

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071379.D
 Acq On : 18 Mar 2022 17:55
 Operator : JC\MD
 Sample : N2009-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31722

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_N\methods\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	35	50	57	rBV	928053	4194422	72.61%	8.891%
2	2.581	95	101	124	rVB	2869590	5777030	100.00%	12.246%
3	3.681	280	288	305	rBV	243272	666716	11.54%	1.413%
4	4.140	354	366	382	rBV	965141	2739356	47.42%	5.807%
5	4.287	384	391	397	rVV	67140	196762	3.41%	0.417%
6	4.363	397	404	417	rVB3	80301	245144	4.24%	0.520%
7	4.569	424	439	450	rBV3	81691	368474	6.38%	0.781%
8	4.852	479	487	506	rVB	111546	363281	6.29%	0.770%
9	5.957	666	675	690	rVB3	23404	80881	1.40%	0.171%
10	6.575	765	780	793	rBV2	263926	845703	14.64%	1.793%
11	7.063	853	863	874	rBV2	109453	341224	5.91%	0.723%
12	7.334	901	909	920	rVB	80990	211120	3.65%	0.448%
13	7.651	955	963	980	rBV2	49095	148285	2.57%	0.314%
14	7.840	985	995	1003	rBV	80214	187194	3.24%	0.397%
15	8.022	1014	1026	1031	rBV	539197	1346962	23.32%	2.855%
16	8.087	1031	1037	1054	rVB	1052352	2388866	41.35%	5.064%
17	8.434	1083	1096	1109	rBV	653010	1547766	26.79%	3.281%
18	8.634	1109	1130	1131	rBV2	76634	362085	6.27%	0.768%
19	8.963	1177	1186	1202	rVB	1537316	3218273	55.71%	6.822%
20	9.163	1210	1220	1234	rBV3	401369	1060505	18.36%	2.248%
21	9.392	1252	1259	1270	rVB	25922	62554	1.08%	0.133%
22	10.251	1398	1405	1413	rBV2	43924	101265	1.75%	0.215%
23	10.439	1425	1437	1457	rVV	2545223	4647903	80.45%	9.852%
24	11.739	1650	1658	1670	rBV	2299886	4038117	69.90%	8.560%
25	12.098	1708	1719	1731	rBV	235109	428479	7.42%	0.908%
26	12.269	1741	1748	1756	rBV2	89001	214516	3.71%	0.455%
27	12.351	1756	1762	1774	rVB	139863	269038	4.66%	0.570%
28	12.727	1818	1826	1838	rVB	1945901	3241955	56.12%	6.872%
29	12.904	1849	1856	1865	rVB	39110	78744	1.36%	0.167%
30	13.010	1865	1874	1879	rBV2	113741	203588	3.52%	0.432%
31	13.586	1965	1972	1979	rBV	287883	477835	8.27%	1.013%
32	13.669	1979	1986	1996	rVV	1895413	3255873	56.36%	6.902%
33	13.769	1996	2003	2030	rVV	2225389	3808235	65.92%	8.072%
34	14.992	2204	2211	2215	rBV4	29674	57910	1.00%	0.123%

