

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
 Data File : VX029010.D
 Acq On : 26 May 2022 19:32
 Operator : JC/MD
 Sample : N3053-06 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 52322-H

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: VX029010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	79	rBV	1976096	2538424	29.36%	10.986%
2	2.081	152	163	193	rBV	4294144	8646203	100.00%	37.418%
3	2.380	206	212	229	rVB	137152	228767	2.65%	0.990%
4	3.861	444	455	476	rBV	80100	238747	2.76%	1.033%
5	4.562	558	570	584	rBV2	31455	97978	1.13%	0.424%
6	4.715	584	595	616	rVB	162753	464075	5.37%	2.008%
7	5.391	694	706	721	rBV	214618	630075	7.29%	2.727%
8	5.556	721	733	751	rVB	337660	965617	11.17%	4.179%
9	5.830	770	778	789	rBV	41786	112459	1.30%	0.487%
10	5.958	789	799	814	rVB2	222132	587226	6.79%	2.541%
11	6.763	921	931	948	rBV	550923	1315019	15.21%	5.691%
12	7.214	997	1005	1024	rBV	238030	522146	6.04%	2.260%
13	8.653	1233	1241	1248	rBV	1147969	1815949	21.00%	7.859%
14	10.055	1465	1471	1481	rBV	1266844	1657046	19.17%	7.171%
15	10.580	1552	1557	1566	rBV	71939	112923	1.31%	0.489%
16	11.079	1634	1639	1653	rBV	996123	1308312	15.13%	5.662%
17	12.024	1788	1794	1802	rBV	1344044	1666099	19.27%	7.210%
18	15.560	2369	2374	2381	rBV	126402	199786	2.31%	0.865%

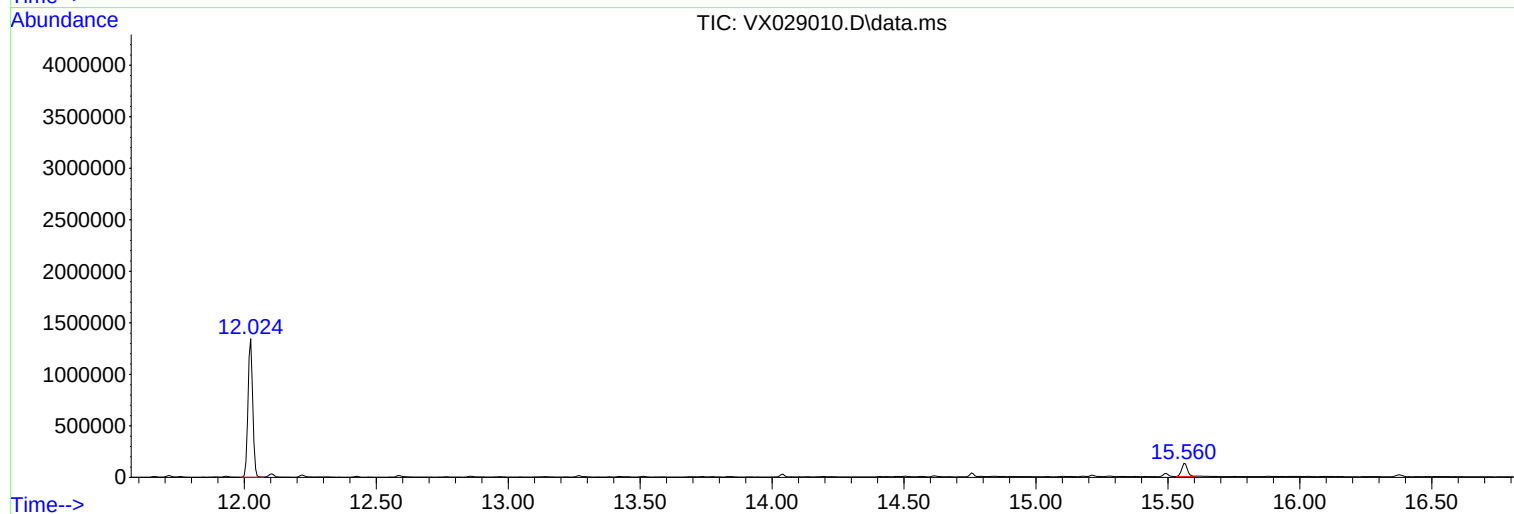
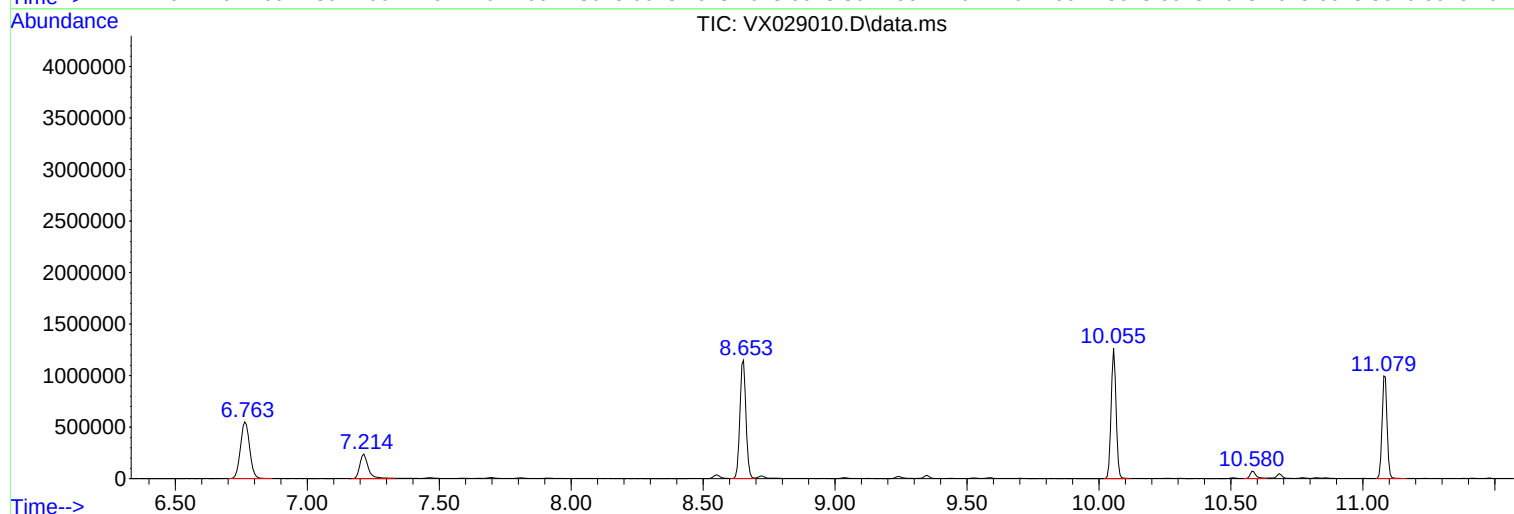
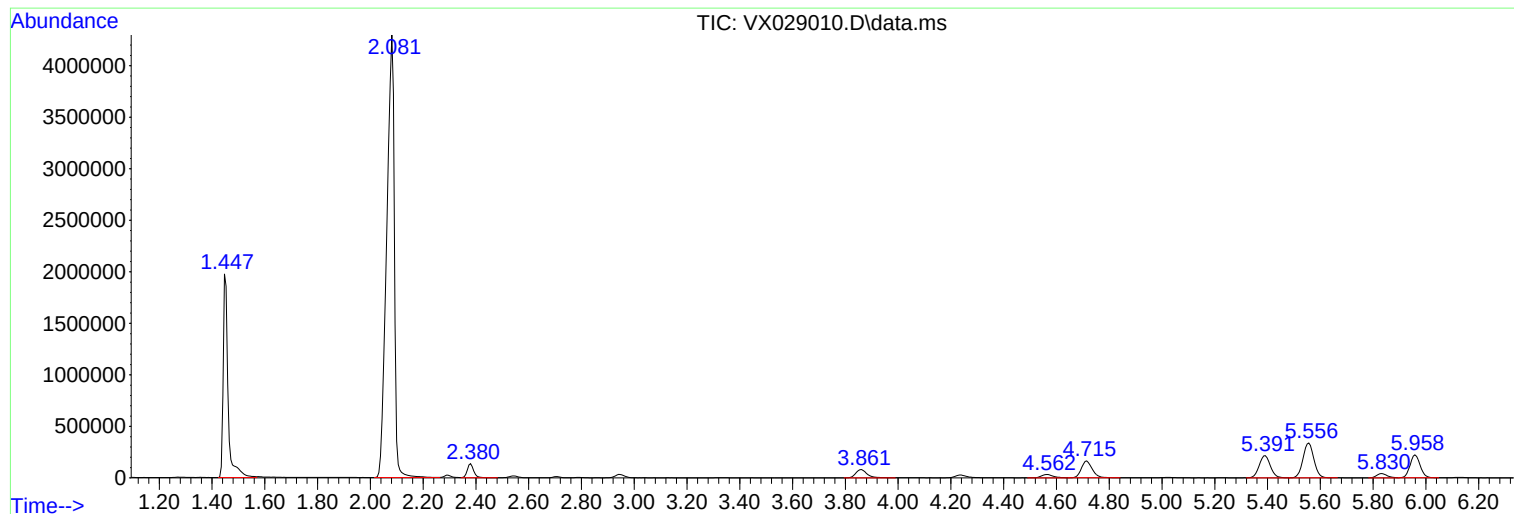
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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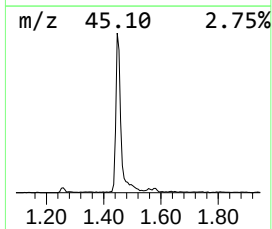
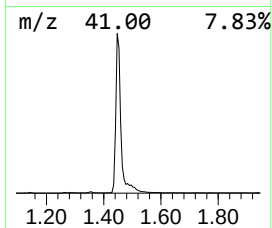
