

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030121\
 Data File : VN066086.D
 Acq On : 1 Mar 2021 19:04
 Operator : JC/MD
 Sample : M1489-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-41706-07

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\82N021721W.M

Title : SW846 8260

Signal : TIC: VN066086.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.309	164	177	196	rBV	357473	585455	6.08%	4.145%
2	3.251	455	470	496	rBV	80180	193792	2.01%	1.372%
3	3.669	562	600	678	rBV	3411503	9636943	100.00%	68.222%
4	5.910	1275	1297	1311	rBV3	41336	144074	1.50%	1.020%
5	5.991	1312	1322	1353	rVB3	35908	116841	1.21%	0.827%
6	6.499	1462	1480	1503	rBV3	31925	97611	1.01%	0.691%
7	7.550	1791	1807	1819	rBV	71938	178900	1.86%	1.266%
8	7.627	1819	1831	1849	rVB	138593	330232	3.43%	2.338%
9	7.991	1926	1944	1964	rBV2	88996	219904	2.28%	1.557%
10	8.550	2105	2118	2138	rVB	200747	418476	4.34%	2.962%
11	10.058	2572	2587	2599	rBV	312479	577758	6.00%	4.090%
12	11.376	2982	2997	3017	rBV	281227	508312	5.27%	3.598%
13	12.338	3284	3296	3299	rBV2	68264	101706	1.06%	0.720%
14	12.373	3299	3307	3320	rVB	211638	367775	3.82%	2.604%
15	13.315	3587	3600	3620	rBV	249358	438700	4.55%	3.106%
16	13.424	3623	3634	3651	rBV	103924	209310	2.17%	1.482%

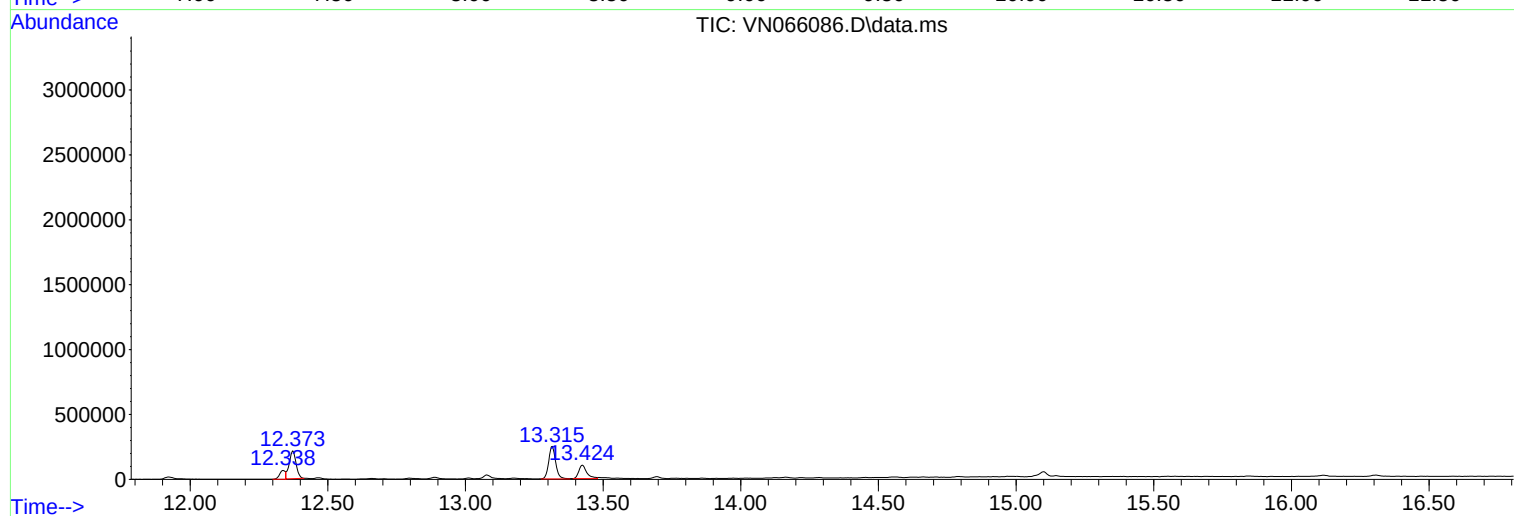
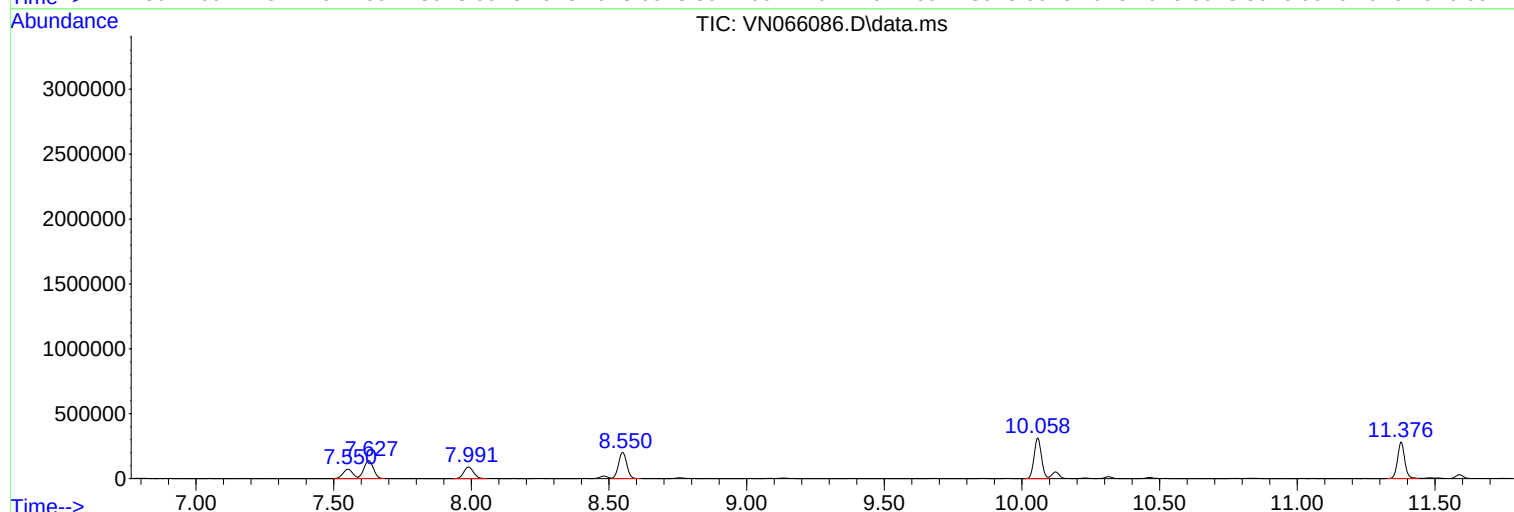
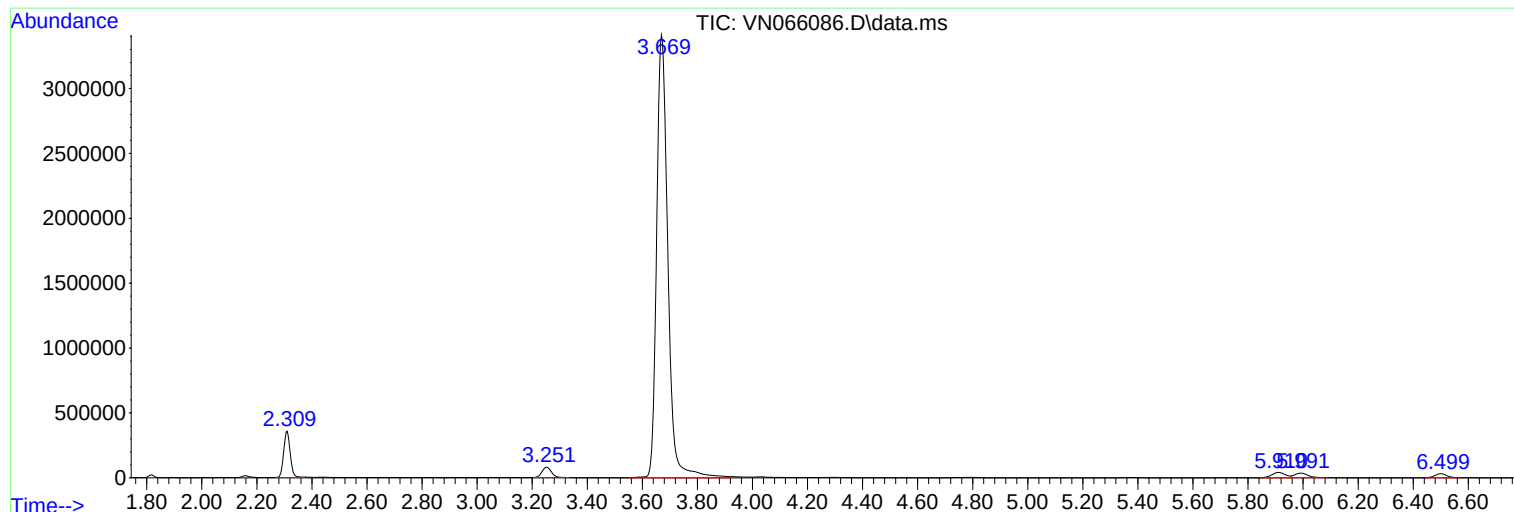
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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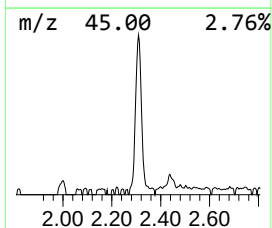
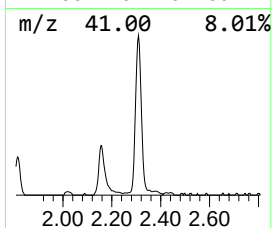
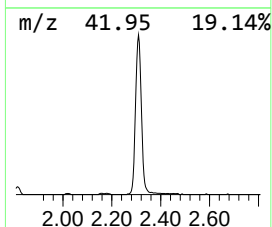
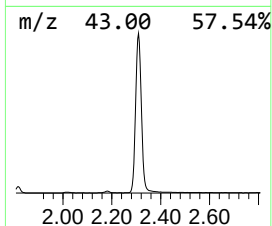
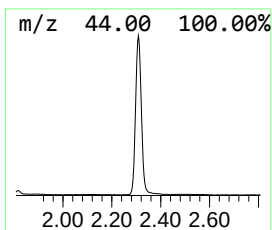
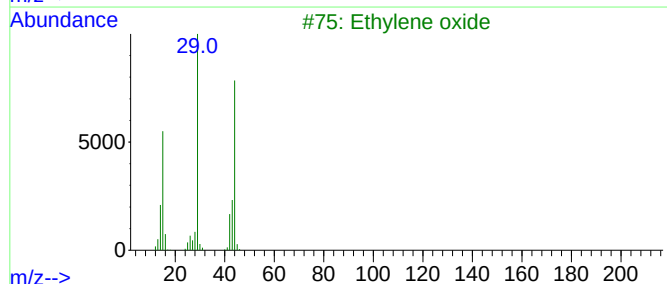
