

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030321\
 Data File : VN066125.D
 Acq On : 3 Mar 2021 15:23
 Operator : JC/MD
 Sample : M1507-08 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41116

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\82N030221W.M

Title : SW846 8260

Signal : TIC: VN066125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	163	176	211	rBV	911912	1505452	100.00%	32.256%
2	3.251	453	470	495	rBV	189571	456591	30.33%	9.783%
3	6.505	1463	1482	1502	rBV4	12462	37499	2.49%	0.803%
4	7.553	1790	1808	1819	rBV2	56088	139247	9.25%	2.984%
5	7.627	1819	1831	1851	rVB	94730	223819	14.87%	4.796%
6	7.991	1928	1944	1967	rBV	62664	146979	9.76%	3.149%
7	8.550	2101	2118	2141	rBV	160019	328324	21.81%	7.035%
8	10.058	2572	2587	2603	rBV	243562	450352	29.91%	9.649%
9	10.846	2822	2832	2843	rBV4	10817	20283	1.35%	0.435%
10	11.376	2983	2997	3021	rBV	238022	434954	28.89%	9.319%
11	11.511	3029	3039	3050	rBV	65140	105995	7.04%	2.271%
12	12.373	3294	3307	3322	rBV	188138	330796	21.97%	7.088%
13	13.077	3515	3526	3533	rBV6	7608	15814	1.05%	0.339%
14	13.312	3587	3599	3619	rBV	213082	377343	25.07%	8.085%
15	13.425	3621	3634	3647	rBV3	29418	64140	4.26%	1.374%
16	13.695	3707	3718	3730	rBV	16917	29590	1.97%	0.634%

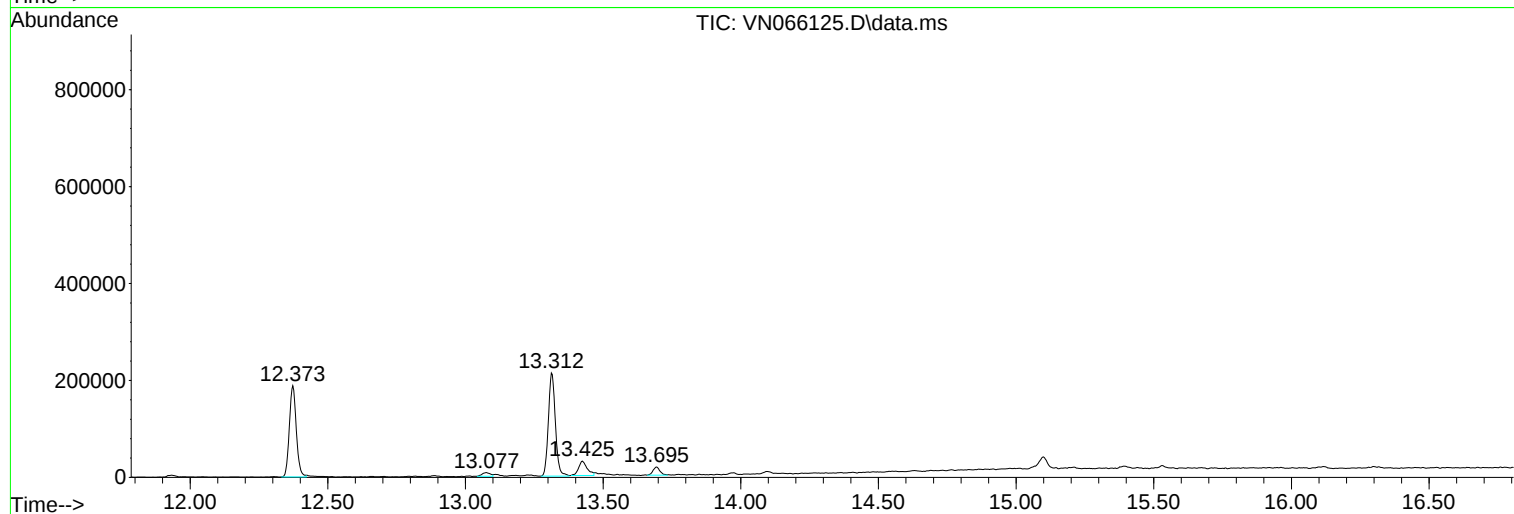
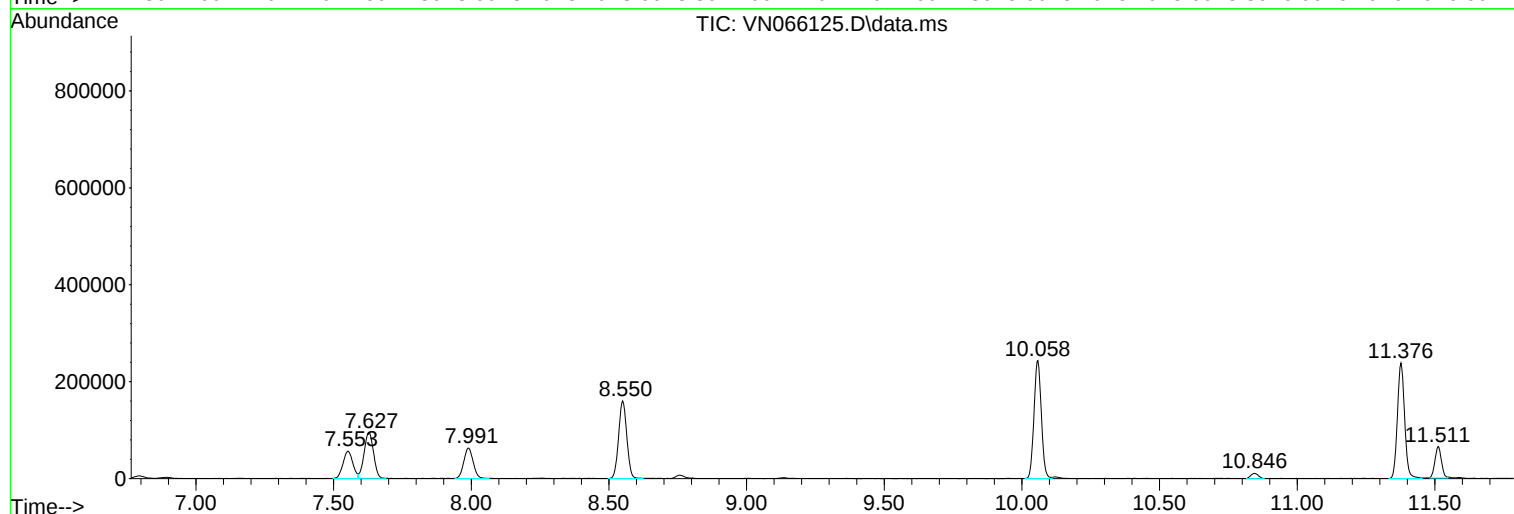
