

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
 Data File : VX029007.D
 Acq On : 26 May 2022 18:22
 Operator : JC/MD
 Sample : N3053-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 52322-E

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: VX029007.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	76	rBV	602908	722997	9.17%	3.528%
2	2.081	152	163	192	rVB	3952807	7881336	100.00%	38.458%
3	2.380	206	212	222	rVB	126672	201783	2.56%	0.985%
4	3.855	442	454	475	rBV	70870	208830	2.65%	1.019%
5	4.562	558	570	585	rBV	31682	95673	1.21%	0.467%
6	4.715	585	595	616	rVB	148525	425570	5.40%	2.077%
7	5.385	693	705	721	rBV	213349	628494	7.97%	3.067%
8	5.556	721	733	750	rVB2	339694	957047	12.14%	4.670%
9	5.830	770	778	789	rBV	36911	99187	1.26%	0.484%
10	5.958	789	799	816	rVB	219112	585331	7.43%	2.856%
11	6.763	921	931	944	rBV	548865	1294164	16.42%	6.315%
12	7.214	997	1005	1022	rBV	193078	440223	5.59%	2.148%
13	8.653	1234	1241	1247	rBV	1150213	1782058	22.61%	8.696%
14	8.720	1247	1252	1259	rVB	321218	483959	6.14%	2.362%
15	10.055	1465	1471	1486	rBV	1243699	1635238	20.75%	7.979%
16	11.085	1634	1640	1651	rBV	968936	1267468	16.08%	6.185%
17	12.024	1788	1794	1802	rBV	1330416	1595257	20.24%	7.784%
18	15.560	2368	2374	2381	rBV	124203	188778	2.40%	0.921%

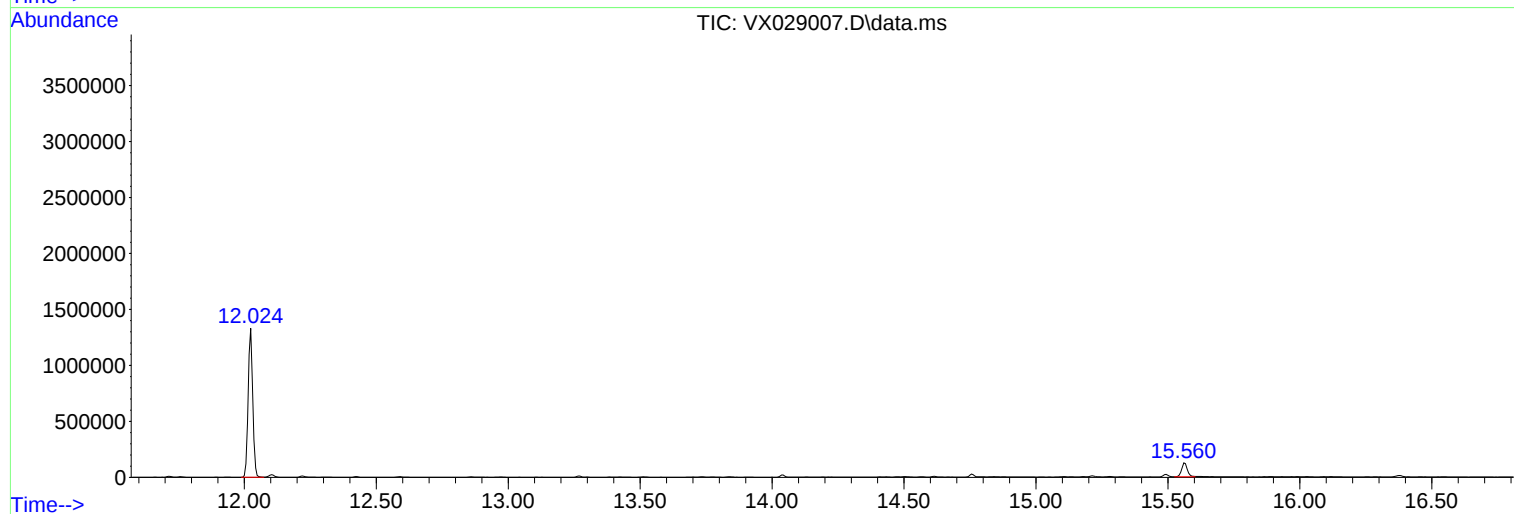
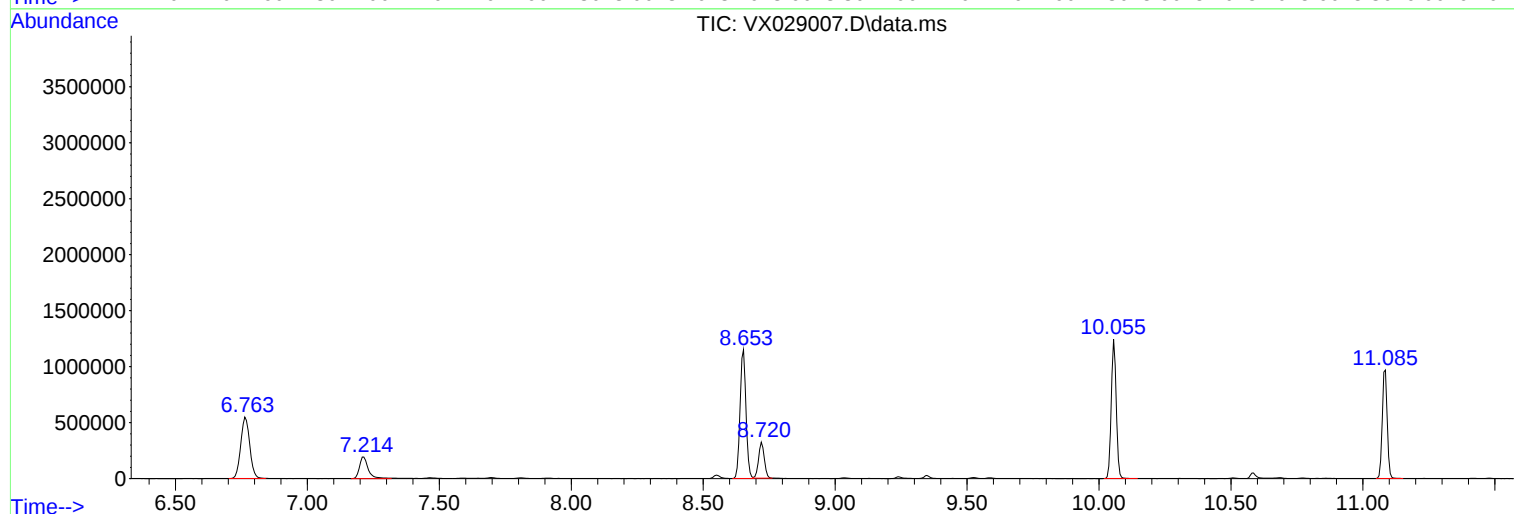
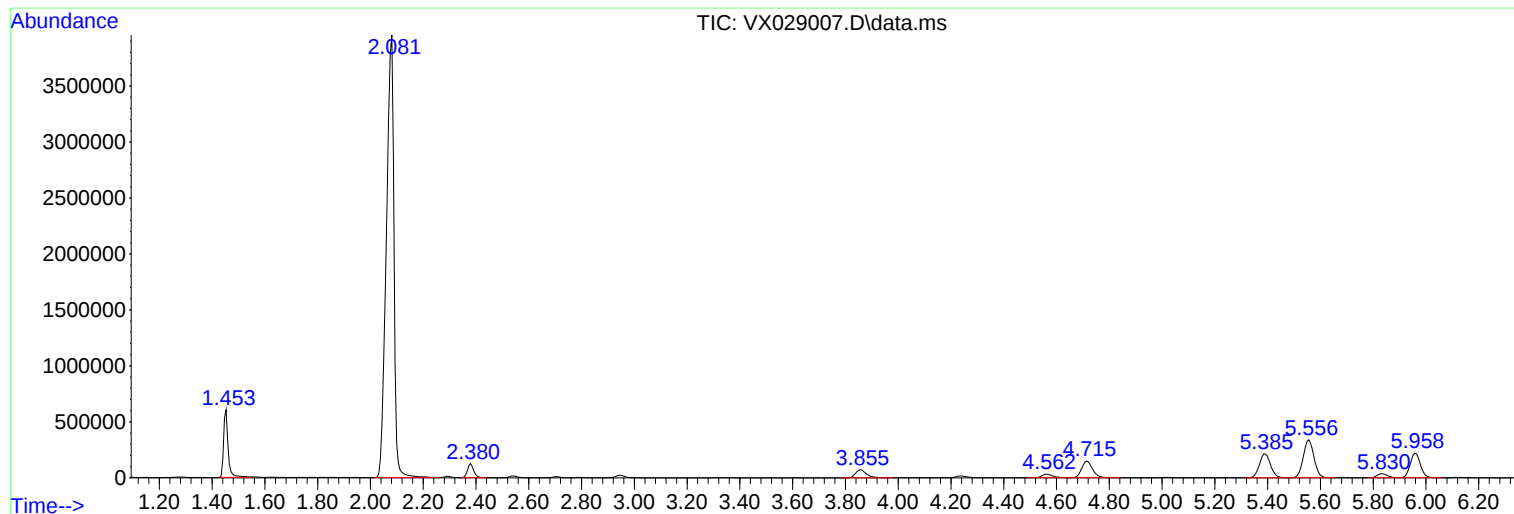