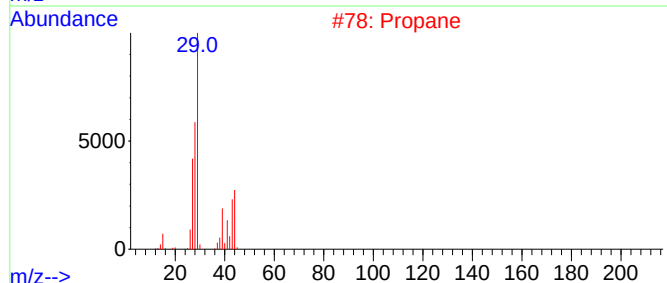
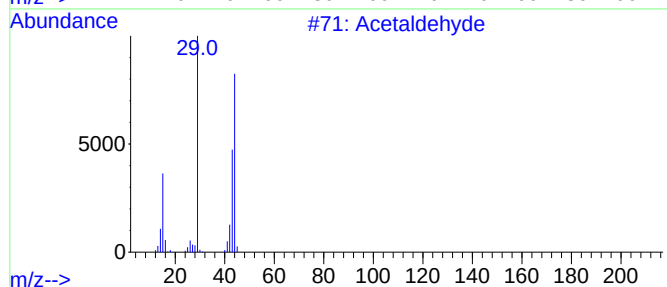
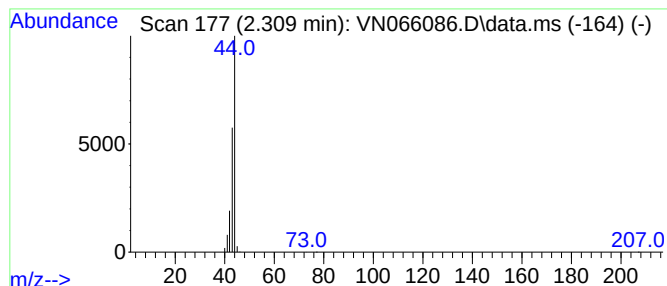
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.309	88.64 ug/l	585455	Pentafluorobenzene	7.627

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			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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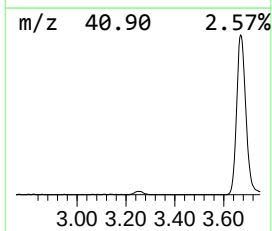
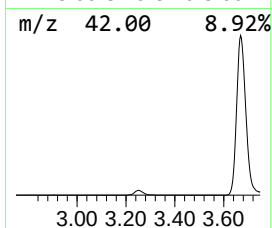
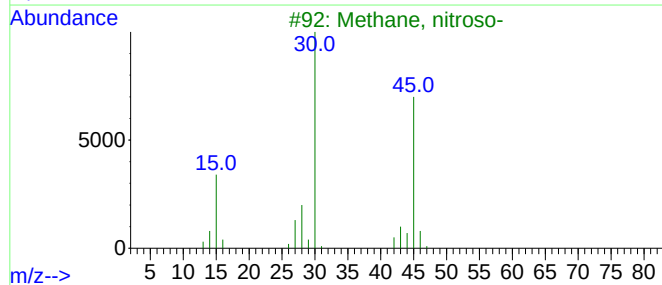
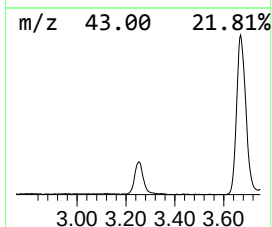
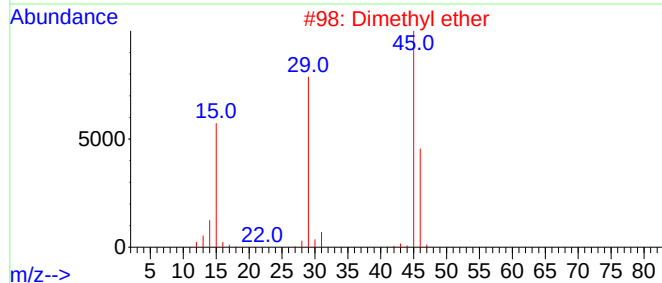
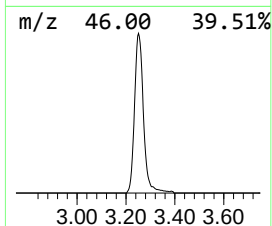
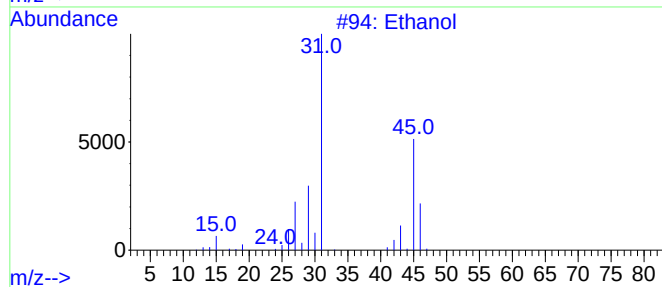
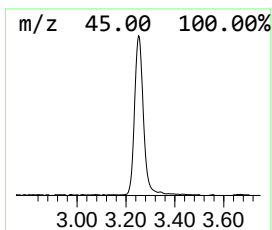
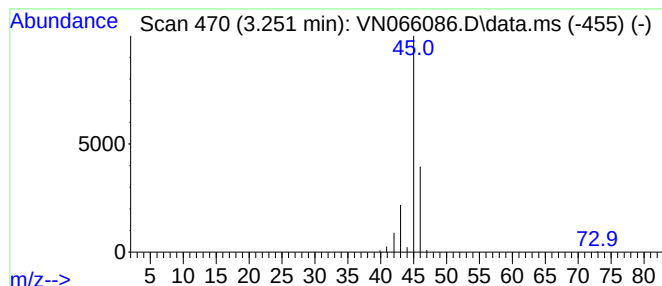
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.251	29.34 ug/l	193792	Pentafluorobenzene	7.627

