

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
 Data File : VX029008.D
 Acq On : 26 May 2022 18:45
 Operator : JC/MD
 Sample : N3053-04 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 52322-F

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\82X051222W.M

Title : SW846 8260

Signal : TIC: VX029008.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	84	rBV	911067	1113112	14.37%	5.484%
2	2.081	150	163	192	rBV	3759408	7748386	100.00%	38.171%
3	2.380	206	212	224	rVB	121033	198286	2.56%	0.977%
4	3.861	443	455	470	rBV	68344	201029	2.59%	0.990%
5	4.562	562	570	584	rBV2	30033	89214	1.15%	0.439%
6	4.715	584	595	612	rVV	145851	408153	5.27%	2.011%
7	5.391	693	706	721	rBV	215953	626411	8.08%	3.086%
8	5.556	721	733	750	rVB	336020	957494	12.36%	4.717%
9	5.830	770	778	789	rBV	35720	98239	1.27%	0.484%
10	5.958	789	799	817	rVB	219420	583508	7.53%	2.875%
11	6.763	921	931	947	rBV	546361	1303725	16.83%	6.423%
12	7.214	998	1005	1030	rBV	191682	438703	5.66%	2.161%
13	8.653	1233	1241	1248	rBV	1170444	1793052	23.14%	8.833%
14	10.055	1465	1471	1483	rBV	1237329	1625094	20.97%	8.006%
15	10.579	1553	1557	1565	rBV	60147	90632	1.17%	0.446%
16	11.085	1634	1640	1651	rBV	962375	1276583	16.48%	6.289%
17	12.024	1788	1794	1802	rBV	1296910	1606791	20.74%	7.916%
18	15.560	2368	2374	2381	rBV	91773	140669	1.82%	0.693%

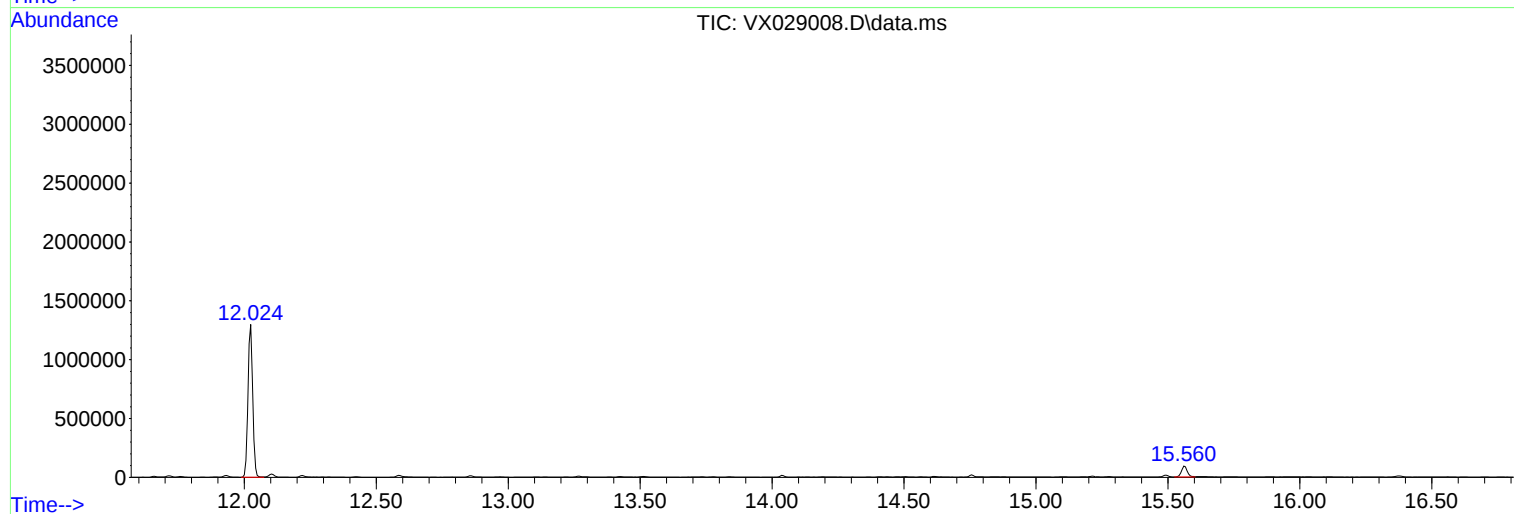
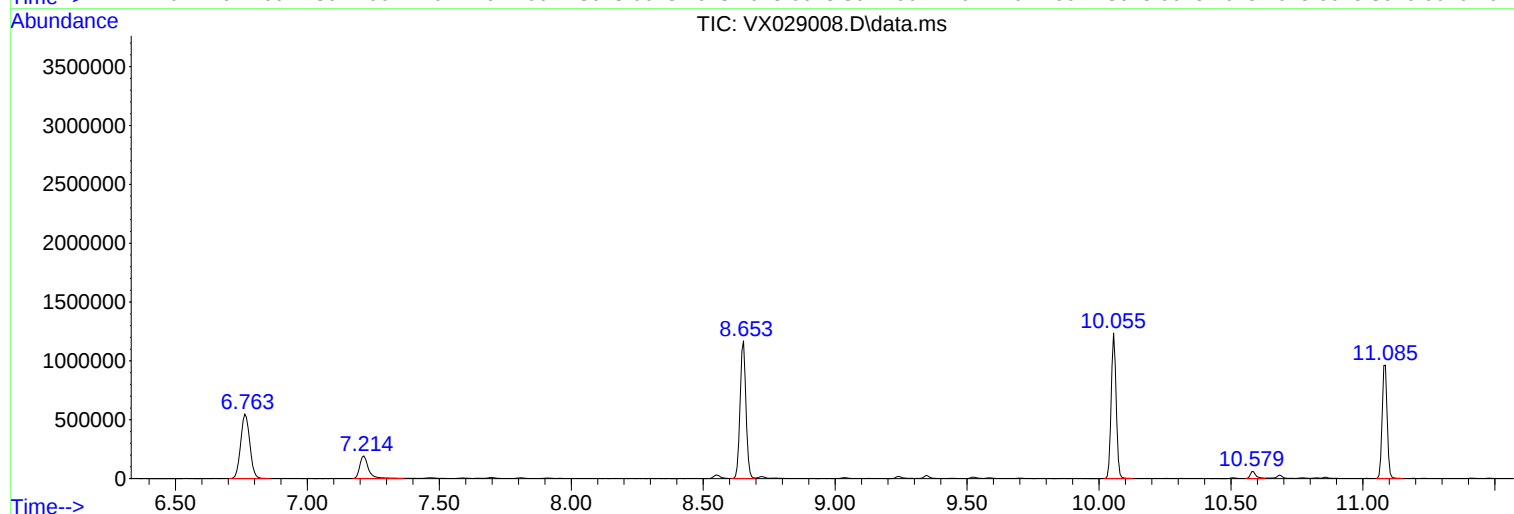
