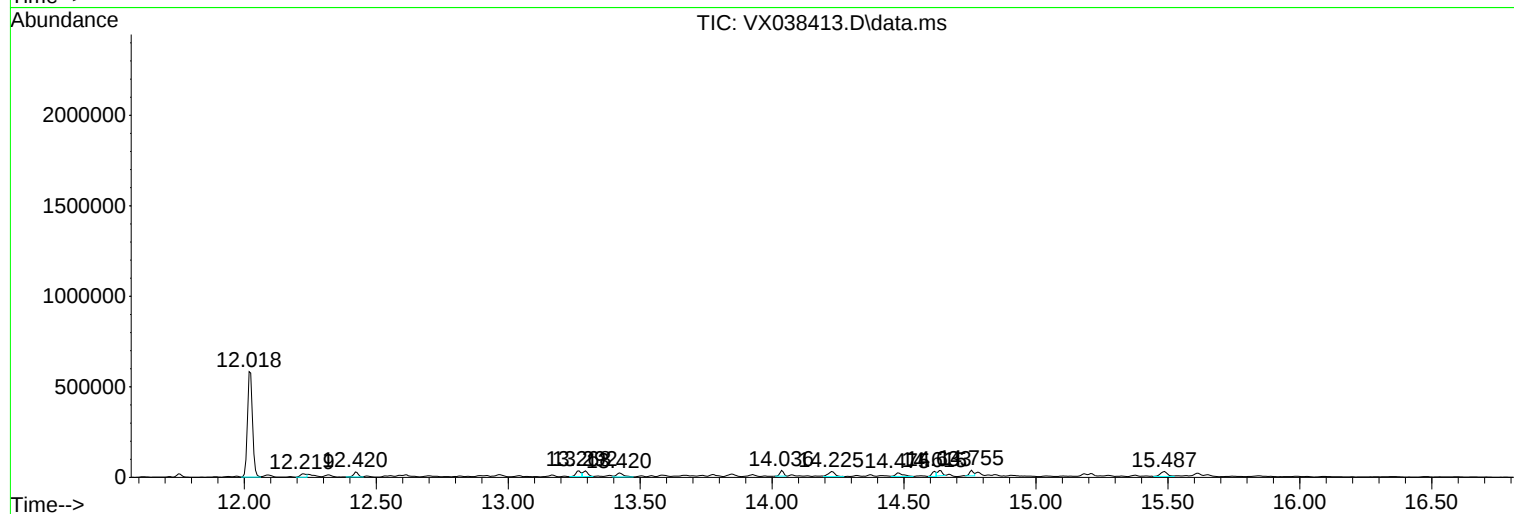
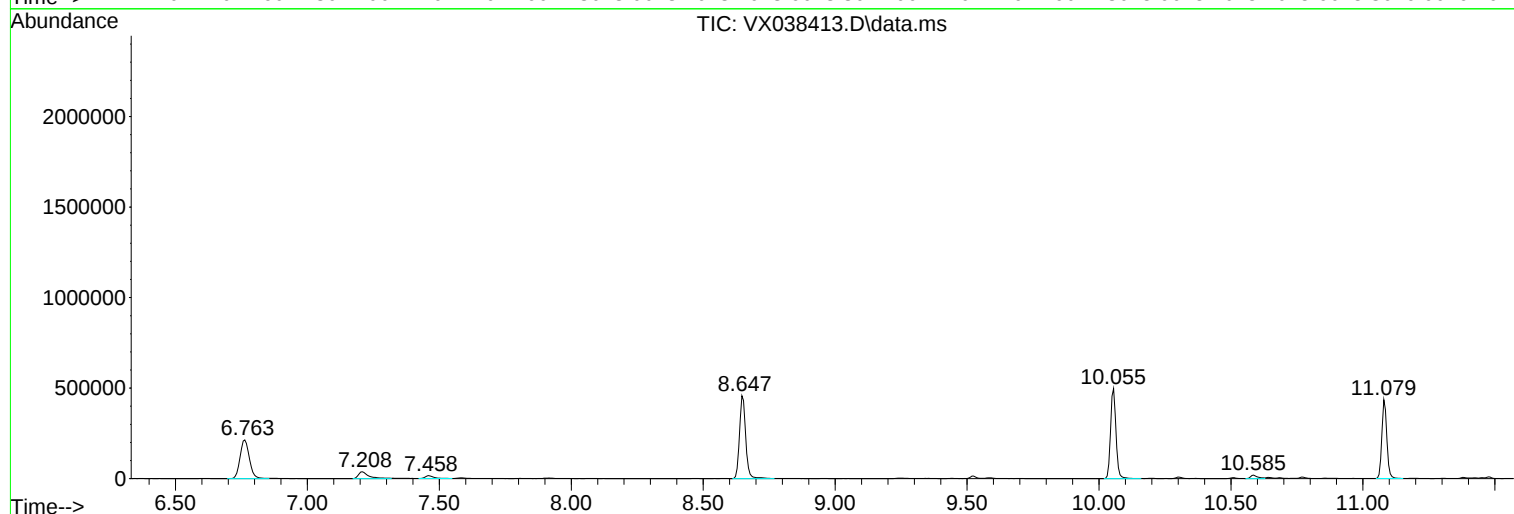
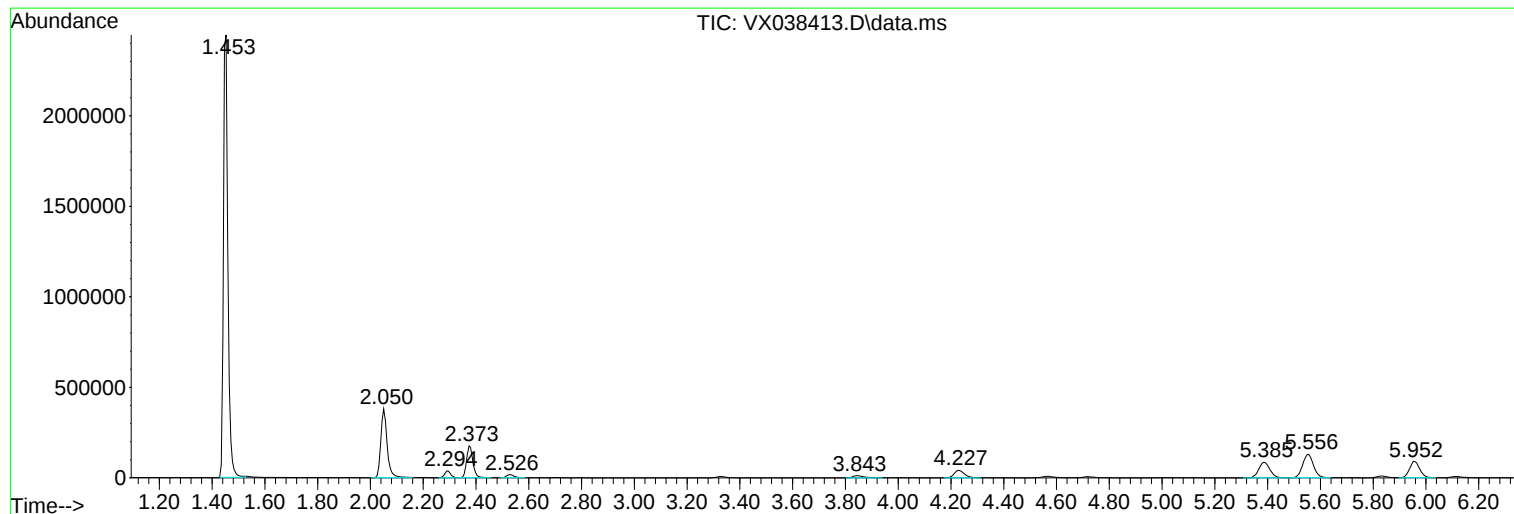
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1021-1024

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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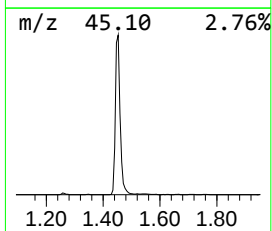
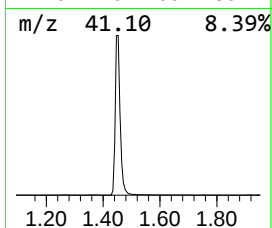
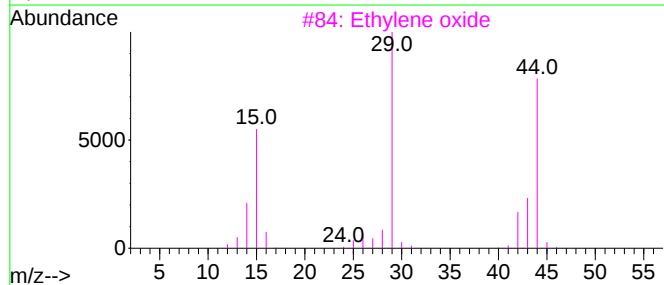
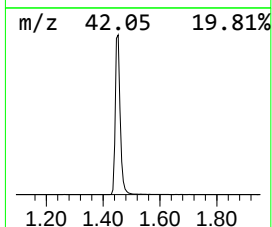
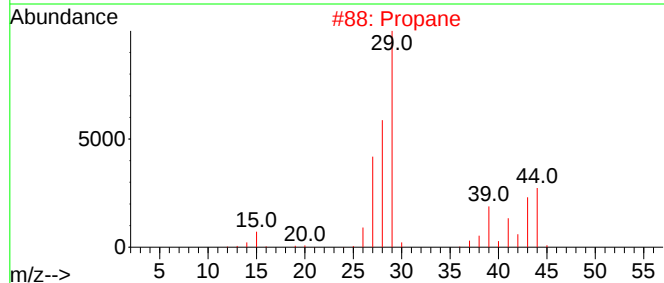
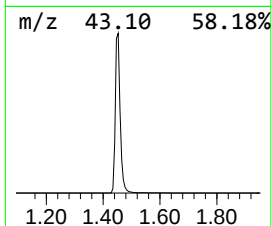