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			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Formic acid	46	CH2O2	000064-18-6	4



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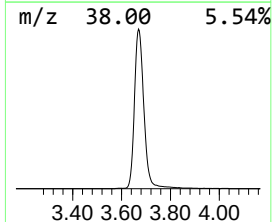
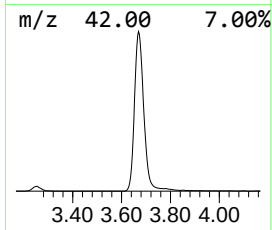
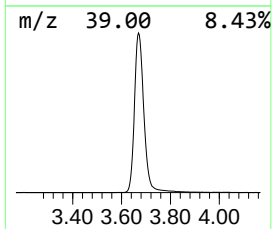
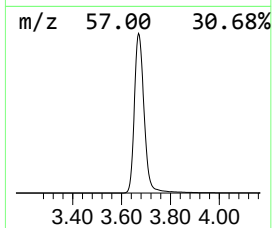
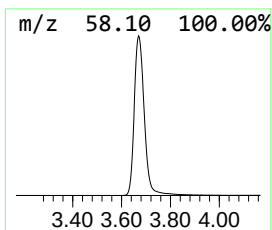
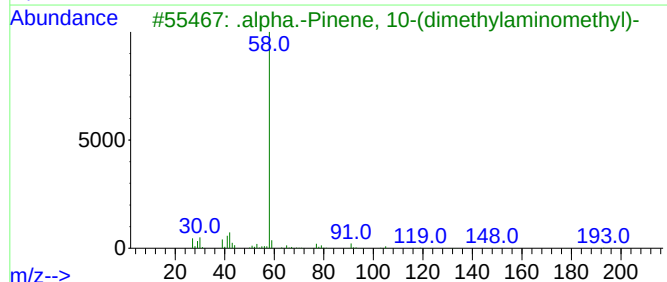
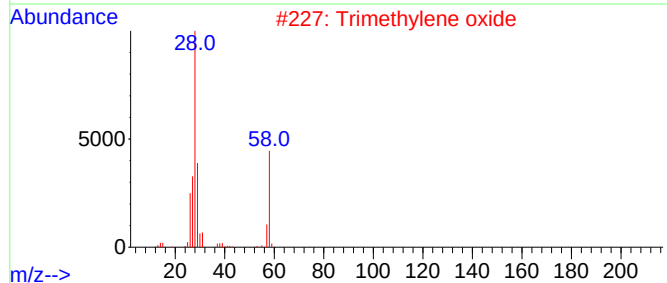
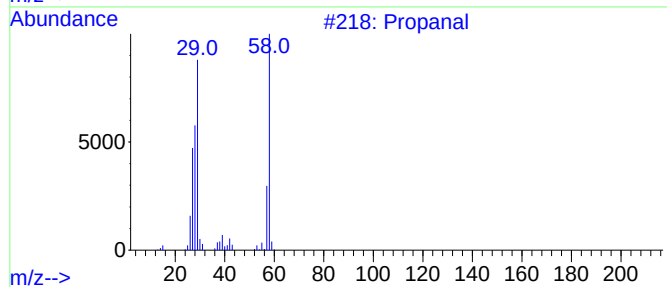
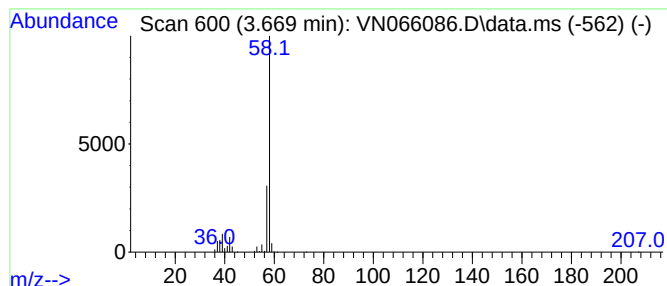
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Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	1459.12 ug/l	9636940	Pentafluorobenzene	7.627

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	9
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			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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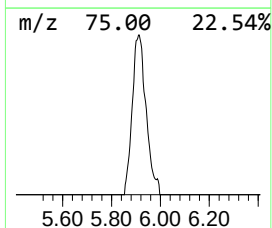