Sum of corrected areas: 47176061

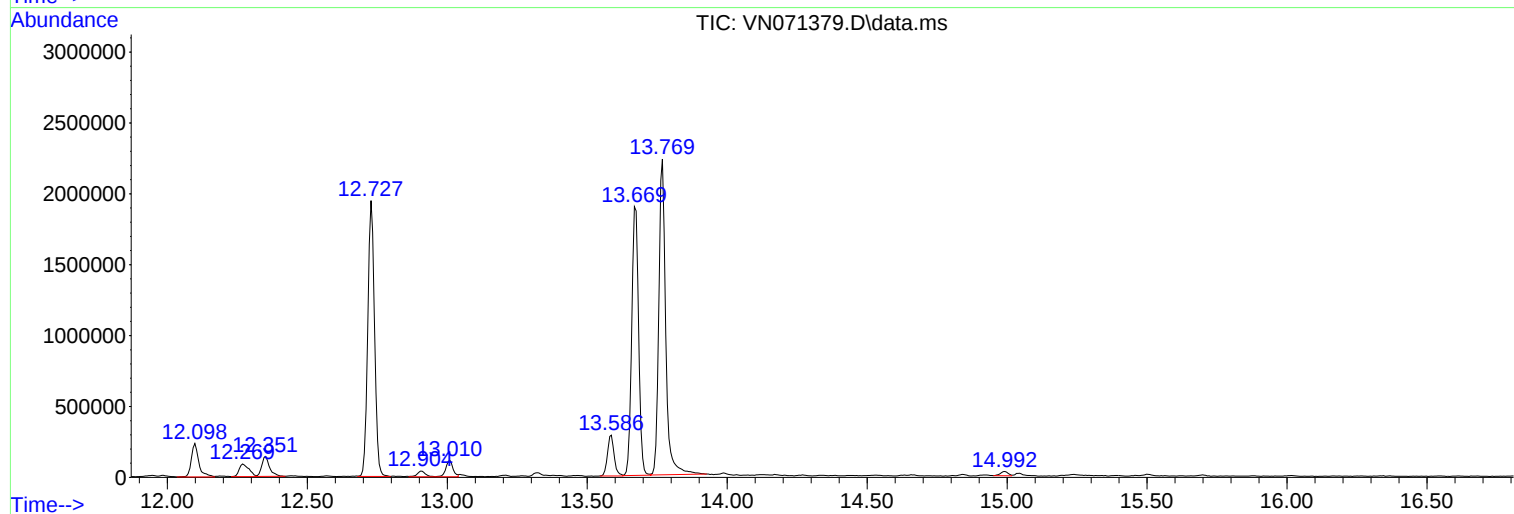
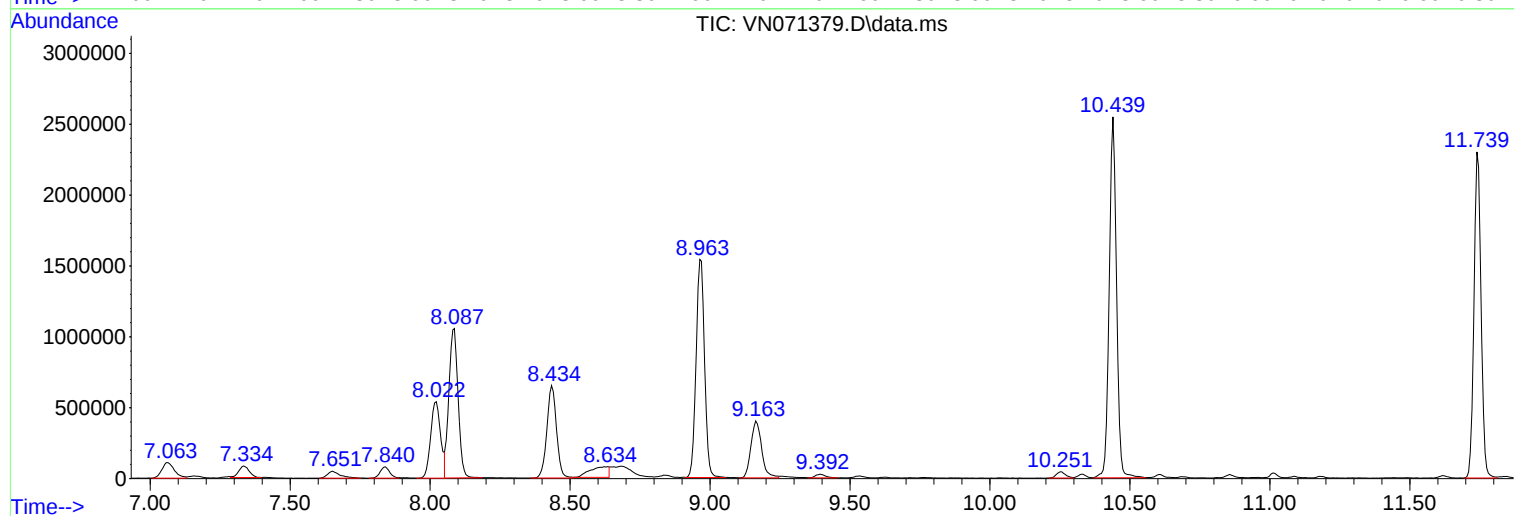
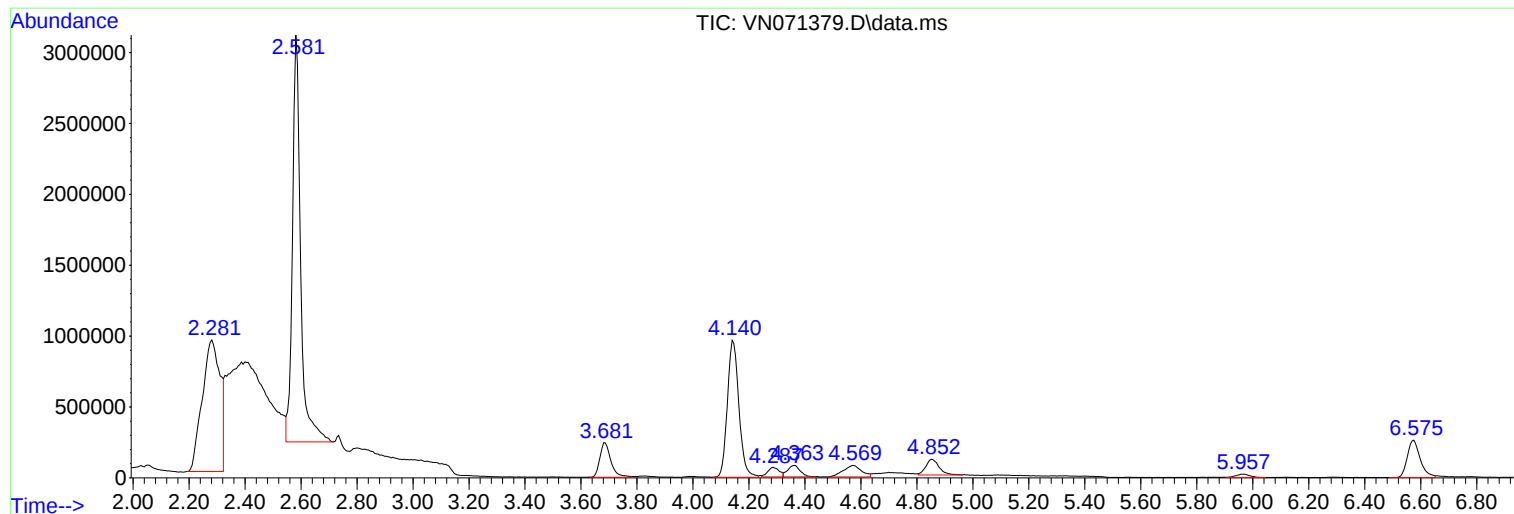
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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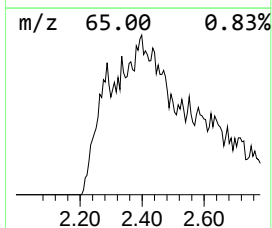
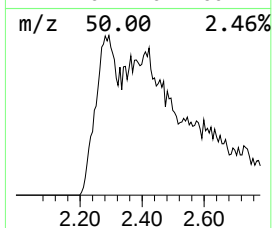
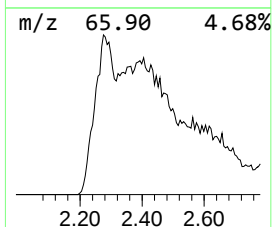
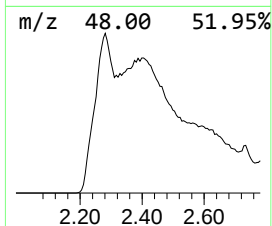
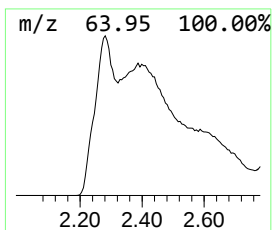
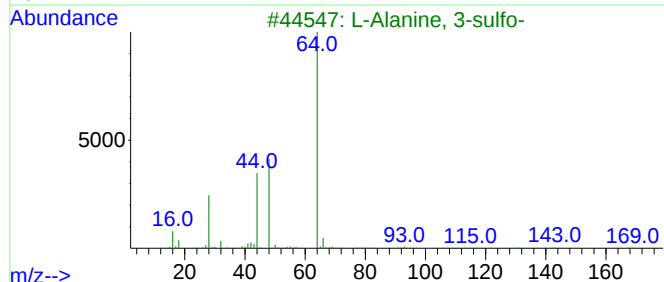
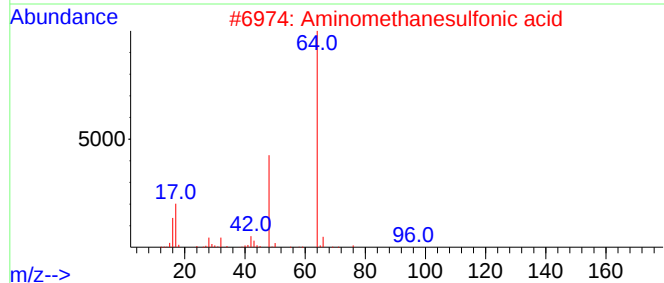
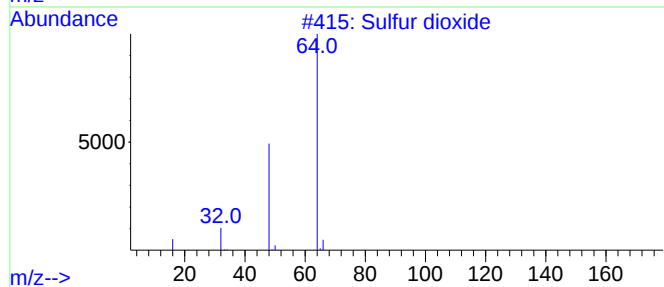
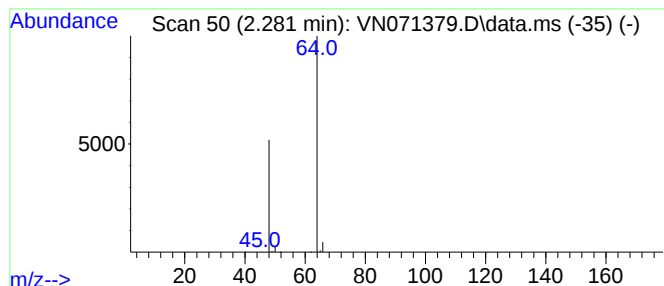
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Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	87.79 ug/l	4194420	