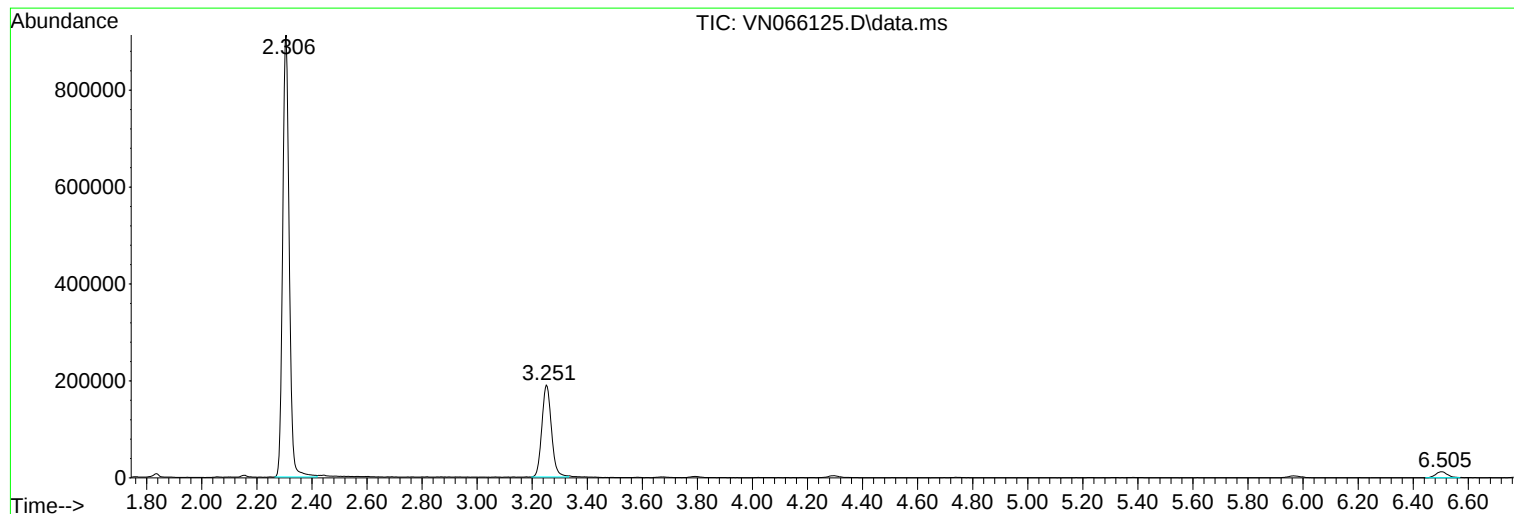
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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



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Instrument :
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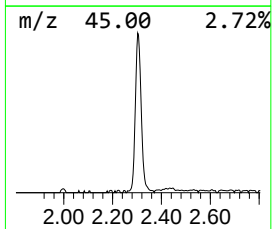
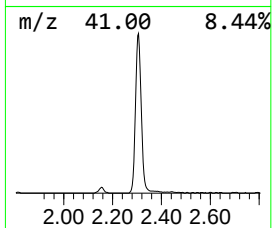
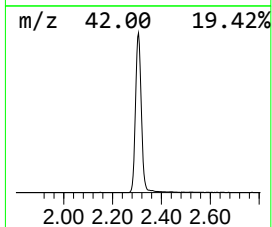
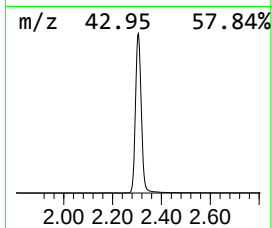
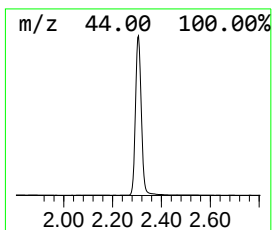
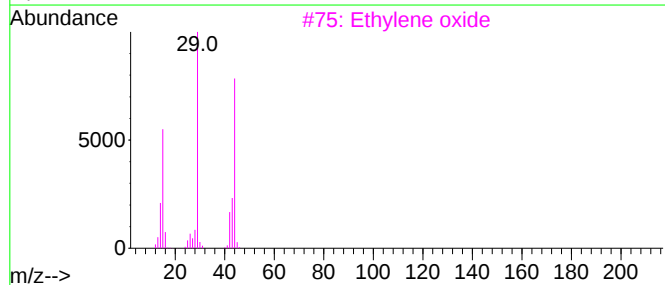
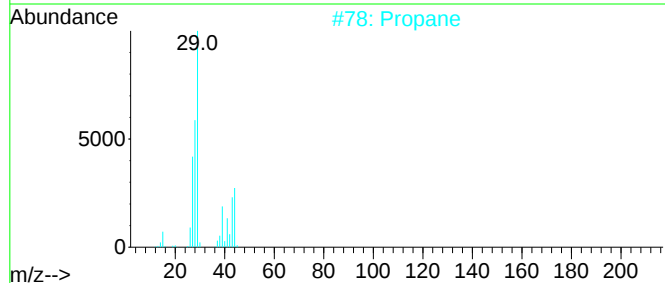
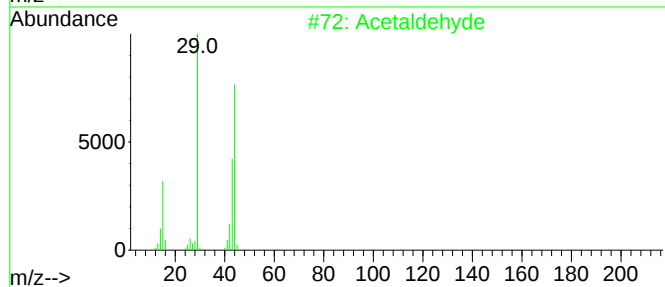
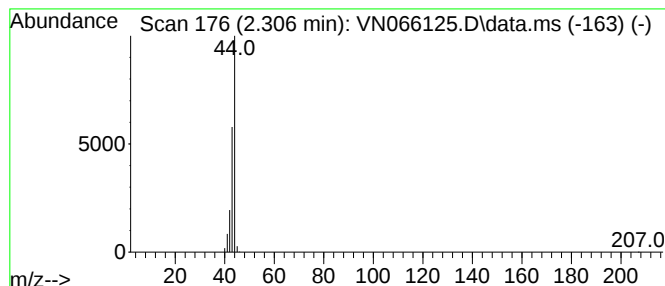