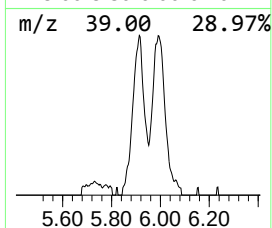
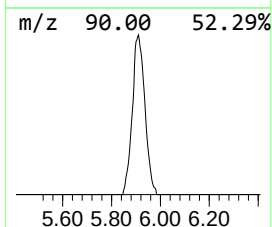
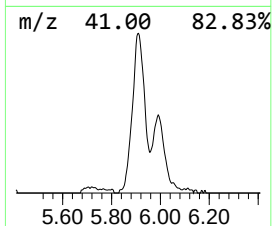
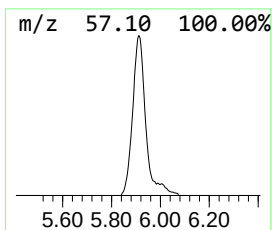
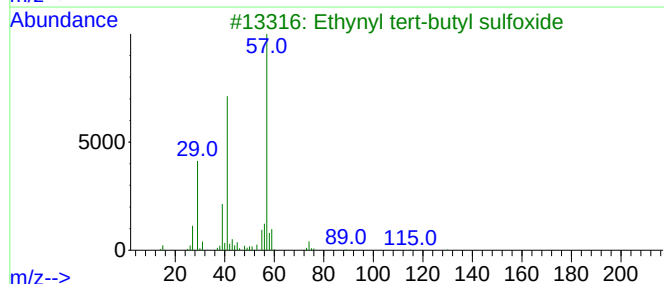
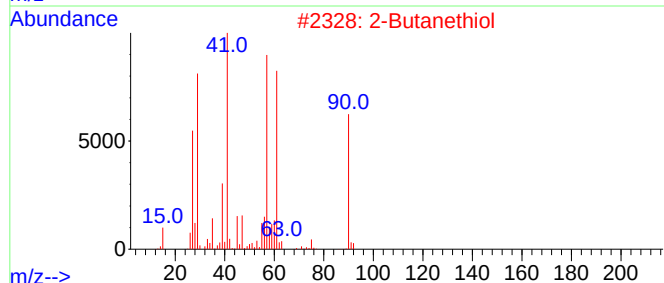
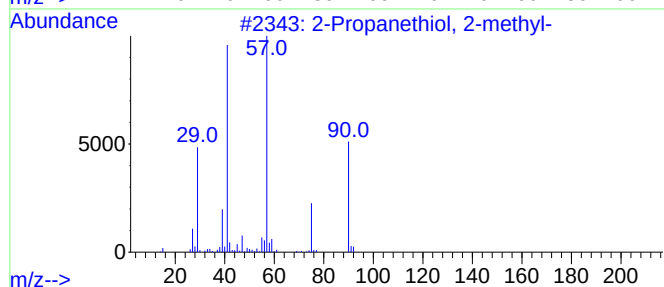
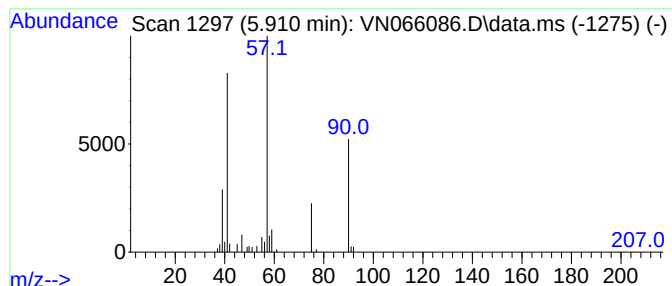
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TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Propanethiol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.910	21.81 ug/l	144074	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2			2-Butanethiol	90	C4H10S	000513-53-1	42
3			Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	25
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
5			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	22