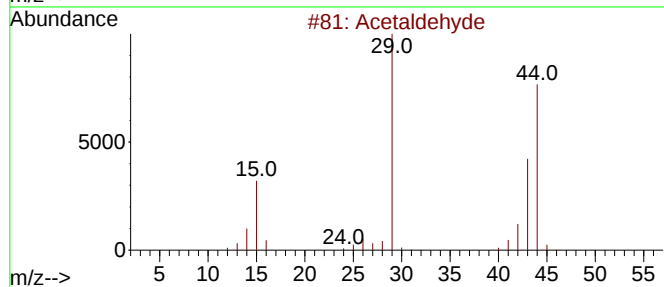
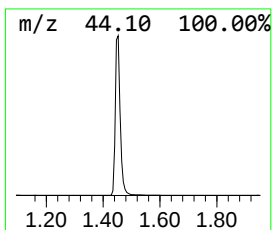
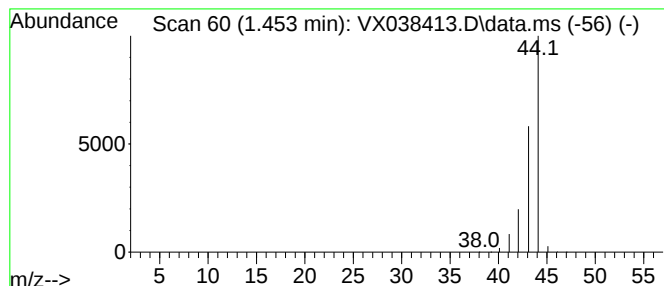
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	386.28 ug/l	2875030	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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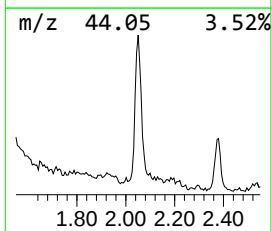
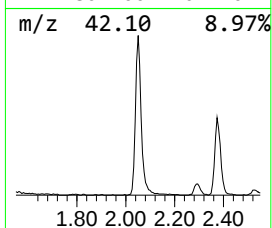
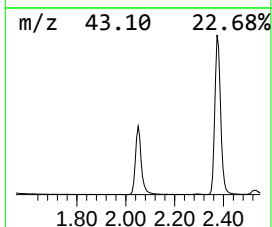
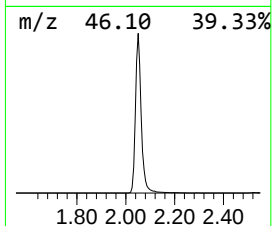
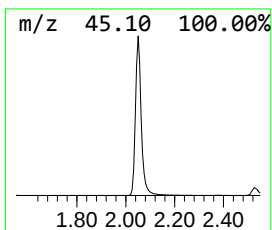
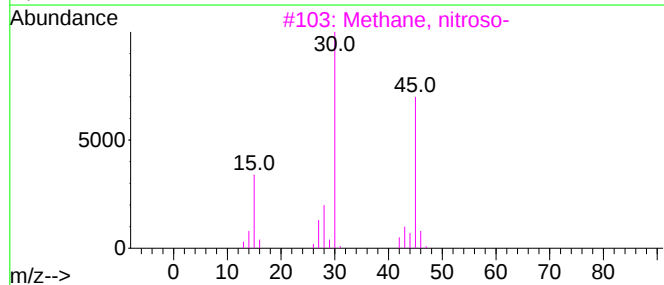