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	336.31 ug/l	1505450	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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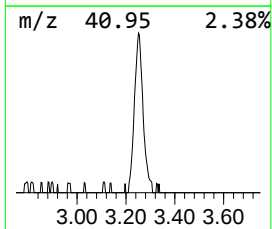
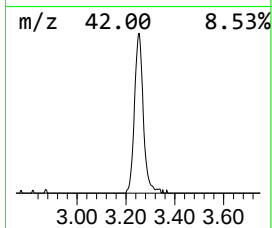
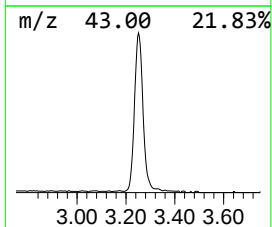
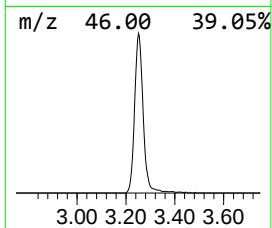
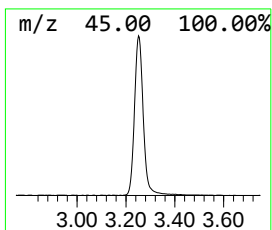
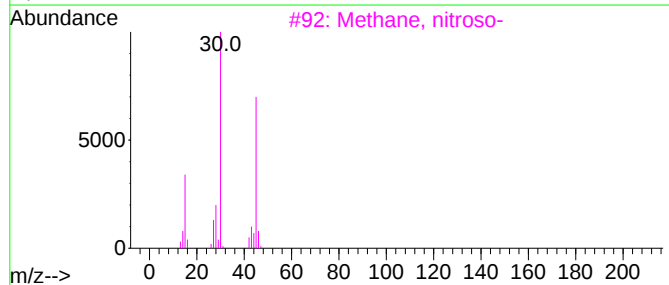
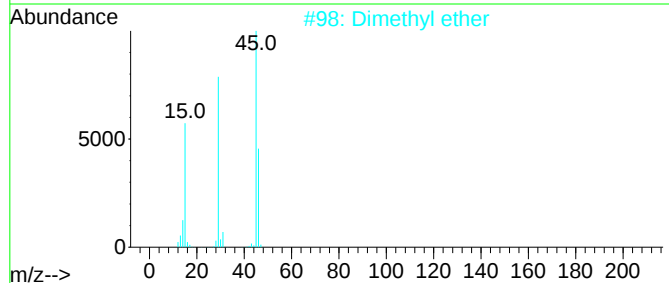
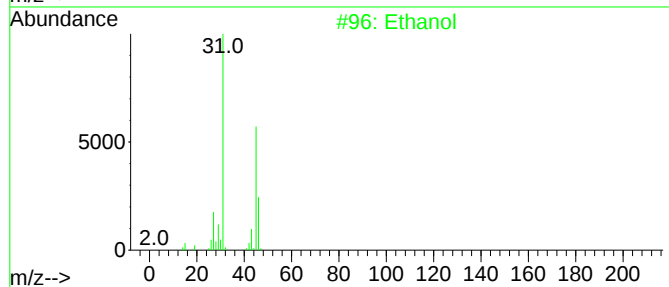
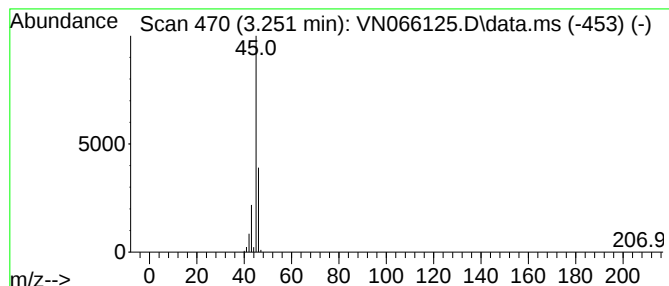
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.251	102.00 ug/l	456591	