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Quant Title : SW846 8260

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



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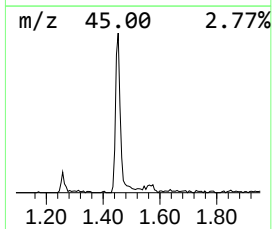
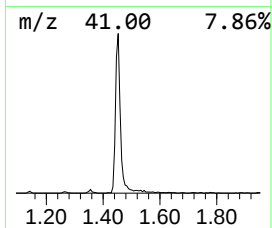
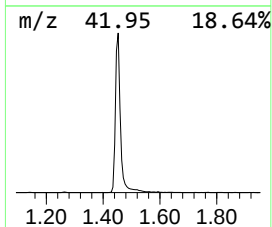
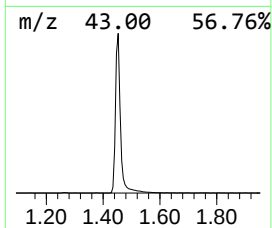
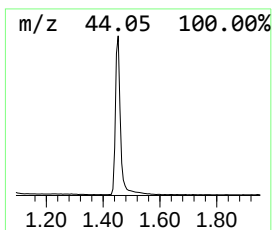
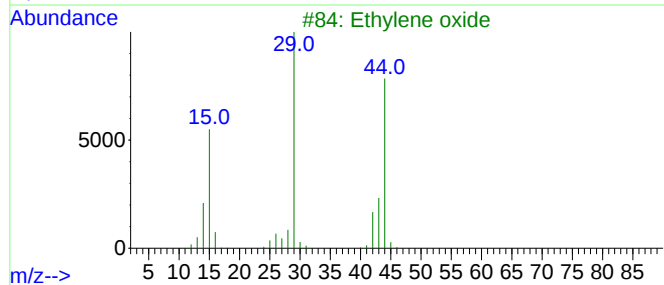
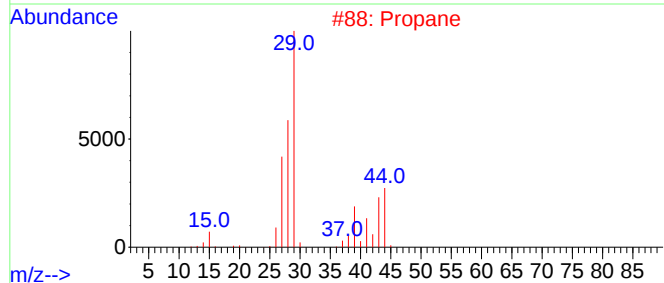
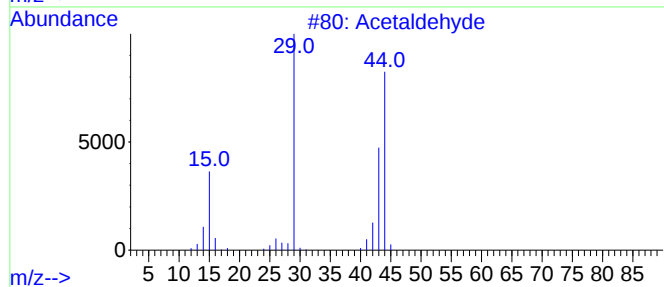
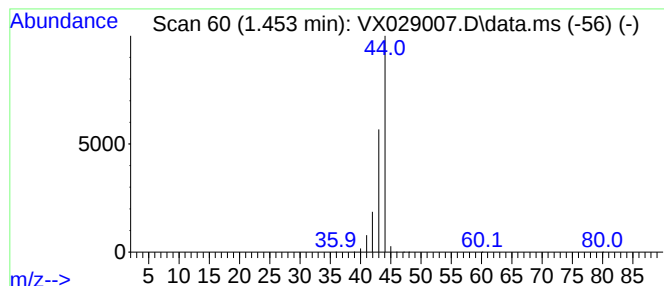
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Quant Title : SW846 8260

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.