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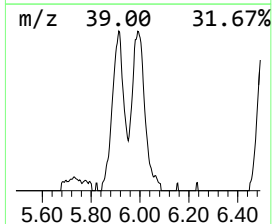
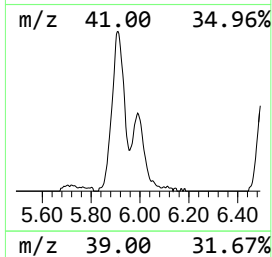
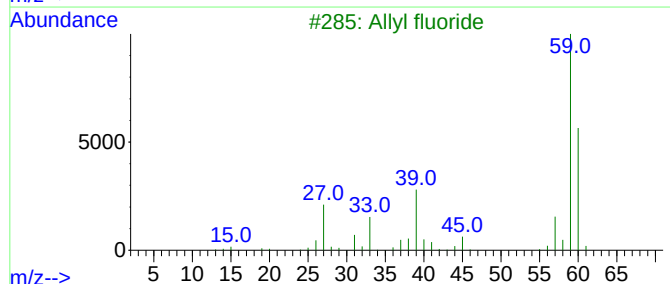
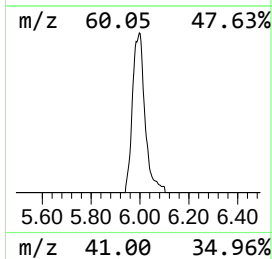
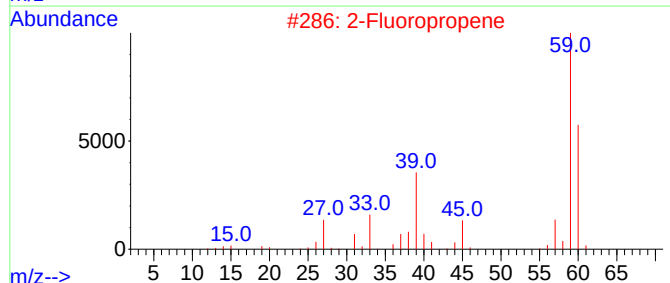
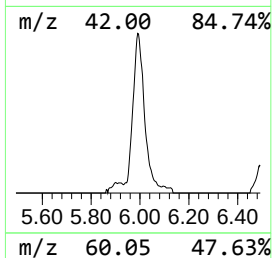
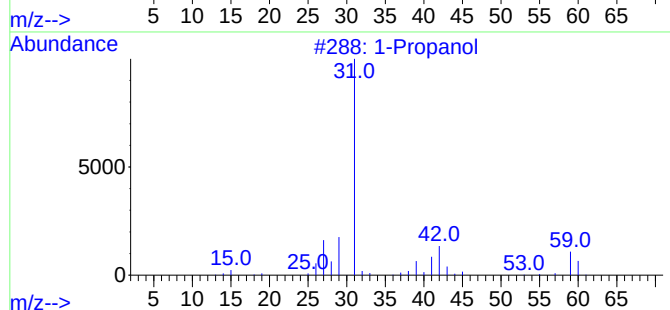
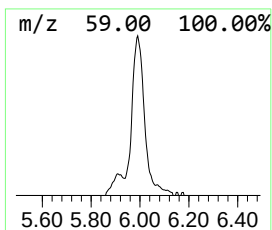
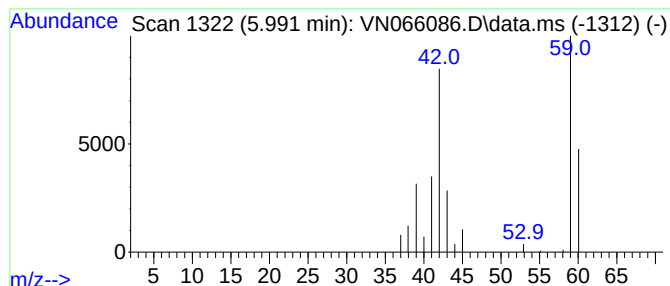
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Propanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.991	17.69 ug/l	116841	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	58
2	2-Fluoropropene			60	C3H5F	001184-60-7	47
3	Allyl fluoride			60	C3H5F	000818-92-8	9
4	Cyclopropane			42	C3H6	000075-19-4	9
5	Ethylenimine			43	C2H5N	000151-56-4	5



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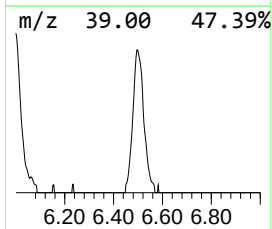