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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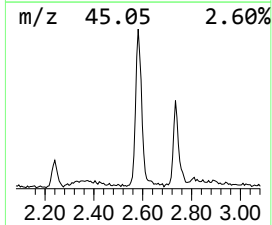
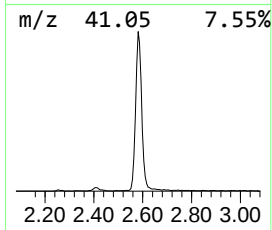
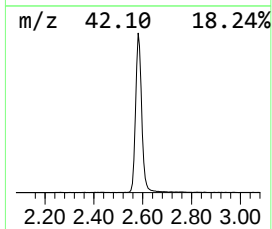
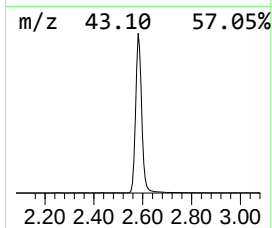
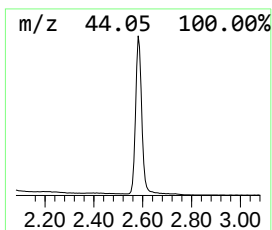
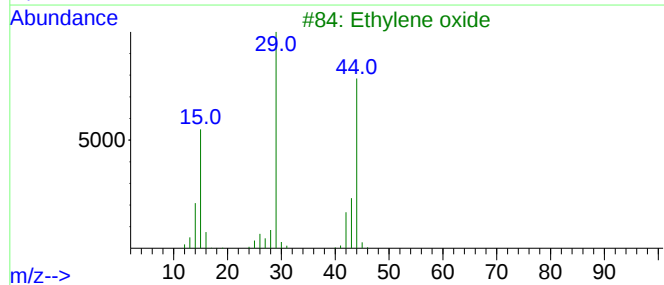
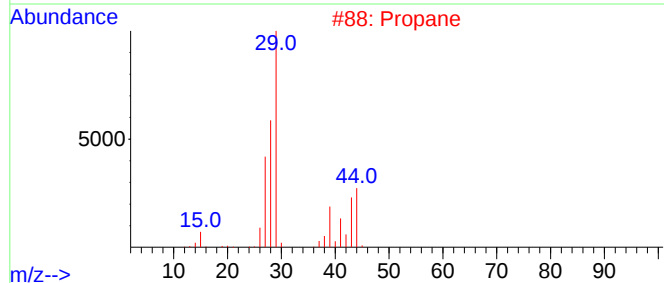
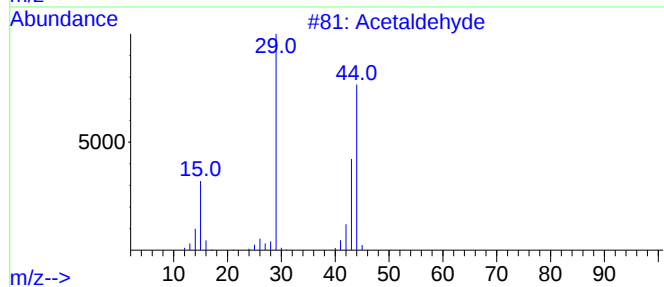
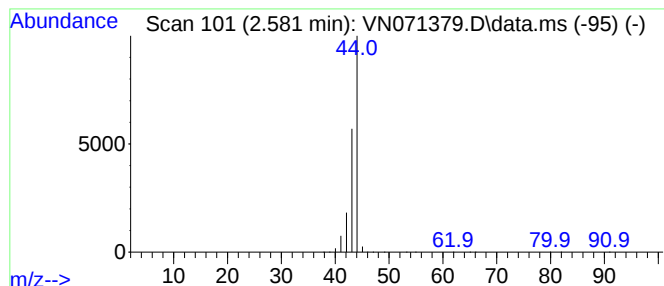
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.581	120.92 ug/l	5777030	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
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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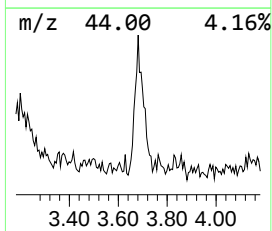
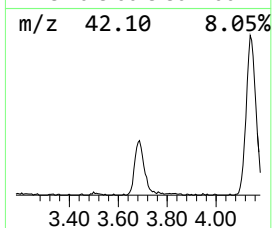