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			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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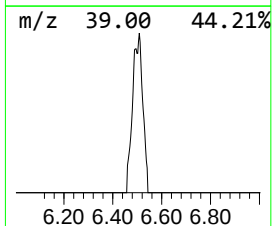
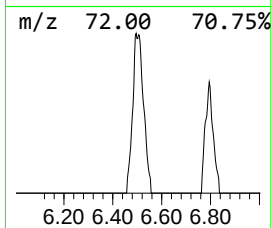
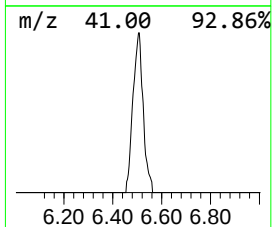
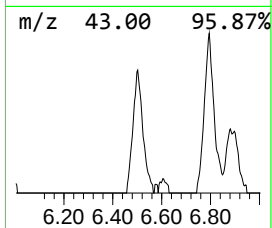
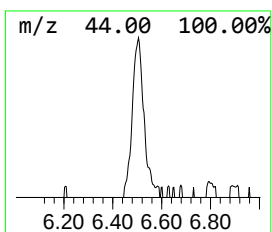
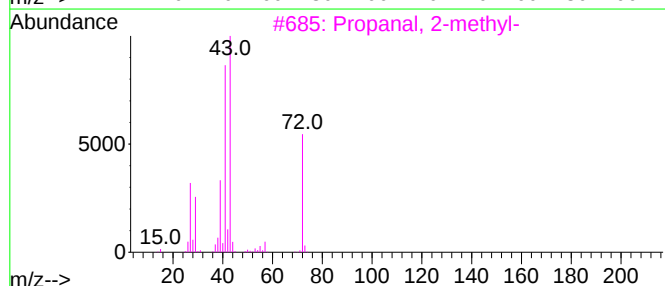
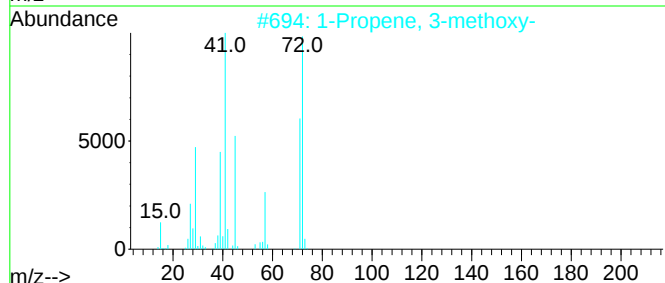
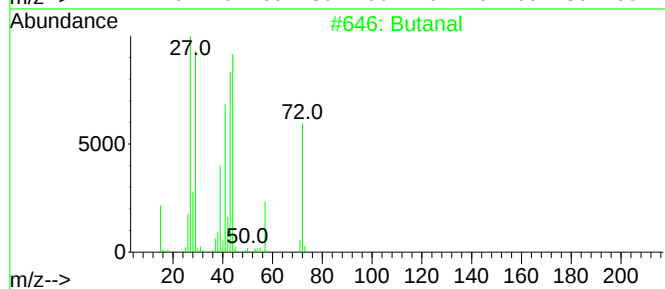
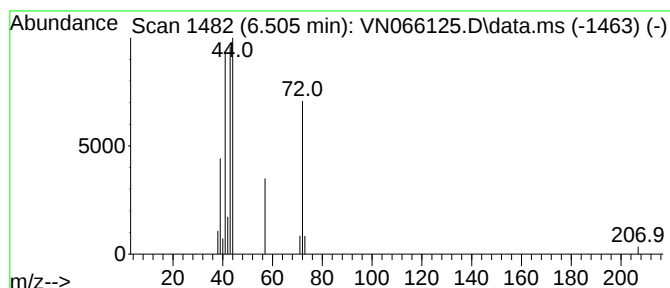
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Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.505	8.38 ug/l	37499	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	25