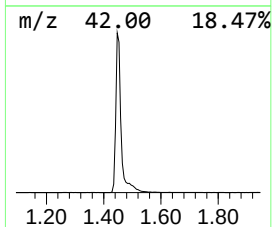
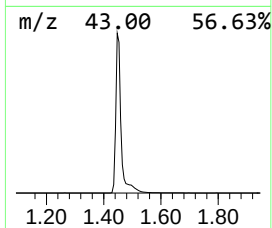
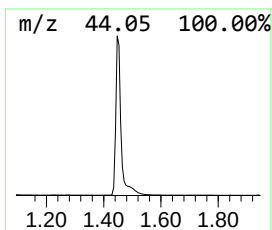
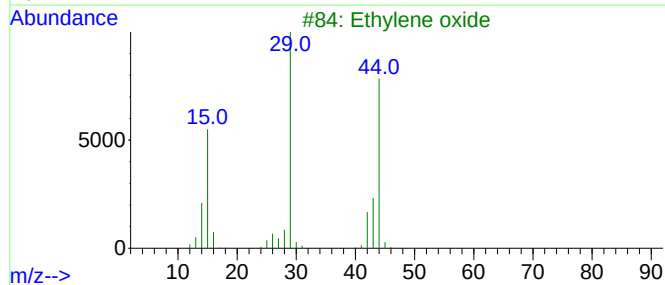
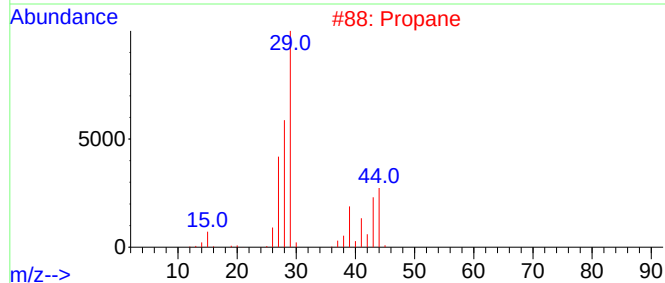
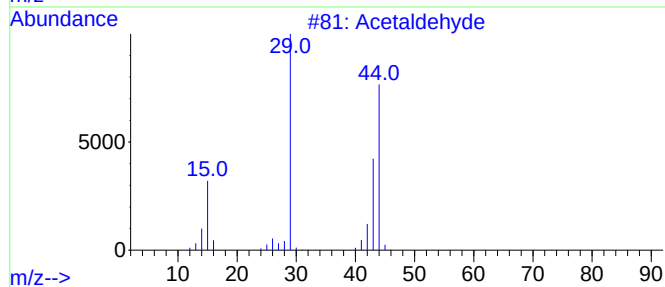
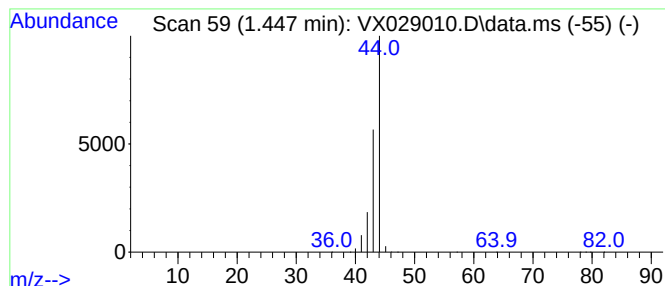
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	131.44 ug/l	2538420	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
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			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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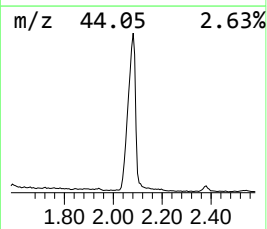
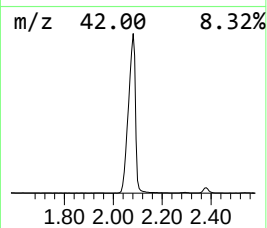
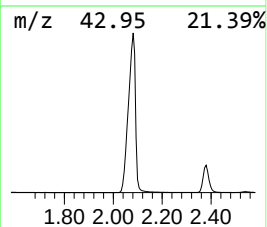
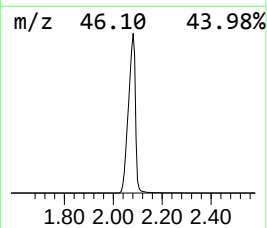
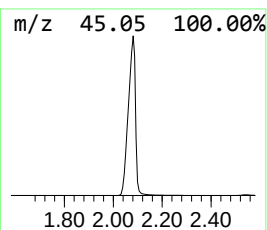