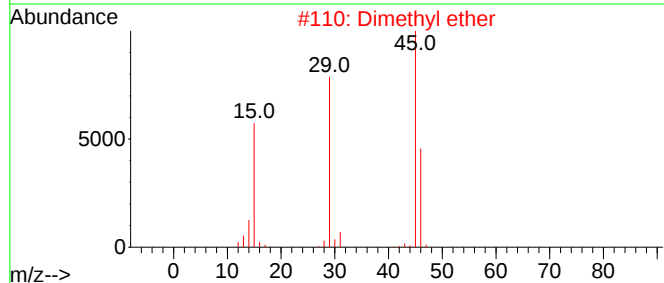
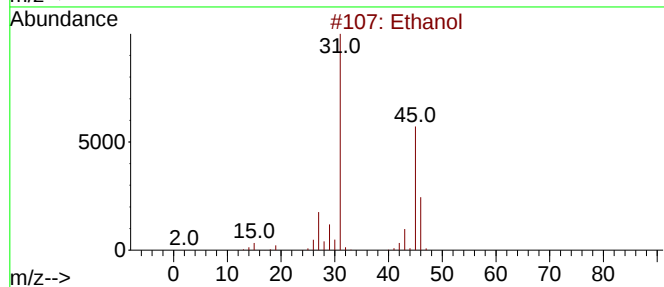
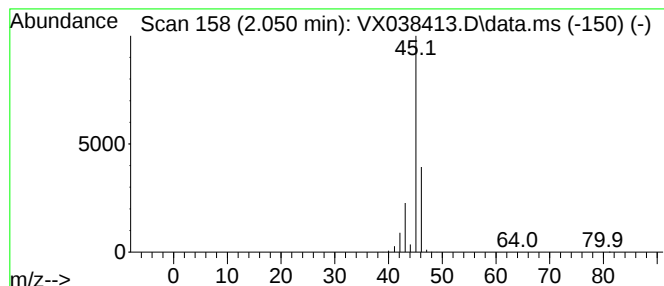
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	84.43 ug/l	628388	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
1021-1024

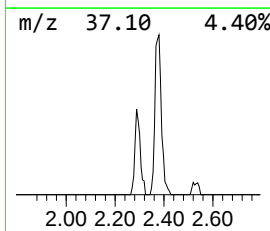
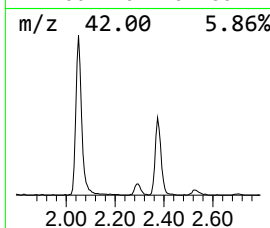
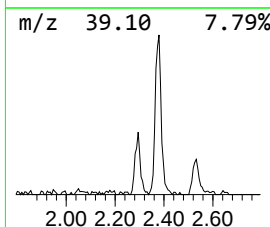
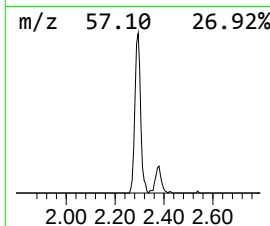
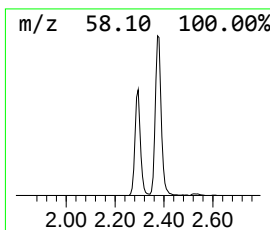
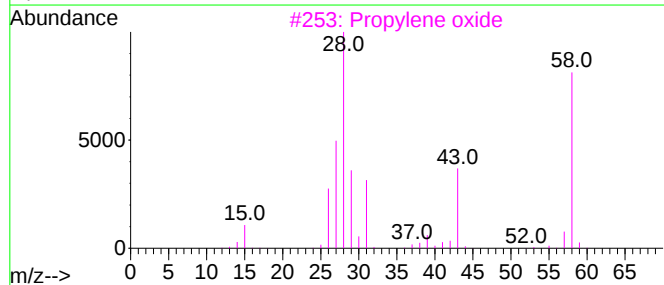
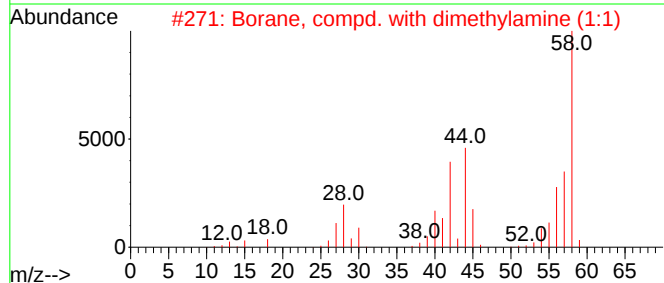