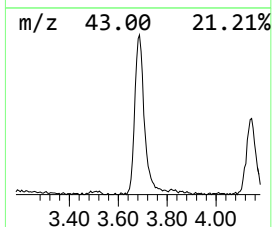
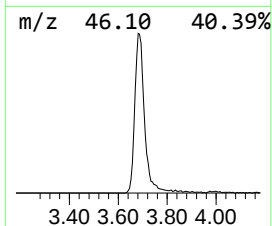
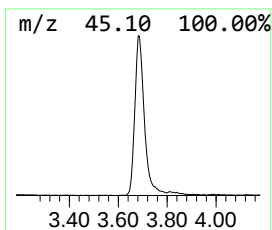
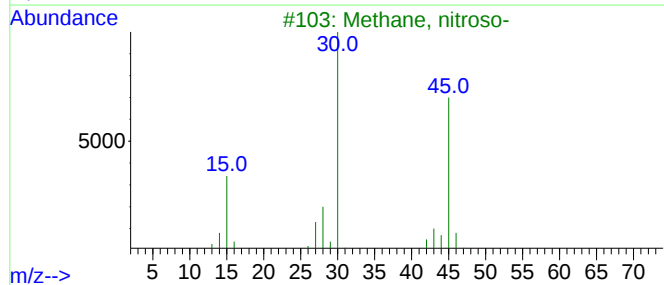
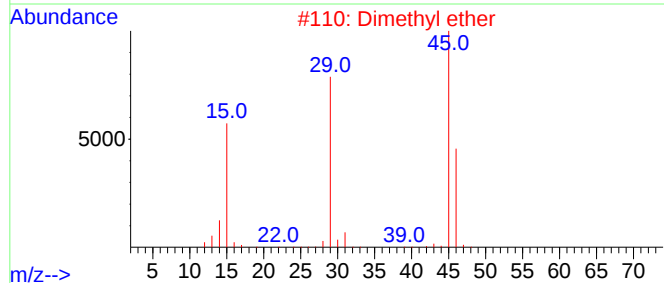
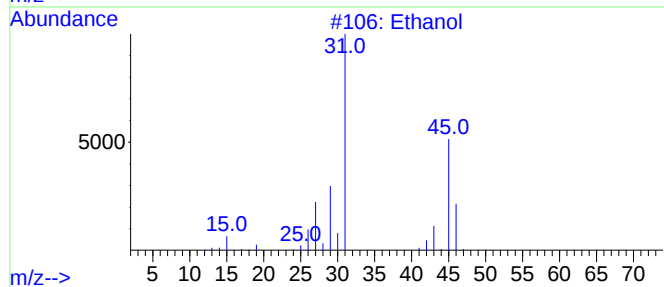
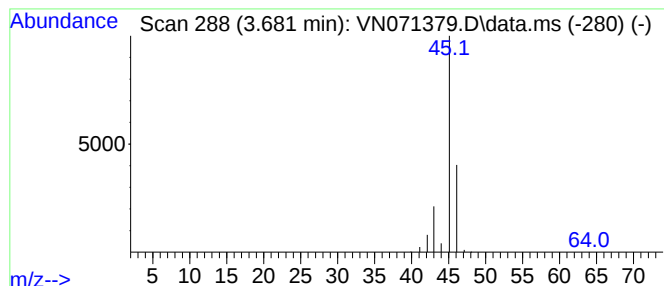
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	13.95 ug/l	666716	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
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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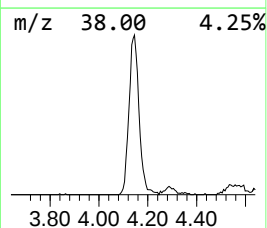
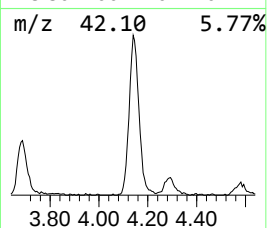
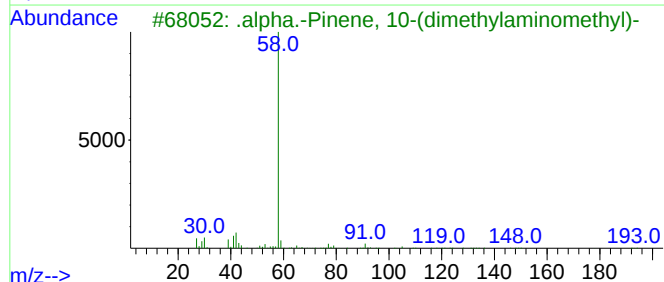
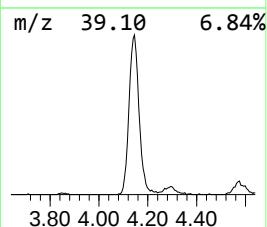
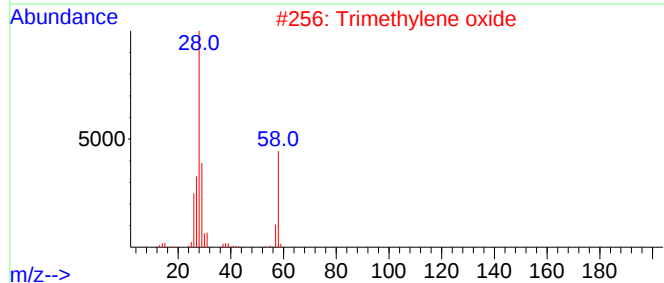
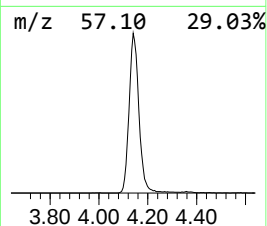