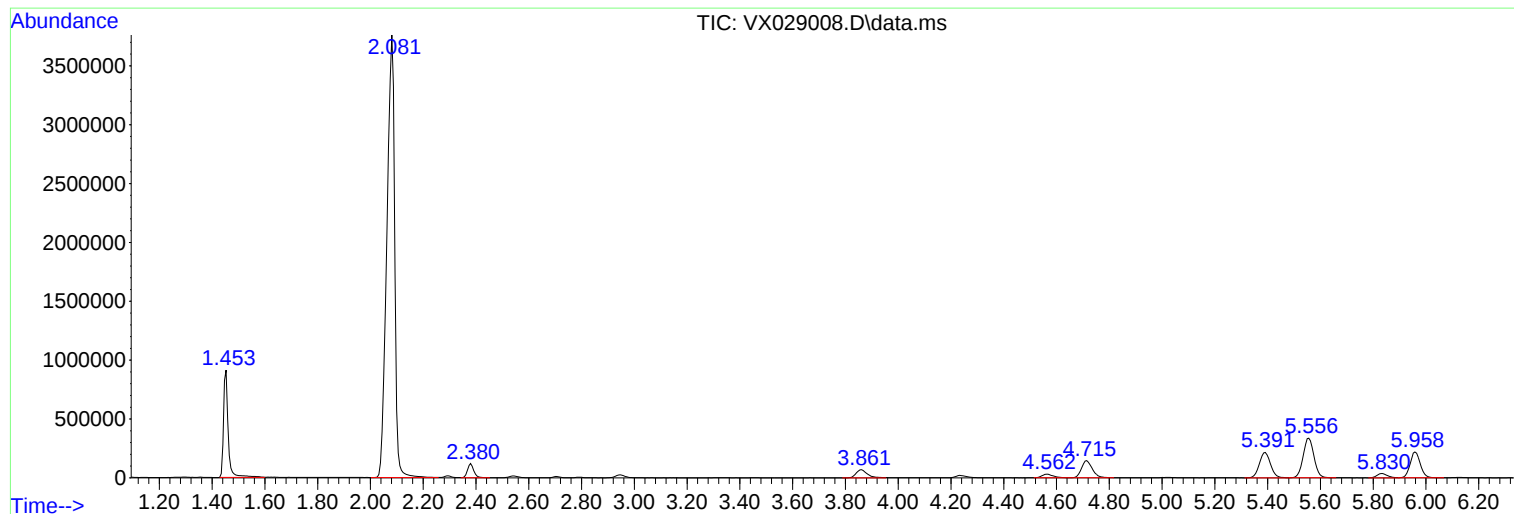
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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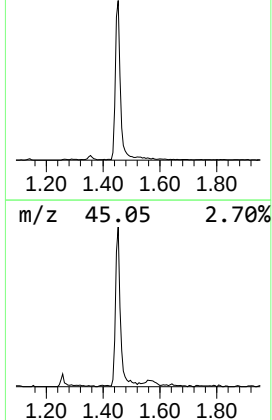
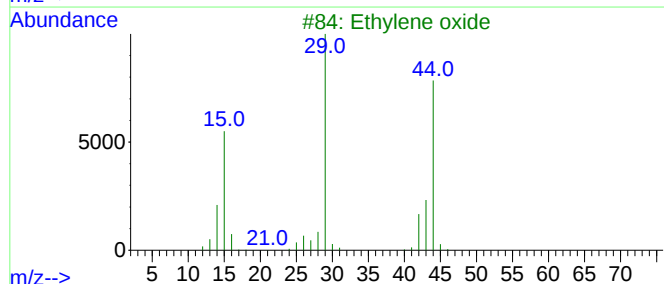
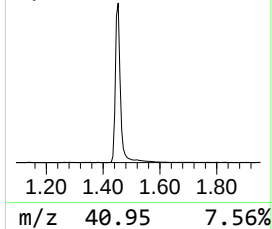
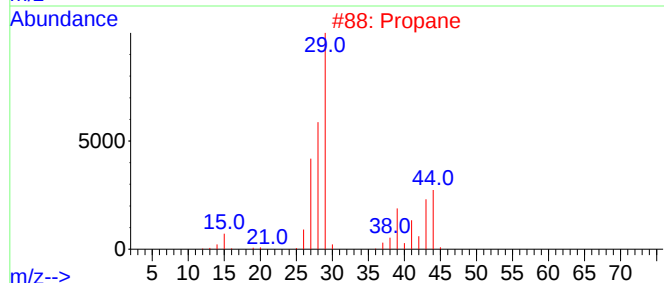
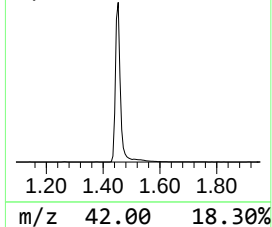
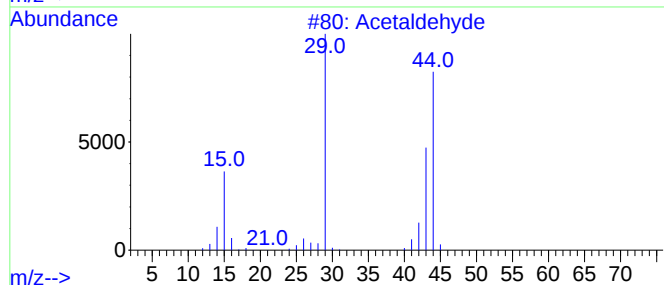
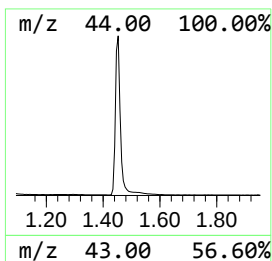
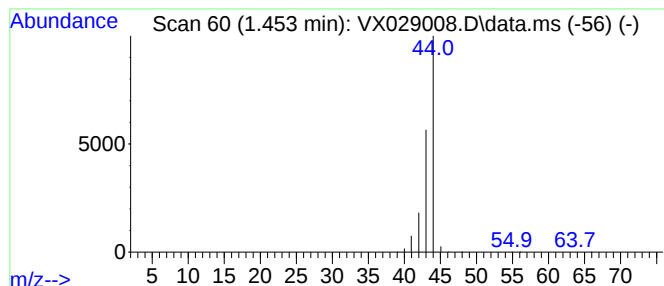
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
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Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	58.13 ug/l	1113110	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			