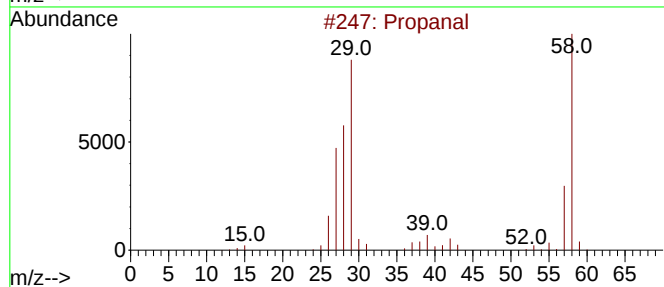
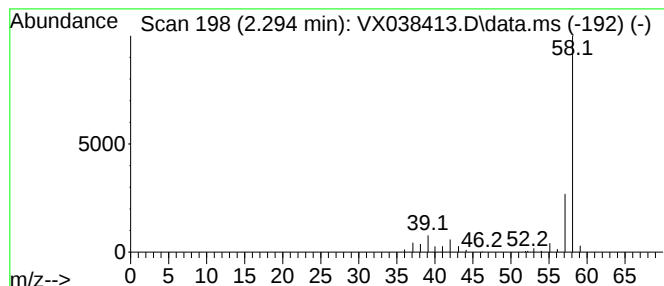
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	8.28 ug/l	61631	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	72
2			Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	9
3			Propylene oxide	58	C3H6O	000075-56-9	9
4			Trimethylene oxide	58	C3H6O	000503-30-0	9
5			Eicosylamine, N,N-dimethyl-	325	C22H47N	1000406-30-5	9



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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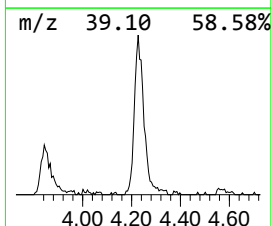