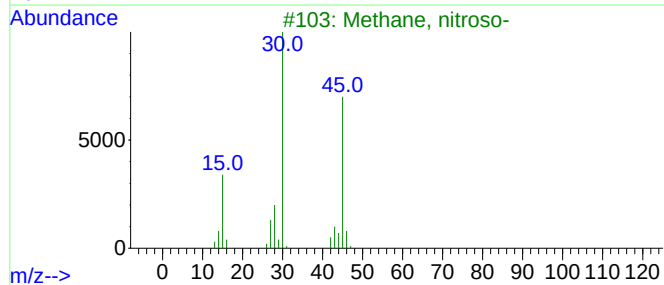
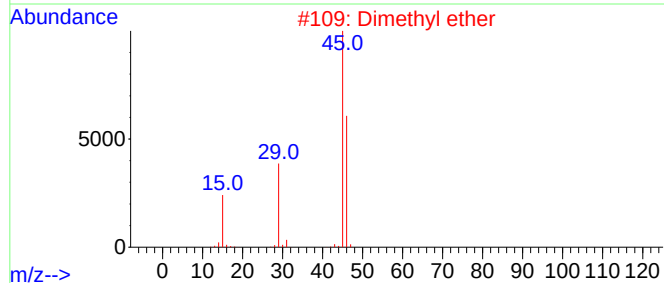
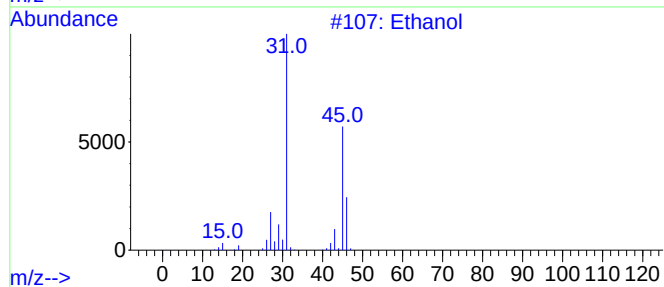
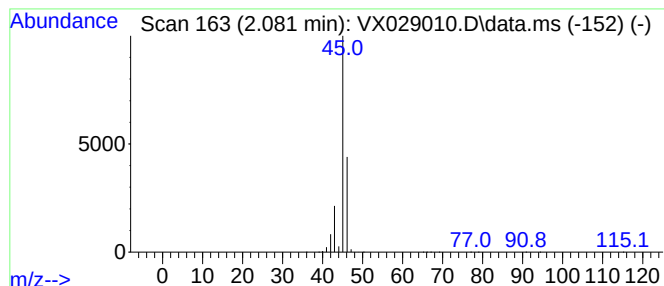
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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	447.70 ug/l	8646200	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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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
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52322-H

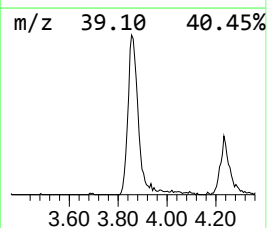
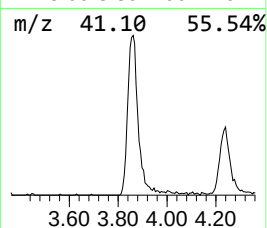
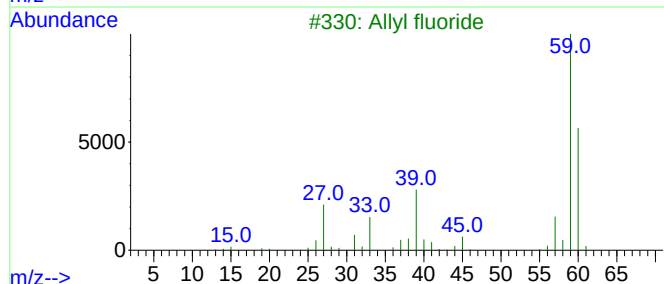
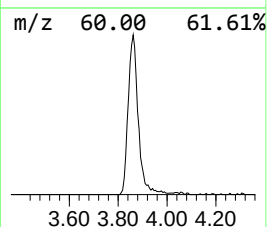
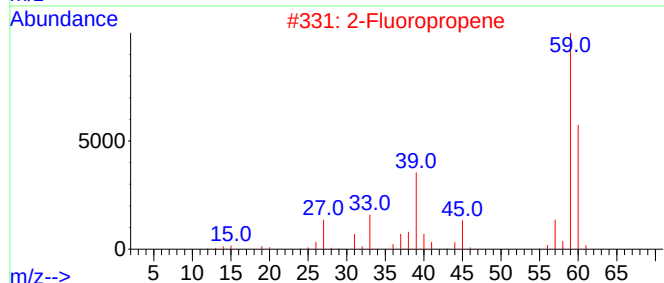
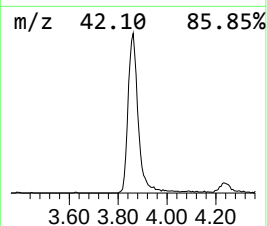
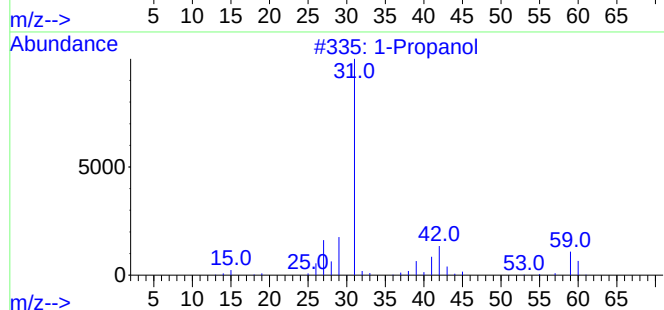