1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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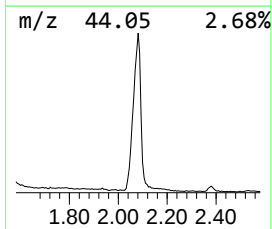
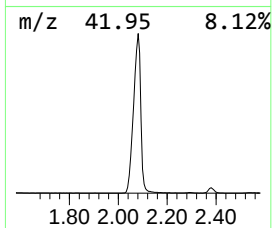
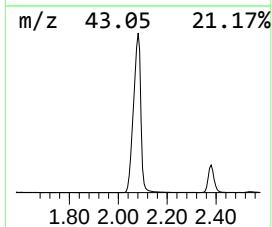
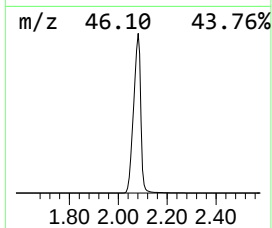
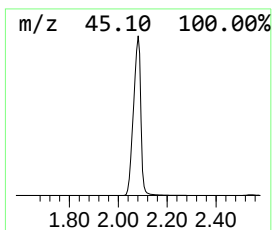
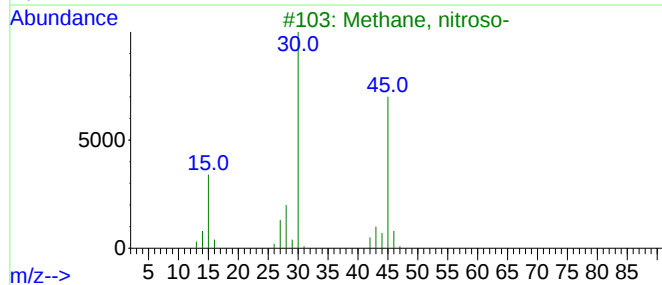
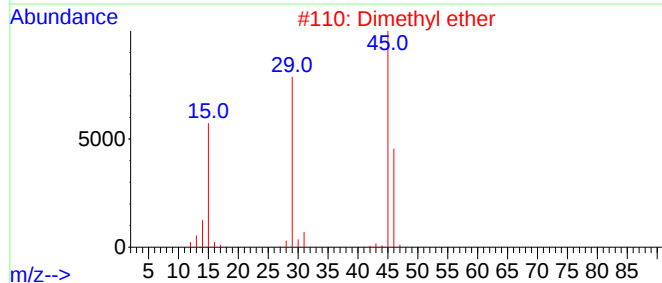
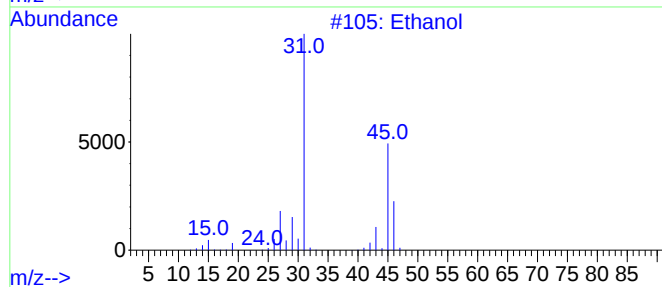
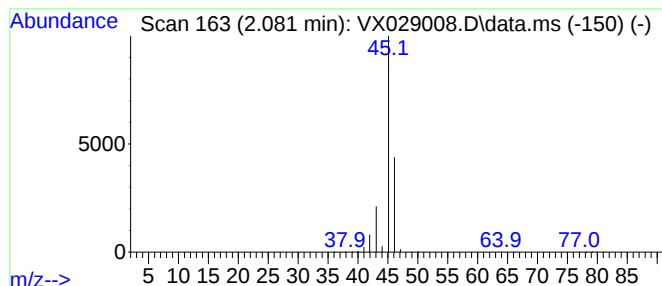
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.081	404.62 ug/l	7748390	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
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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Instrument :