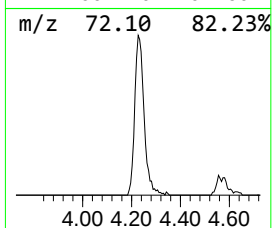
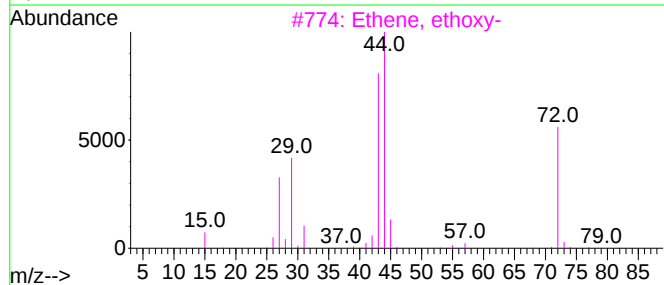
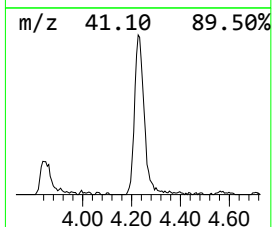
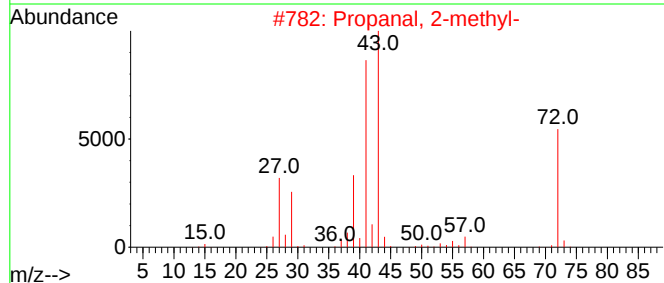
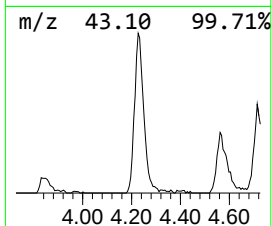
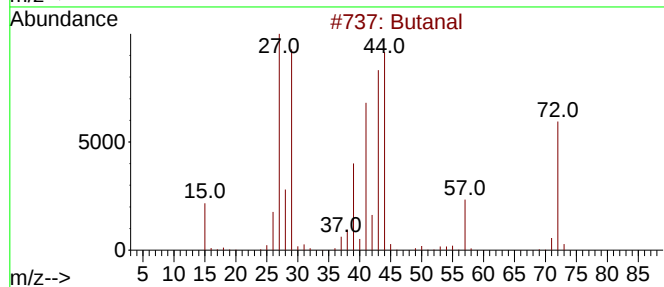
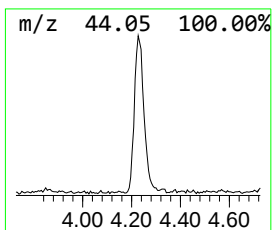
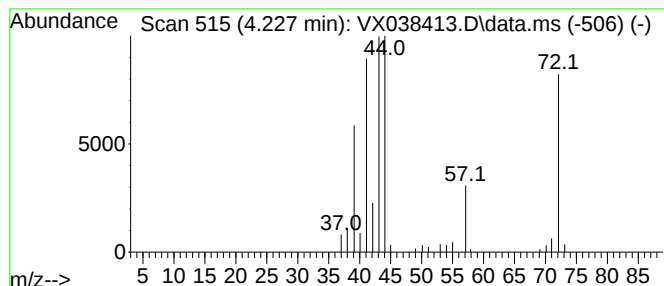
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	15.13 ug/l	112587	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4			Propane	44	C3H8	000074-98-6	38
5			Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	27