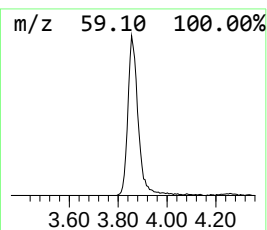
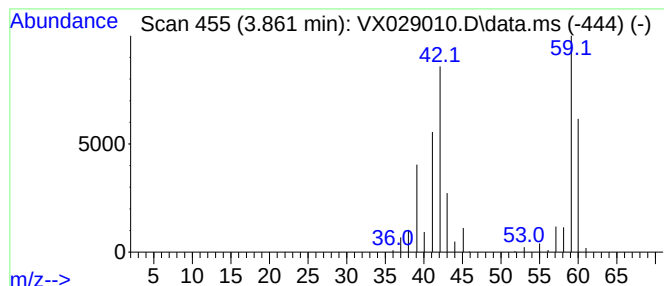
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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	12.36 ug/l	238747	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	64
2	2-Fluoropropene			60	C3H5F	001184-60-7	52
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	Formamidoxime			60	CH4N2O	000624-82-8	9



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

Instrument :
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ClientSampleId :
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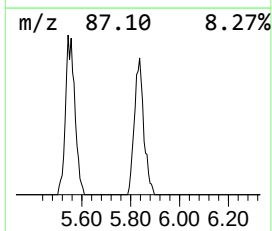
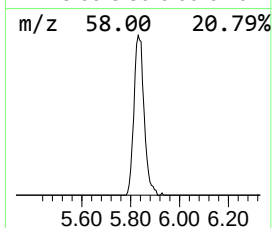
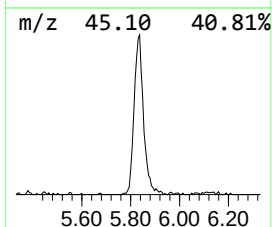
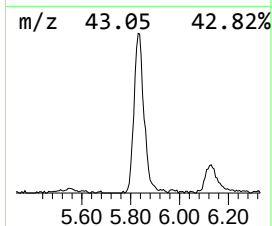