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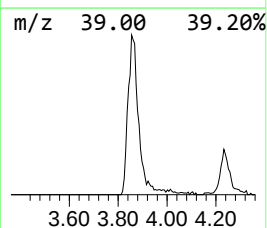
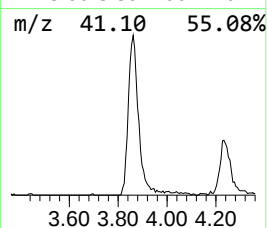
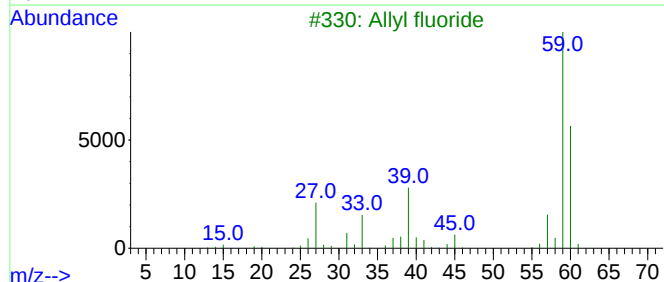
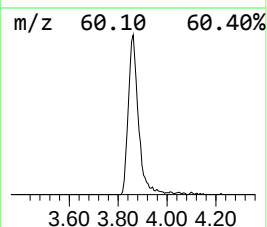
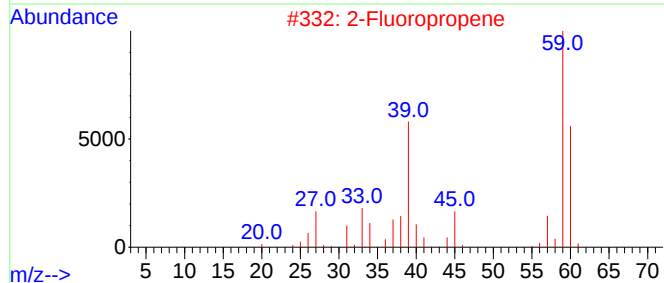
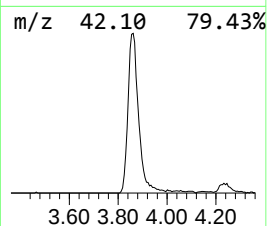
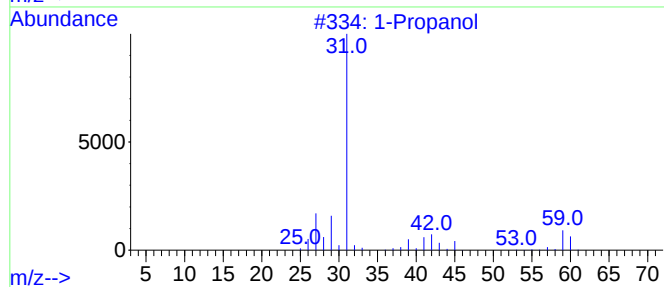
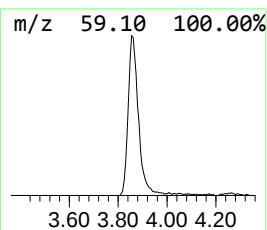
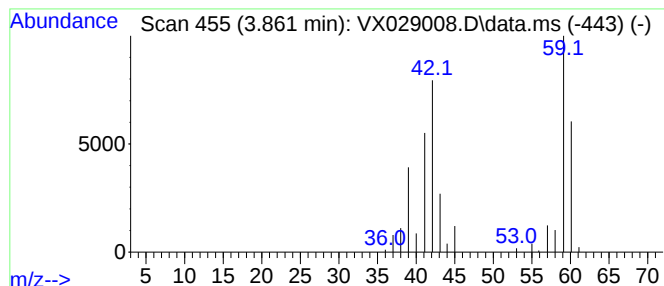
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	10.50 ug/l	201029	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	50
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	1,2-Butanediol			90	C4H10O2	000584-03-2	9