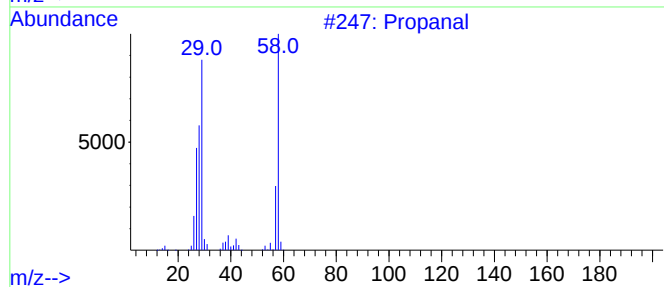
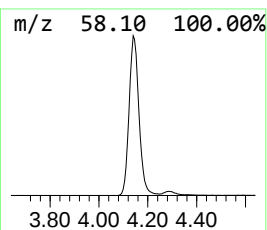
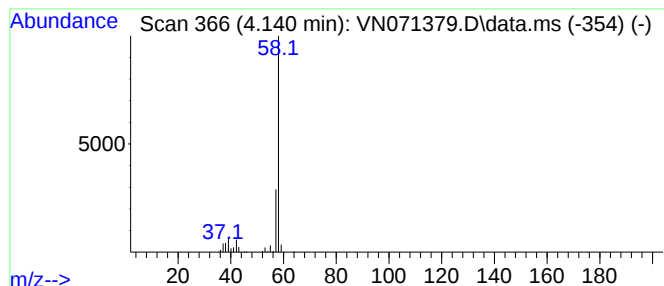
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.140	57.34 ug/l	2739360	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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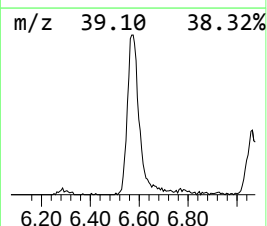
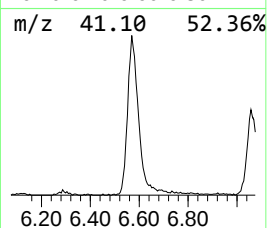
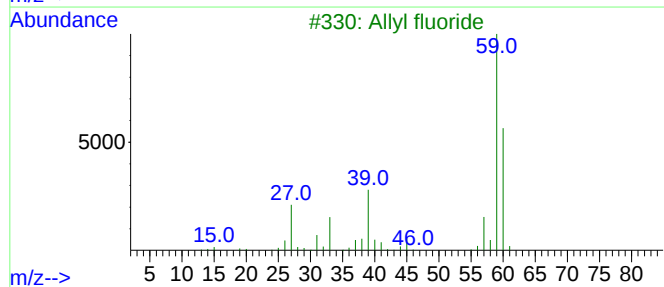
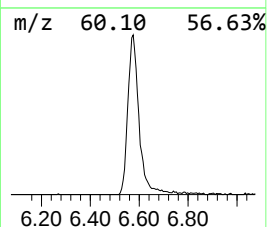
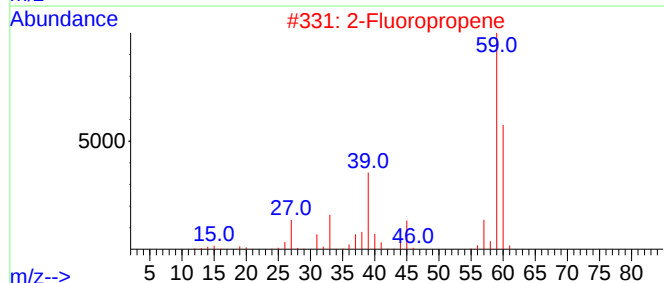
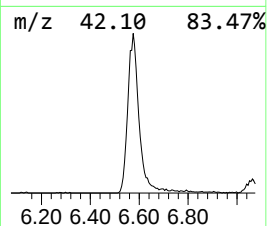
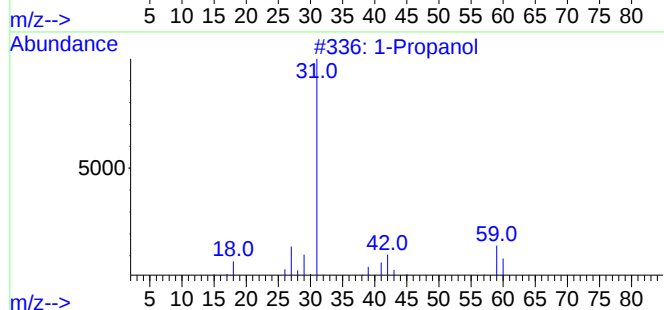
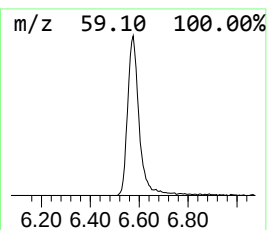
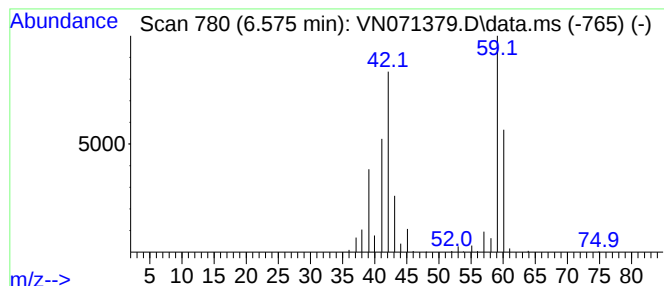
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.575	17.70 ug/l	845703	Pentafluorobenzene	8.087