1.453	37.77 ug/l	722997	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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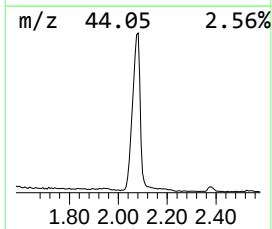
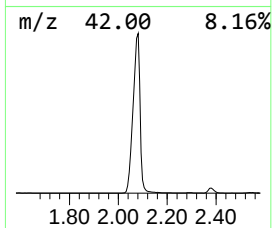
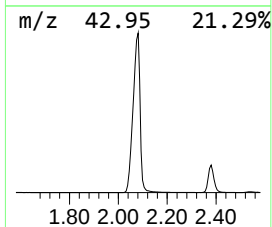
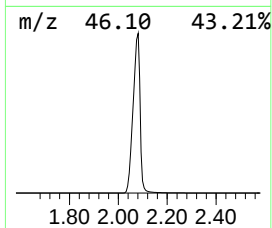
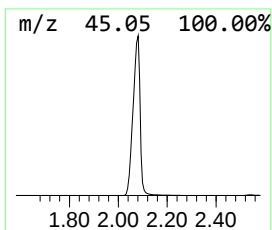
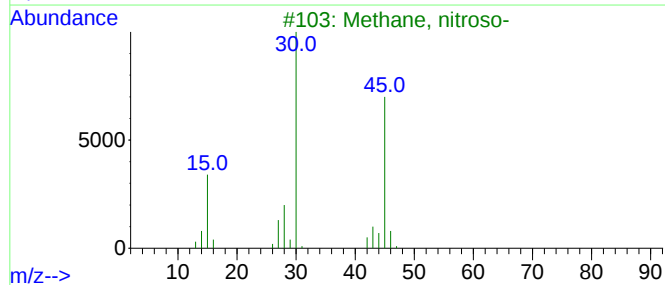
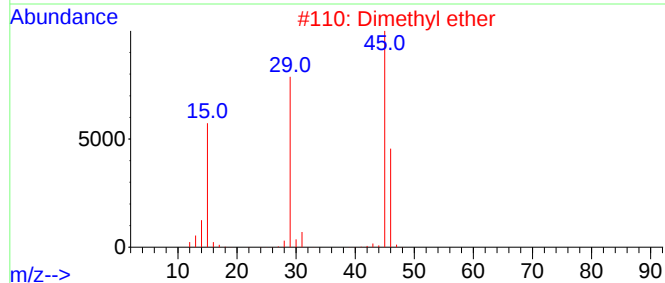
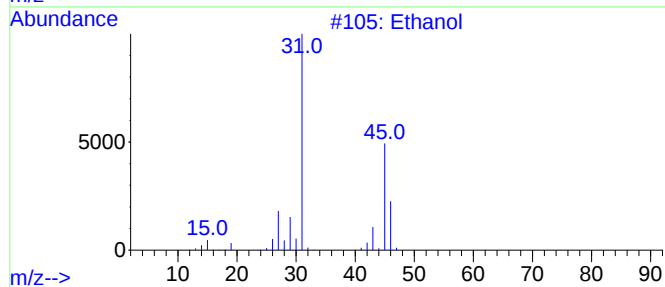
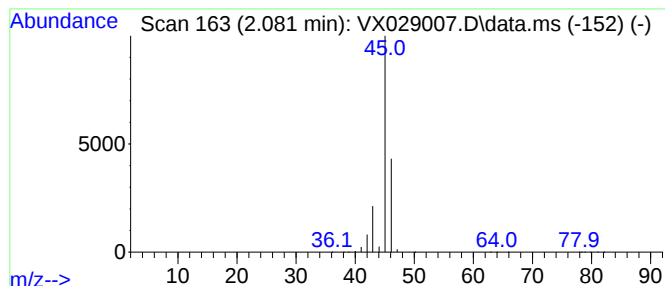
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Quant Title : SW846 8260

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	411.75 ug/l	7881340	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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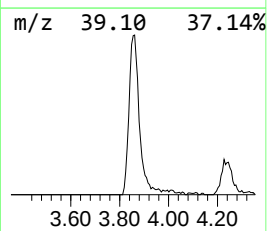
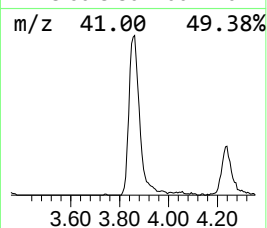
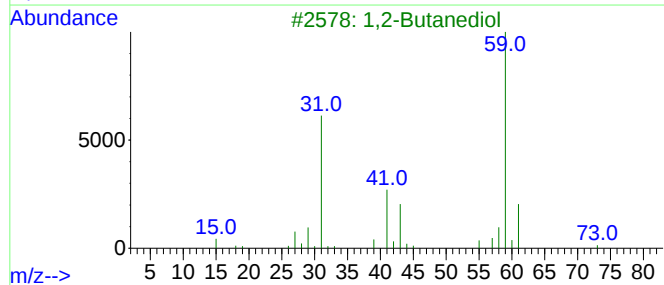