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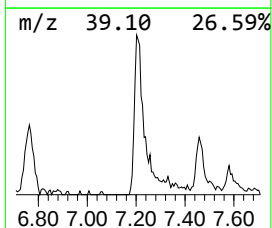
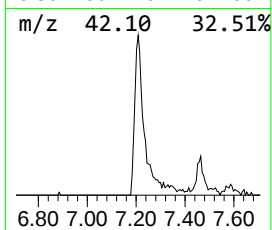
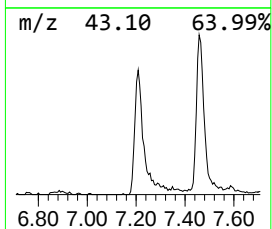
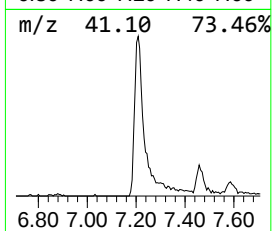
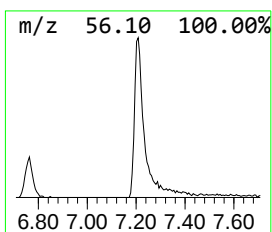
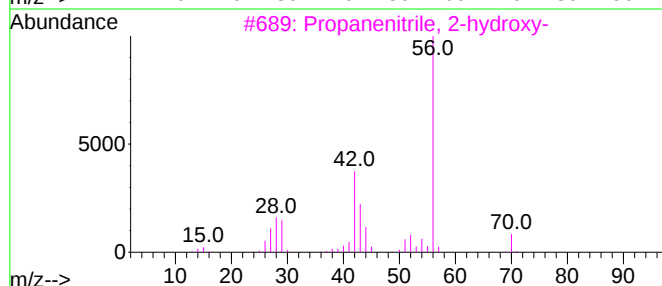
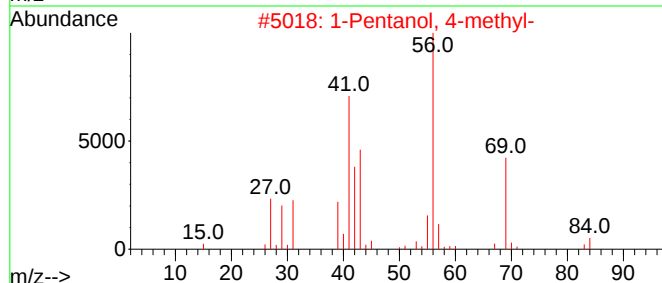
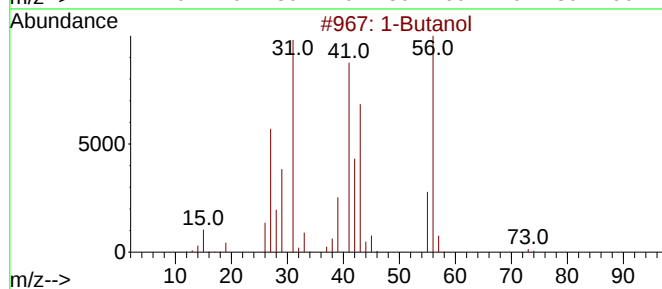
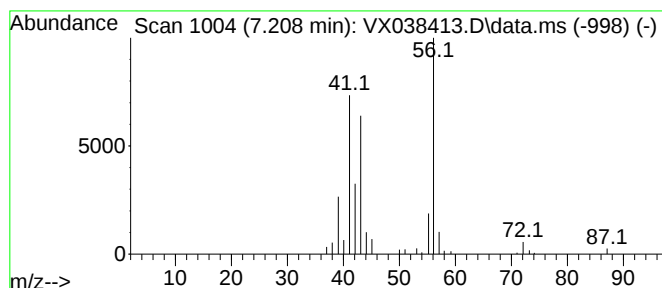
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	9.97 ug/l	103808	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol	74	C4H10O	000071-36-3	80
2		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	56
3		Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	45
4		Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	40
5		2-Butene	56	C4H8	000107-01-7	40



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	386.3	ug/l	2875030	1	5.556	372142	50.0
Ethanol	2.050	84.4	ug/l	628388	1	5.556	372142	50.0
Propanal	2.294	8.3	ug/l	61631	1	5.556	372142	50.0
Butanal	4.227	15.1	ug/l	112587	1	5.556	372142	50.0
1-Butanol	7.208	10.0	ug/l	103808	2	6.763	520395	50.0