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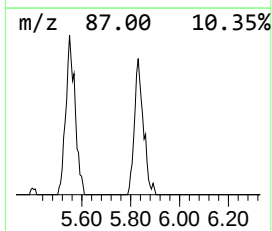
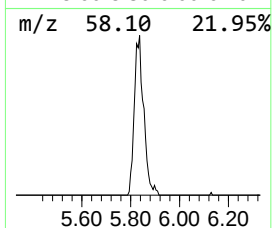
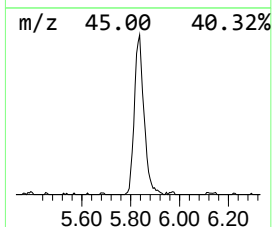
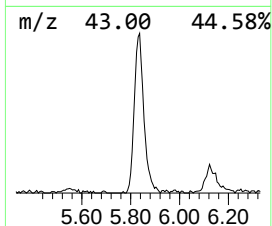
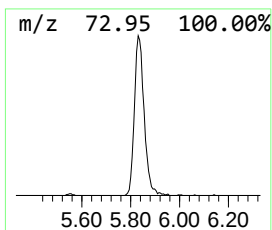
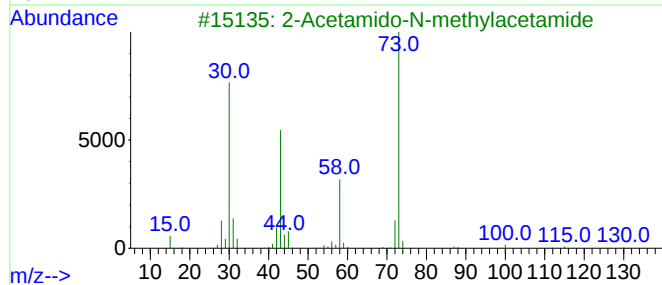
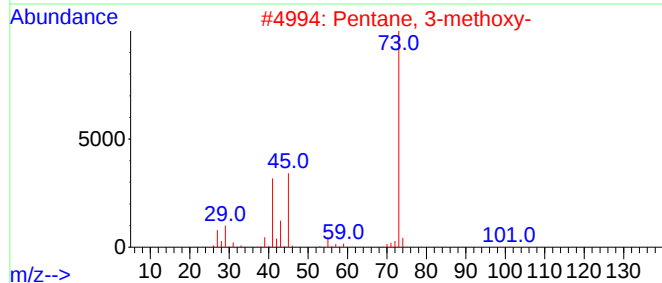
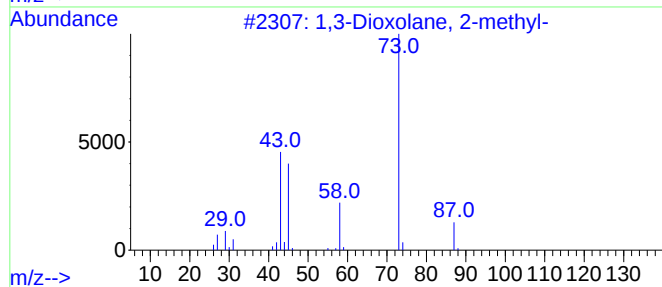
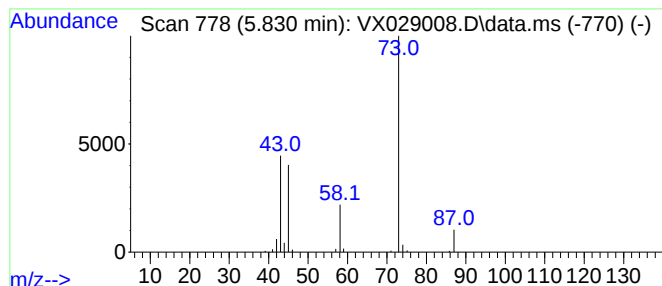
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	5.13 ug/l	98239	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	23
4			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9



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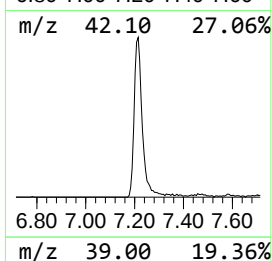
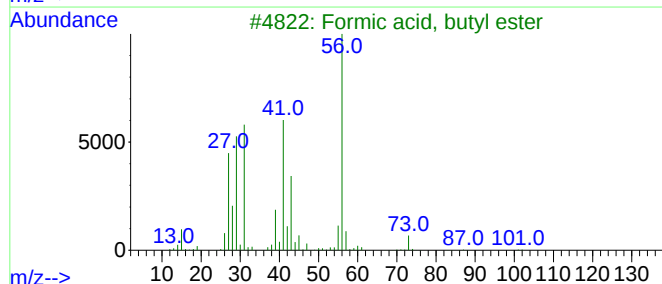