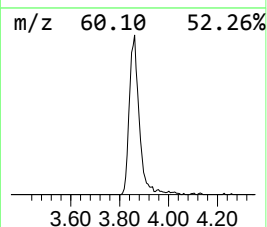
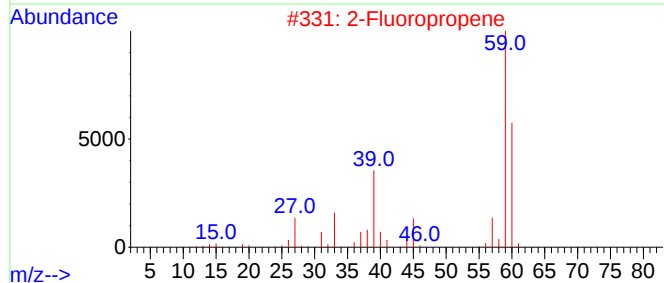
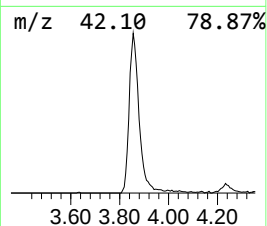
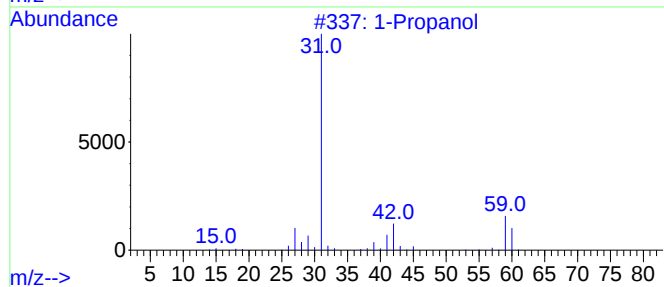
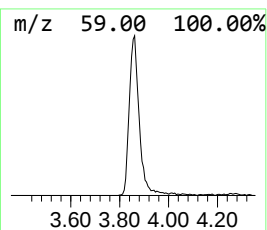
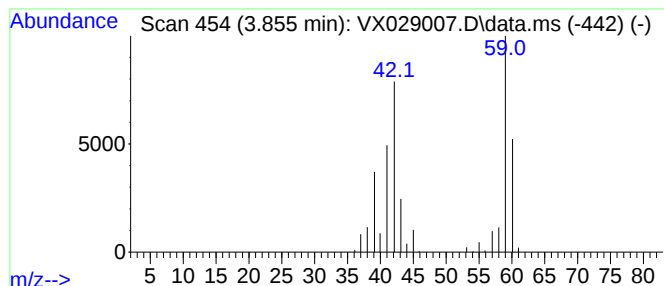
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.855	10.91 ug/l	208830	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	72
2	2-Fluoropropene			60	C3H5F	001184-60-7	49
3	1,2-Butanediol			90	C4H10O2	000584-03-2	17
4	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	17
5	Cyclopropane			42	C3H6	000075-19-4	12



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Instrument :
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ClientSampleId :
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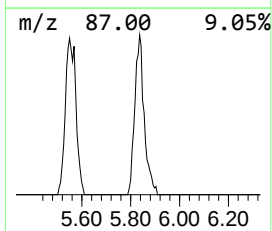
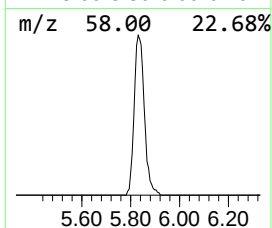
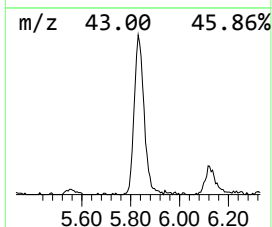