4			3-Bromopropyl isothiocyanate	179	C4H6BrNS	002799-73-7	25
5			Ethene, ethoxy-	72	C4H8O	000109-92-2	9



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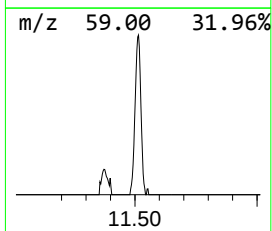
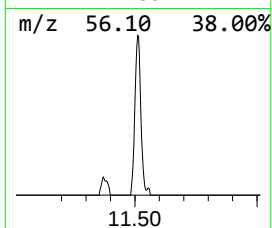
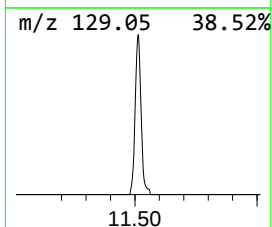
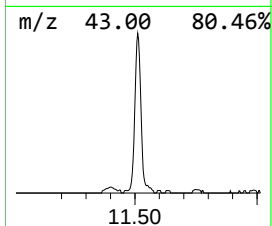
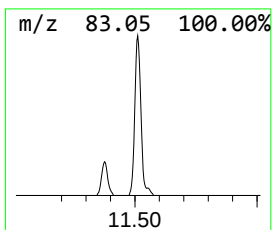
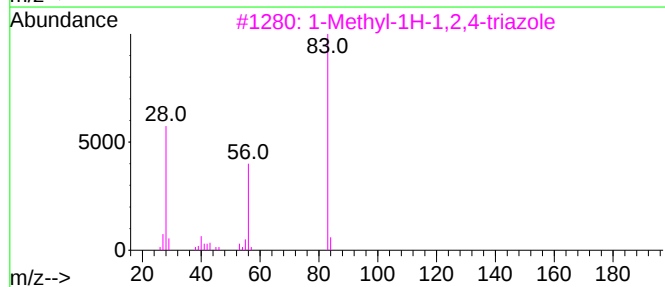
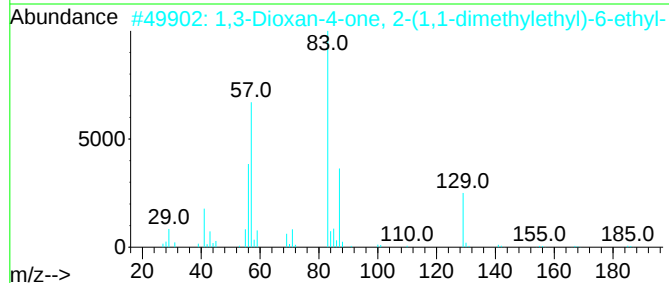
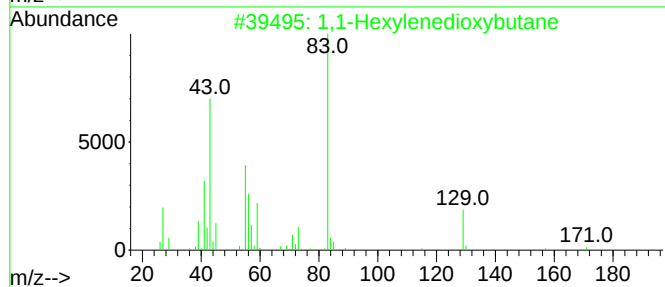
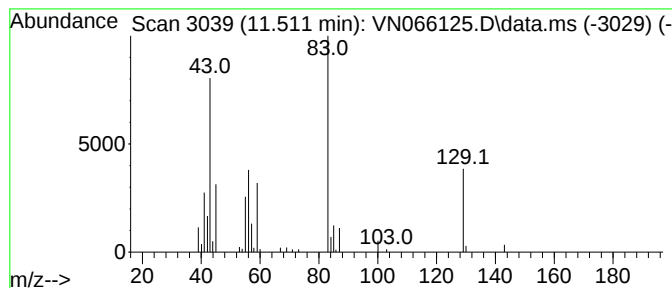