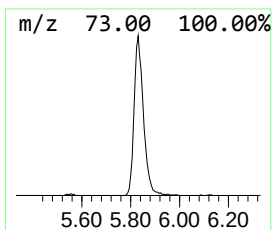
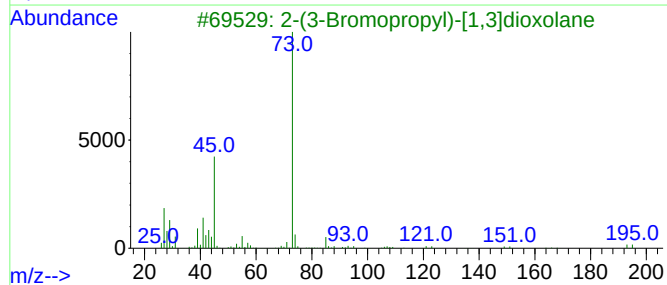
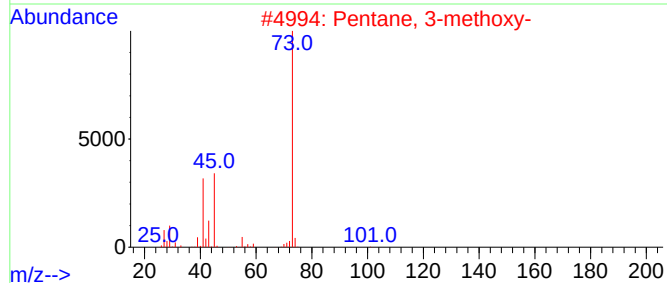
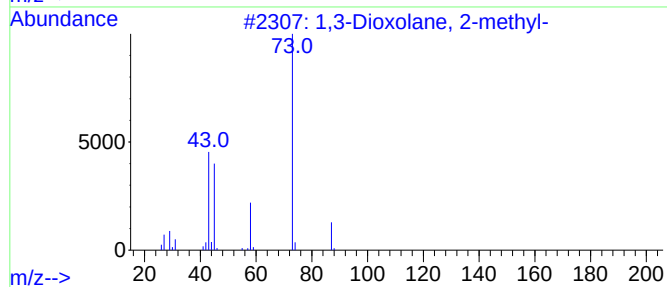
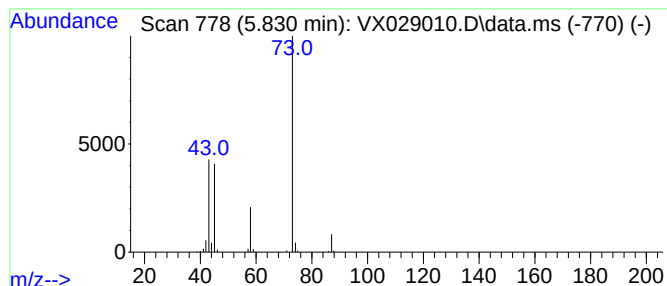
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Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	5.82 ug/l	112459	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	40
3			2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	33
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9



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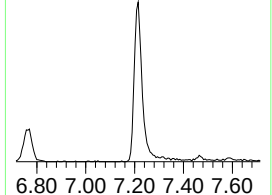
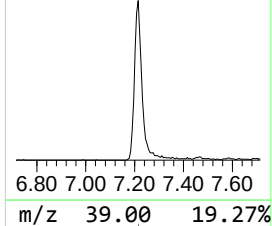
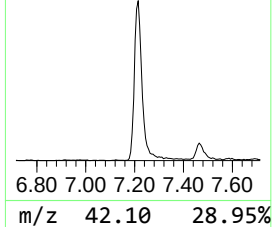
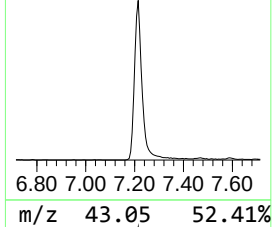
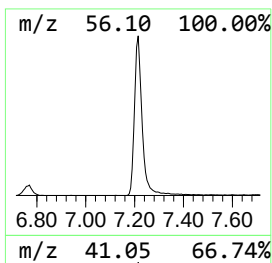
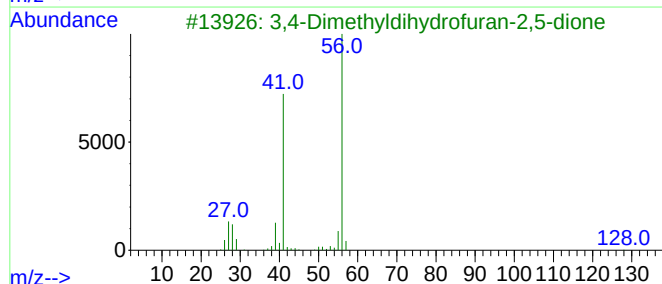