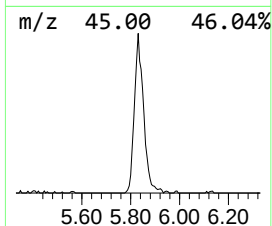
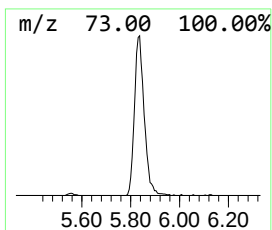
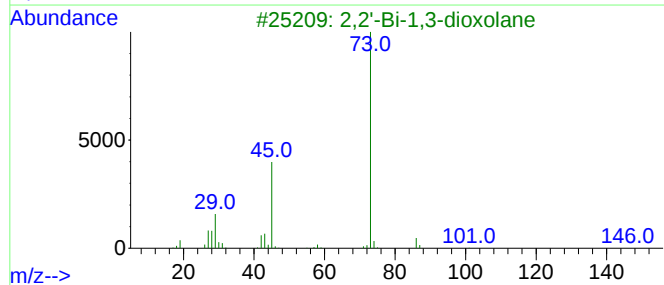
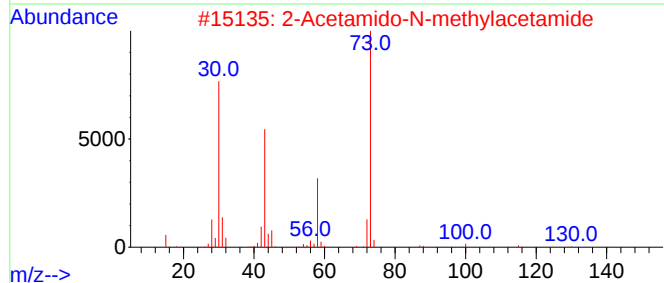
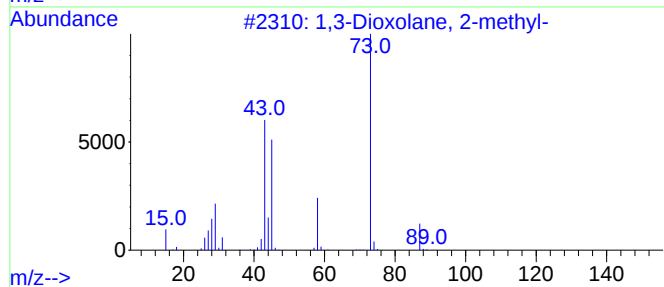
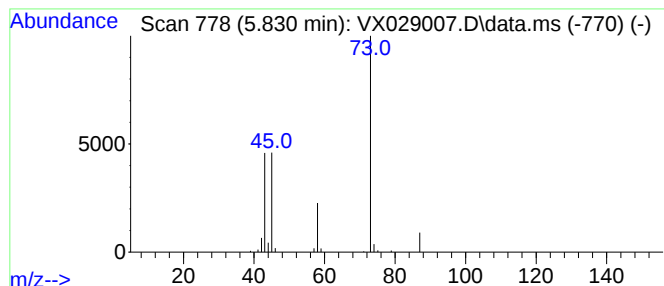
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Quant Title : SW846 8260

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	5.18 ug/l	99187	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			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	47
3			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
4			Ethene, methoxy-	58	C3H6O	000107-25-5	7
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	7



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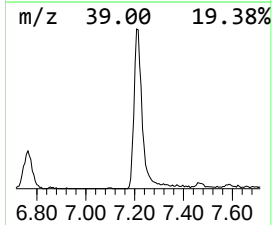
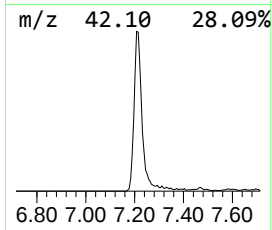
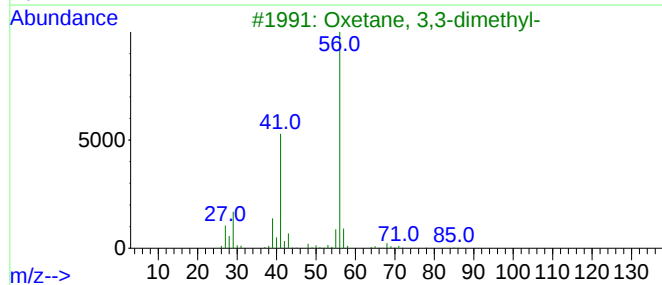
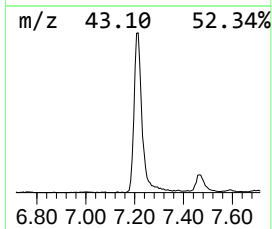
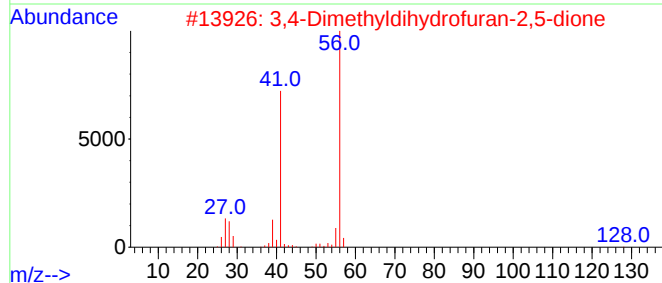