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	46
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			Cyclopropane	42	C3H6	000075-19-4	25
5			3-Buten-1-ol	72	C4H8O	000627-27-0	23



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31722

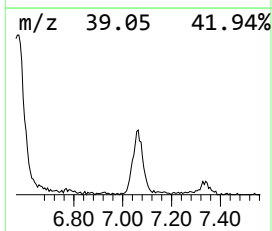
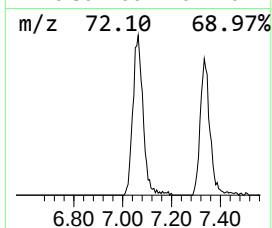
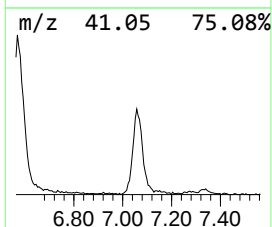
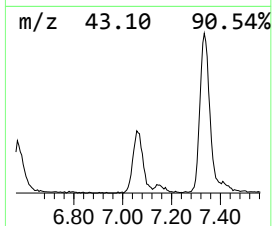
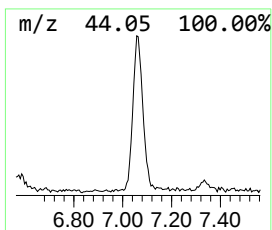
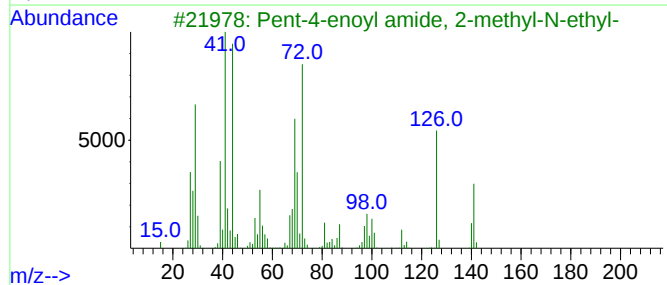
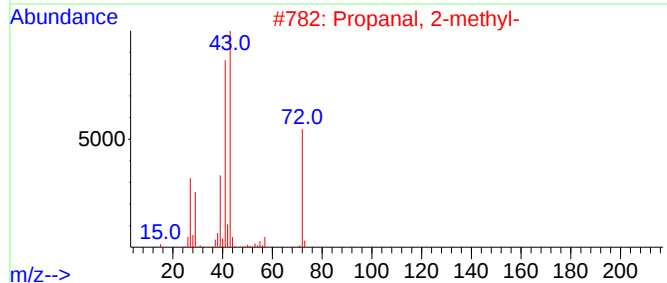
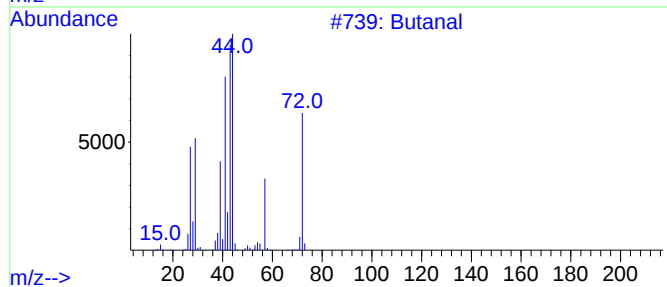
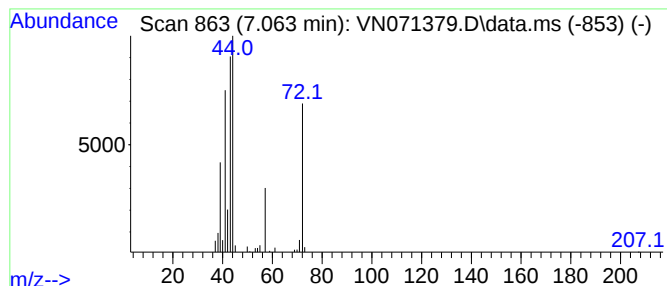
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Quant Title : SW846 8260

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

Peak Number 6 Butanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	7.14 ug/l	341224	Pentafluorobenzene	8.087

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	49
3			Pent-4-enoyl amide, 2-methyl-N-e...	141	C8H15NO	1000420-35-1	38
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071379.D
Acq On : 18 Mar 2022 17:55
Operator : JC\MD
Sample : N2009-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31722

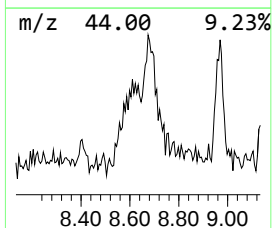
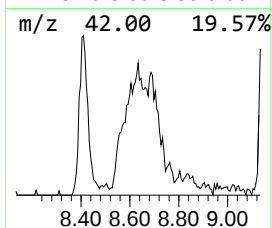
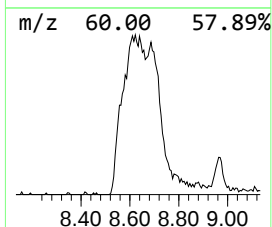
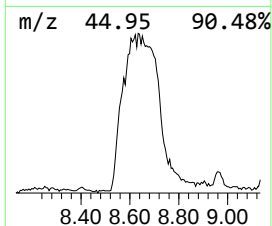
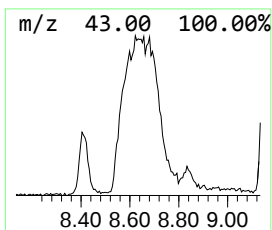
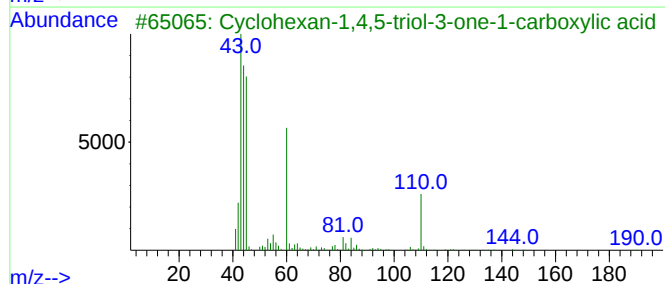
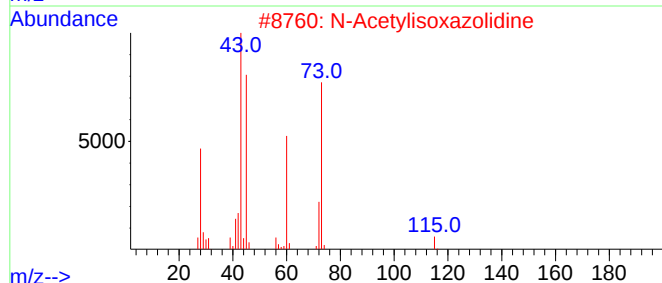
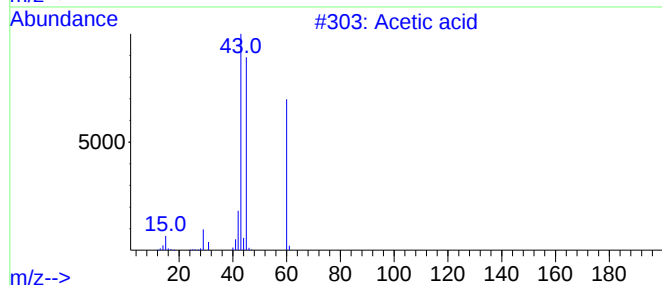
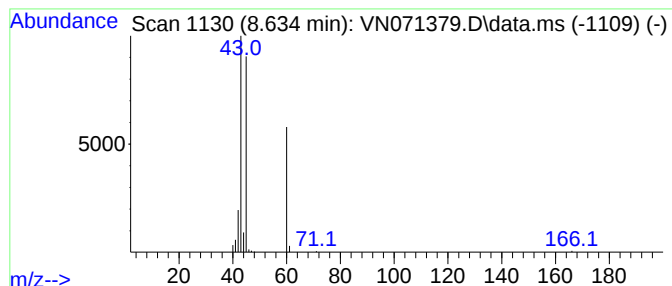
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Quant Title : SW846 8260