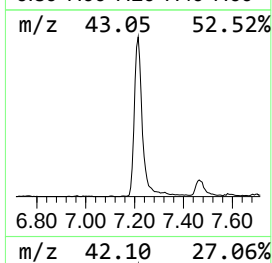
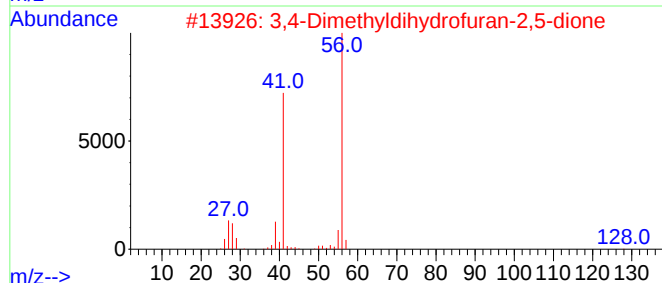
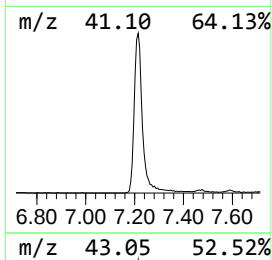
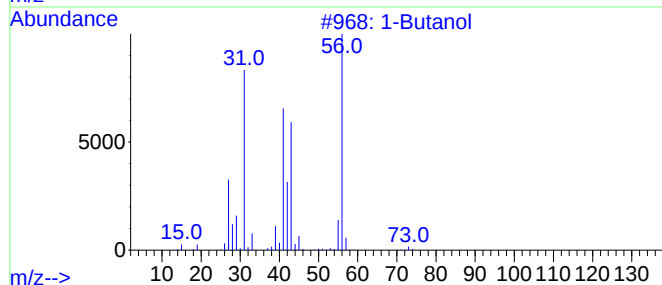
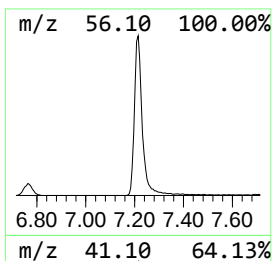
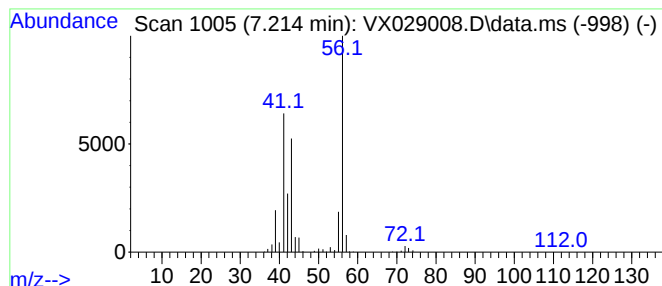
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	16.82 ug/l	438703	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
3			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	58.1	ug/l	1113110	1	5.556	957494	50.0
Ethanol	2.081	404.6	ug/l	7748390	1	5.556	957494	50.0
1-Propanol	3.861	10.5	ug/l	201029	1	5.556	957494	50.0
1,3-Dioxolane, ...	5.830	5.1	ug/l	98239	1	5.556	957494	50.0
1-Butanol	7.214	16.8	ug/l	438703	2	6.763	1303730	50.0