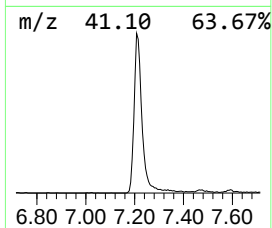
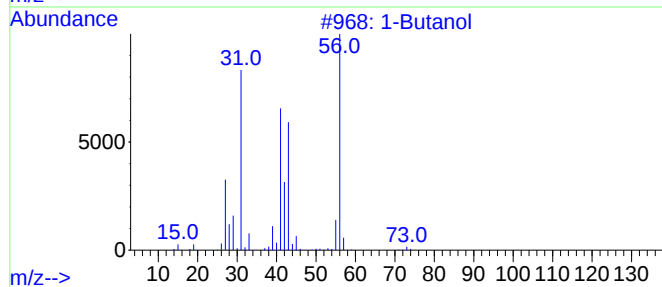
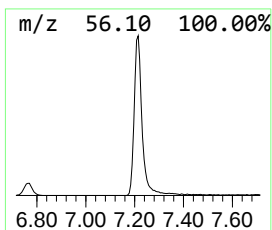
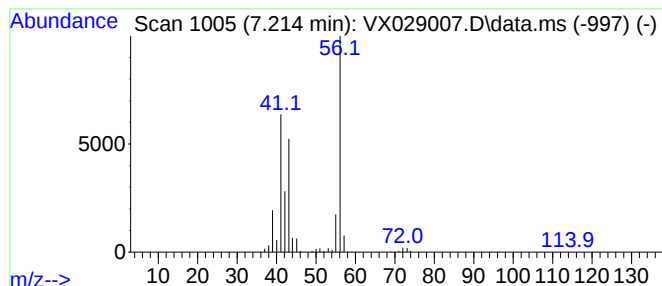
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Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	17.01 ug/l	440223	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			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4			Methoxyacetonitrile	71	C3H5NO	001738-36-9	9
5			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9



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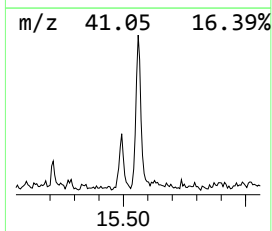
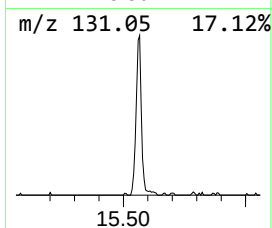
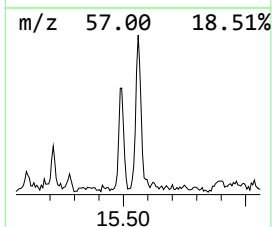
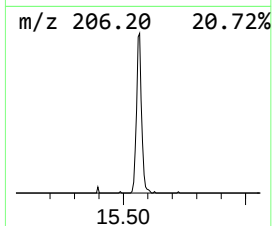
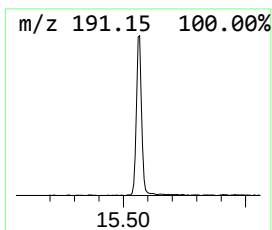
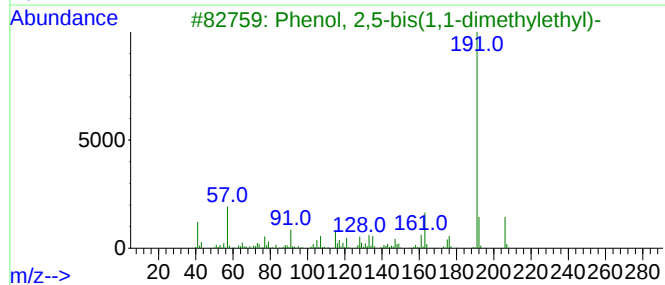
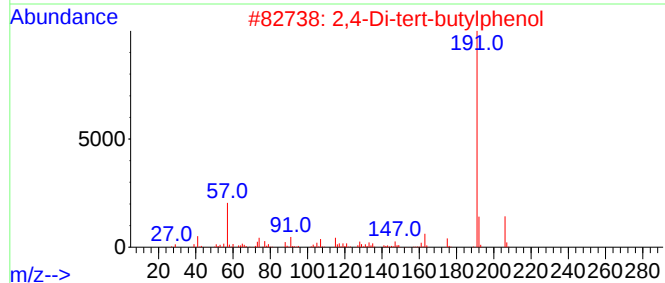
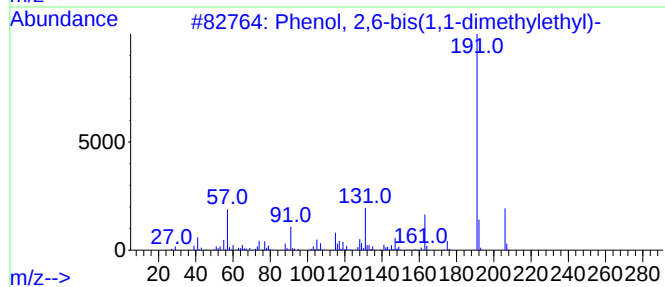