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

Peak Number 7 Acetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.634	5.63 ug/l	362085	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	64
3			Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	43
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	16
5			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071379.D
Acq On : 18 Mar 2022 17:55
Operator : JC\MD
Sample : N2009-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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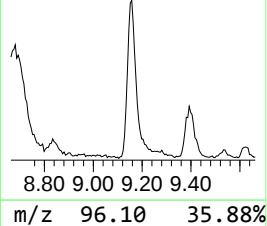
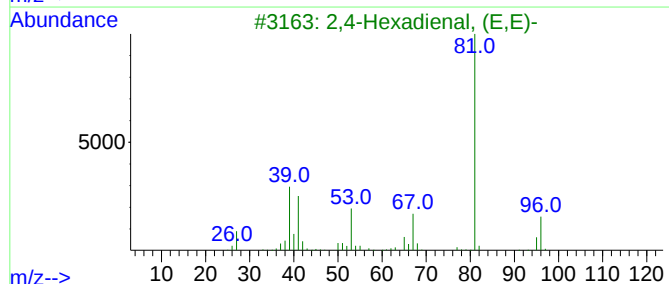
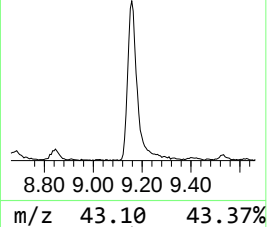
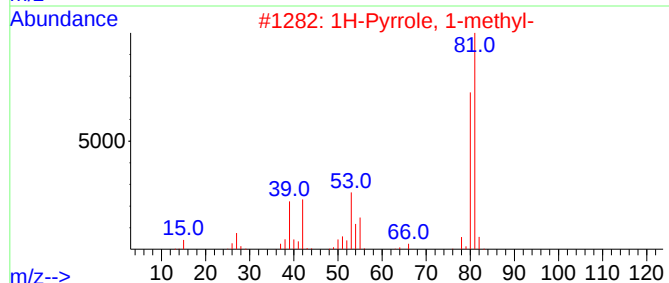
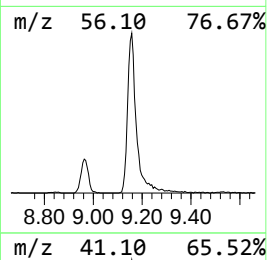
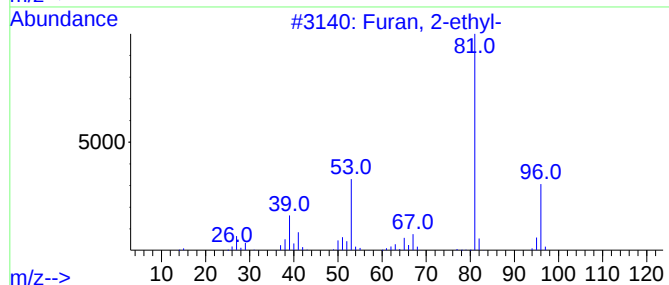
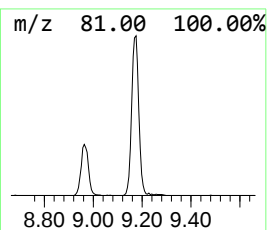
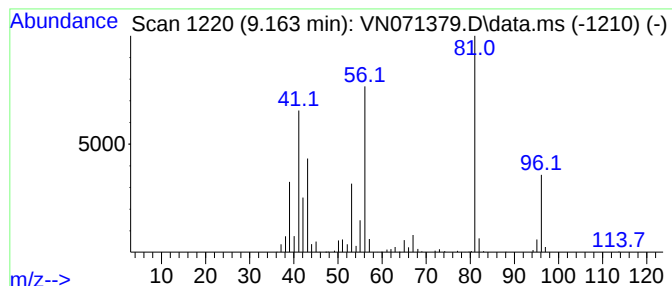
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Quant Title : SW846 8260

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

Peak Number 8 Furan, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.163	16.48 ug/l	1060510	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-ethyl-	96	C6H8O	003208-16-0	89
2			1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	45
3			2,4-Hexadienal, (E,E)-	96	C6H8O	000142-83-6	43
4			1-Butanol	74	C4H10O	000071-36-3	38
5			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071379.D
Acq On : 18 Mar 2022 17:55
Operator : JC\MD
Sample : N2009-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31722

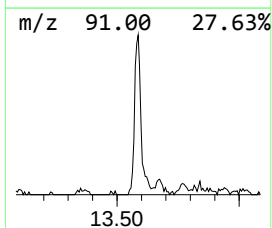
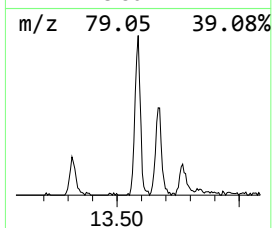
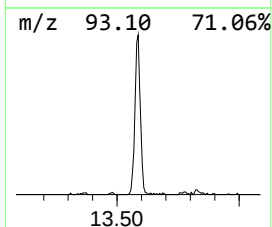
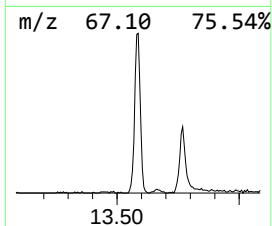
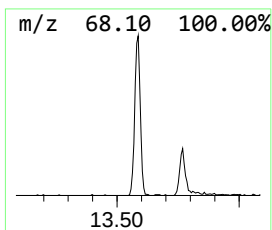
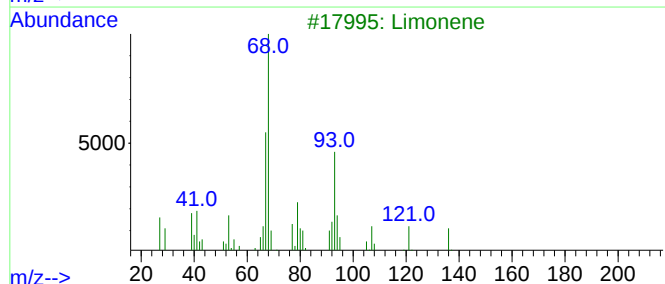
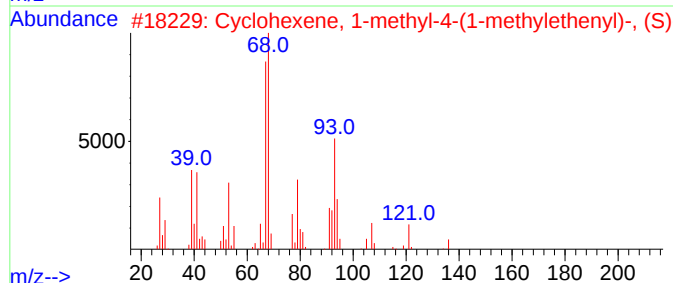
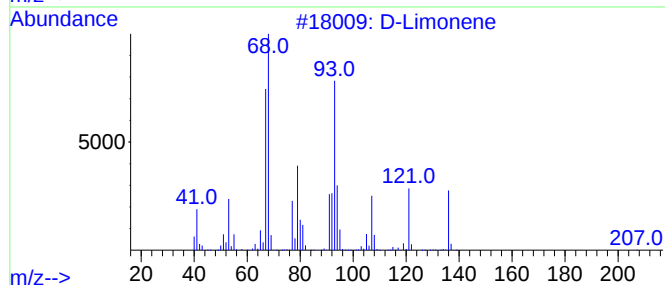
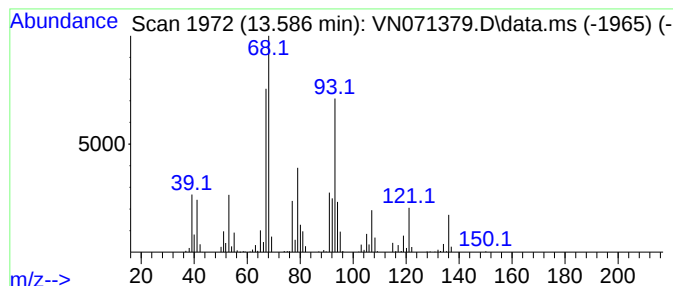
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Quant Title : SW846 8260