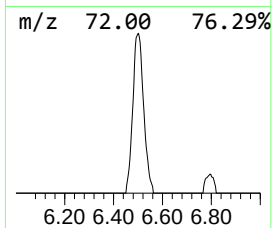
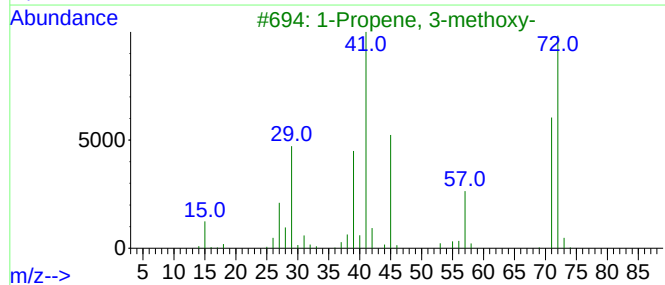
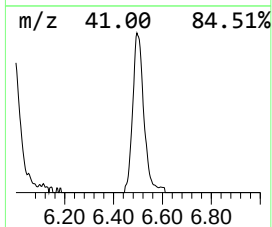
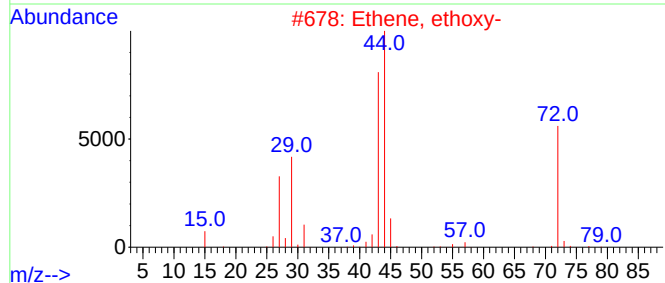
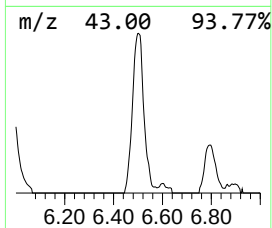
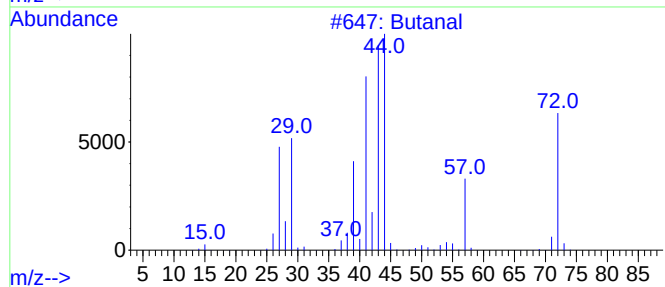
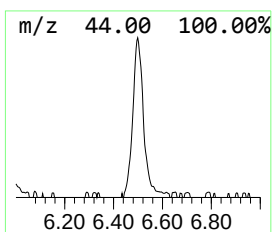
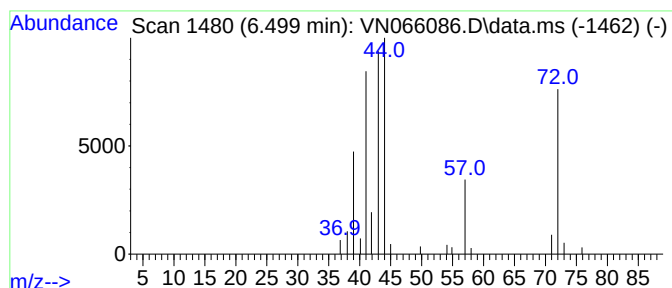
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.499	14.78 ug/l	97611	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030121\
Data File : VN066086.D
Acq On : 1 Mar 2021 19:04
Operator : JC/MD
Sample : M1489-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41706-07

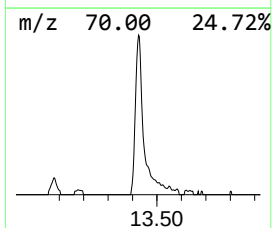
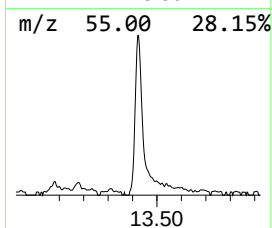
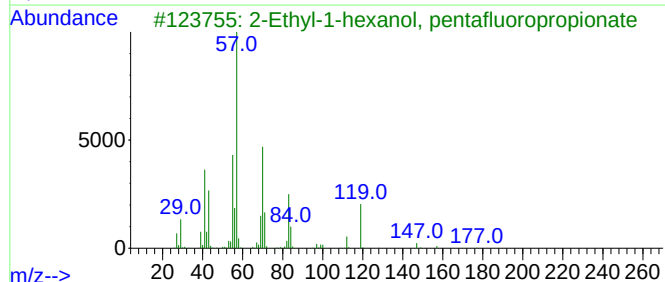
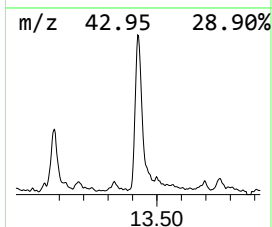
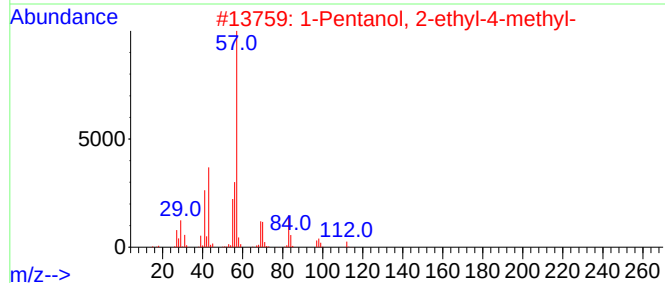