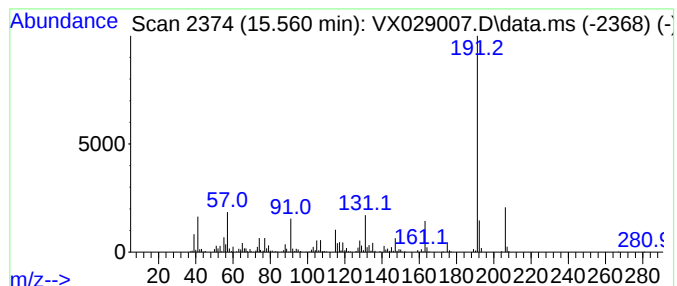
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	5.92 ug/l	188778	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	91
3			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	87
4			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	81
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052622\
Data File : VX029007.D
Acq On : 26 May 2022 18:22
Operator : JC/MD
Sample : N3053-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
52322-E

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	1.453	37.8	ug/l	722997	1	5.556	957047	50.0
Ethanol	2.081	411.8	ug/l	7881340	1	5.556	957047	50.0
1-Propanol	3.855	10.9	ug/l	208830	1	5.556	957047	50.0
1,3-Dioxolane, ...	5.830	5.2	ug/l	99187	1	5.556	957047	50.0
1-Butanol	7.214	17.0	ug/l	440223	2	6.763	1294160	50.0
Phenol, 2,6-bis...	15.560	5.9	ug/l	188778	4	12.024	1595260	50.0