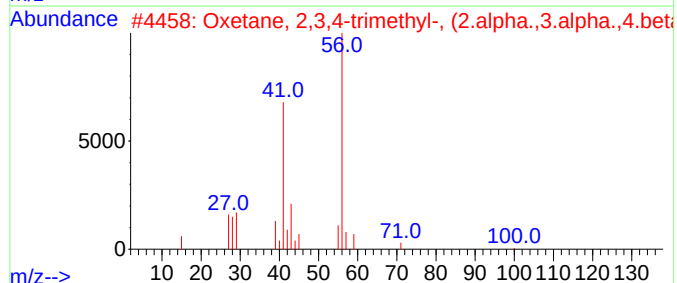
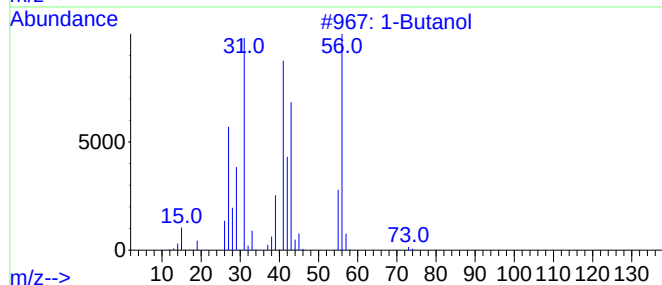
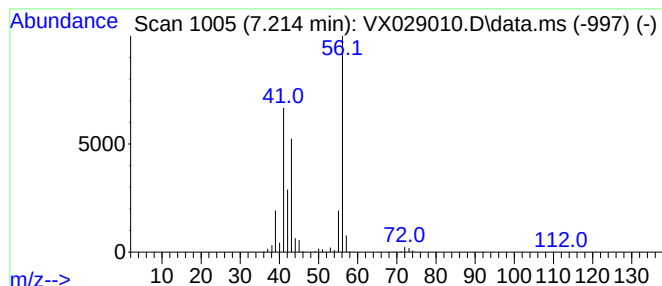
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	19.85 ug/l	522146	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	39
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	36
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



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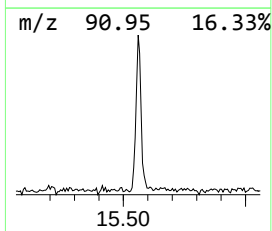
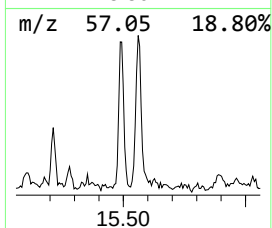
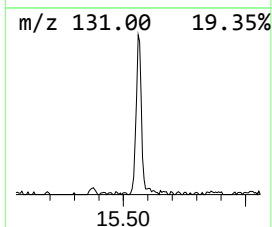
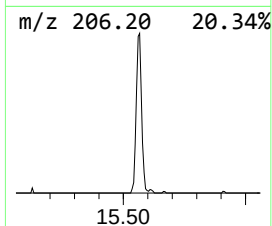
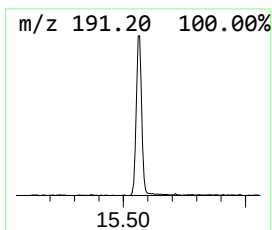
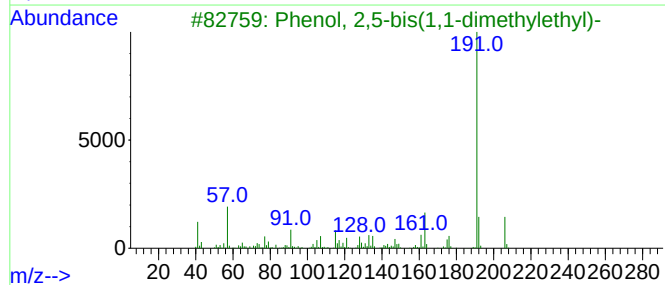
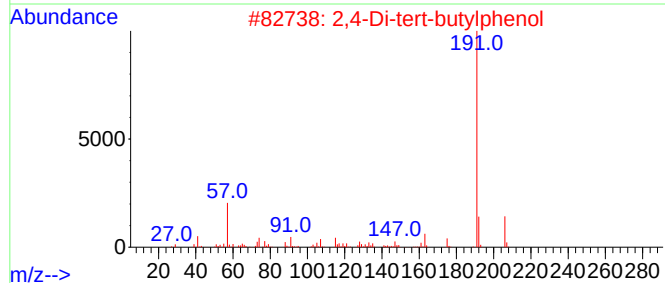
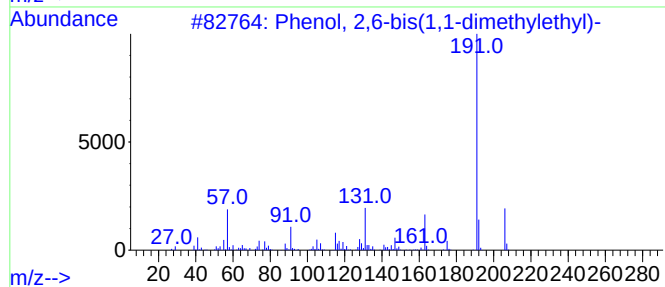
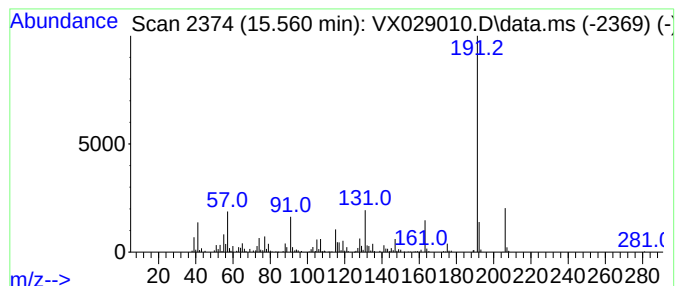
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	6.00 ug/l	199786	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	87
4			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	83
5			2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
Data File : VX029010.D
Acq On : 26 May 2022 19:32
Operator : JC/MD
Sample : N3053-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
52322-H

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
Acetaldehyde	1.447	131.4	ug/l	2538420	1	5.556	965617	50.0
Ethanol	2.081	447.7	ug/l	8646200	1	5.556	965617	50.0
1-Propanol	3.861	12.4	ug/l	238747	1	5.556	965617	50.0
1,3-Dioxolane, ...	5.830	5.8	ug/l	112459	1	5.556	965617	50.0
1-Butanol	7.214	19.9	ug/l	522146	2	6.763	1315020	50.0
Phenol, 2,6-bis...	15.560	6.0	ug/l	199786	4	12.024	1666100	50.0