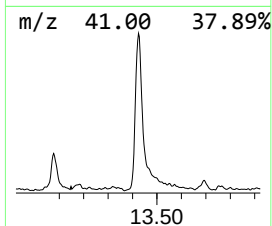
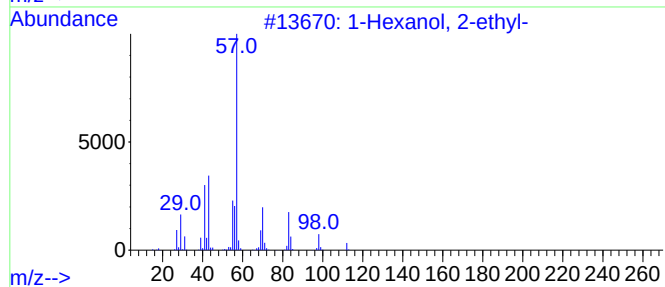
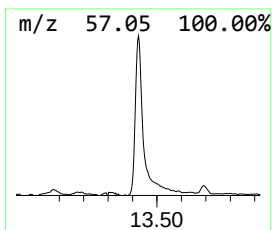
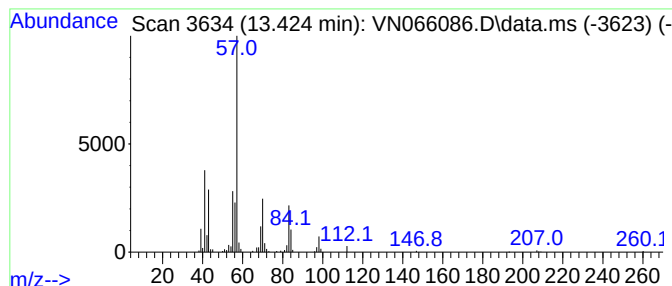
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.424	23.86 ug/l	209310	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030121\
Data File : VN066086.D
Acq On : 1 Mar 2021 19:04
Operator : JC/MD
Sample : M1489-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41706-07

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.309	88.6	ug/l	585455	1	7.627	330232	50.0
Ethanol	3.251	29.3	ug/l	193792	1	7.627	330232	50.0
Propanal	3.669	1459.1	ug/l	9636940	1	7.627	330232	50.0
2-Propanethiol,...	5.910	21.8	ug/l	144074	1	7.627	330232	50.0
1-Propanol	5.991	17.7	ug/l	116841	1	7.627	330232	50.0
Butanal	6.499	14.8	ug/l	97611	1	7.627	330232	50.0
1-Hexanol, 2-et...	13.424	23.9	ug/l	209310	4	13.315	438700	50.0