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

Peak Number 9 D-Limonene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	7.34 ug/l	477835	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	93
3			Limonene	136	C10H16	000138-86-3	91
4			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	56
5			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071379.D
Acq On : 18 Mar 2022 17:55
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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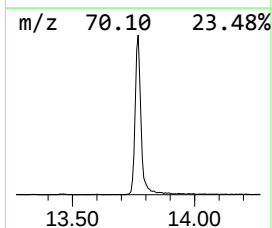
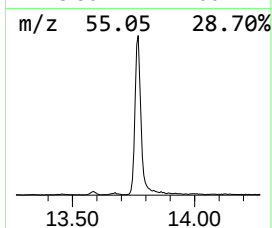
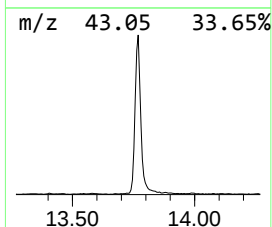
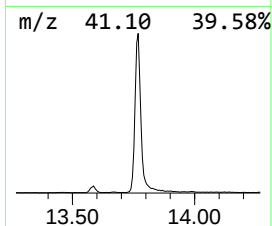
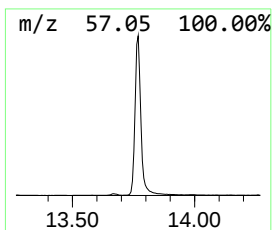
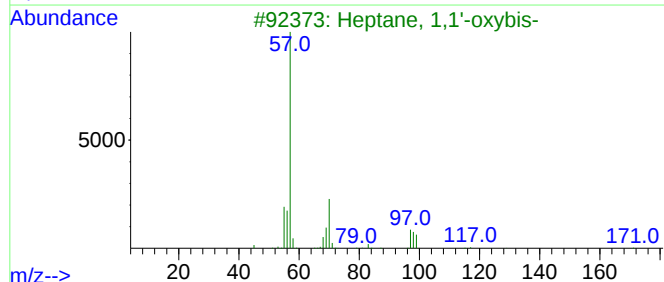
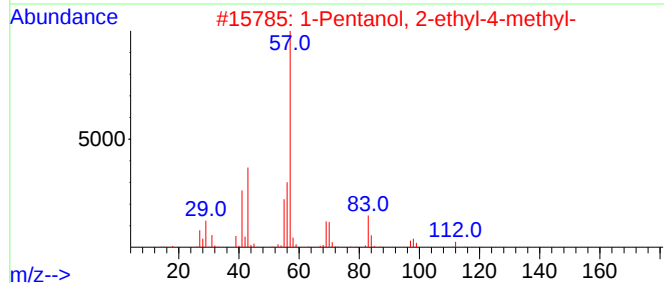
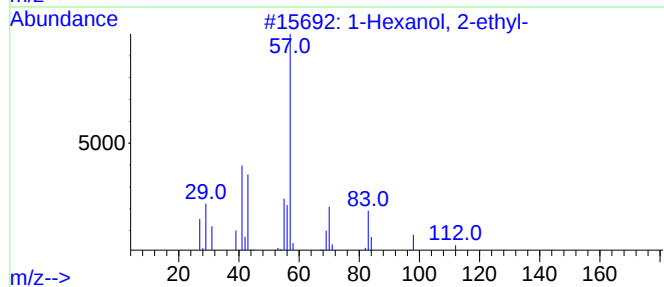
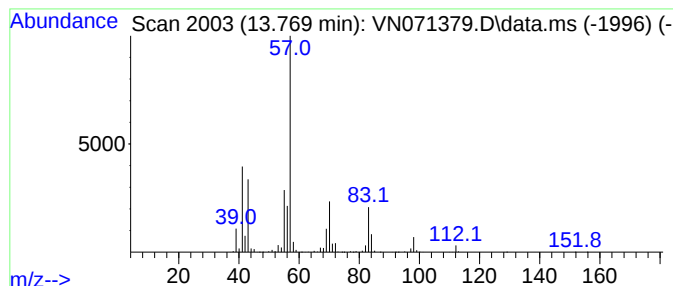
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	58.48 ug/l	3808240	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071379.D
Acq On : 18 Mar 2022 17:55
Operator : JC\MD
Sample : N2009-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31722

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.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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Acetaldehyde	2.581	120.9	ug/l	5777030	1	8.087	2388870	50.0
Ethanol	3.681	13.9	ug/l	666716	1	8.087	2388870	50.0
Propanal	4.140	57.3	ug/l	2739360	1	8.087	2388870	50.0
1-Propanol	6.575	17.7	ug/l	845703	1	8.087	2388870	50.0
Butanal	7.063	7.1	ug/l	341224	1	8.087	2388870	50.0
Acetic acid	8.634	5.6	ug/l	362085	2	8.969	3218270	50.0
Furan, 2-ethyl-	9.163	16.5	ug/l	1060510	2	8.969	3218270	50.0
D-Limonene	13.586	7.3	ug/l	477835	4	13.669	3255870	50.0
1-Hexanol, 2-et...	13.769	58.5	ug/l	3808240	4	13.669	3255870	50.0