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.512 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.512	12.18 ug/l	105995	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	36
2			1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	33
3			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	32
4			Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	25
5			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	25



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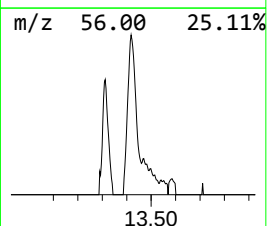
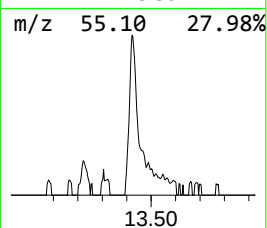
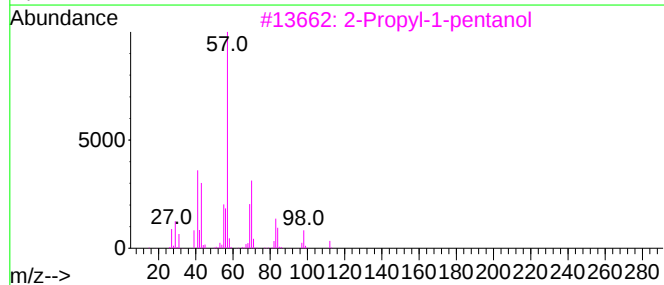
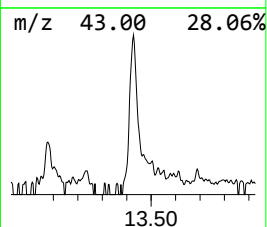
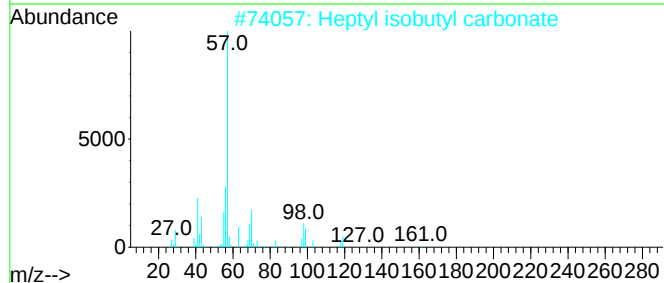
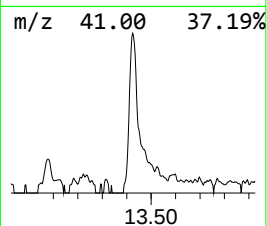
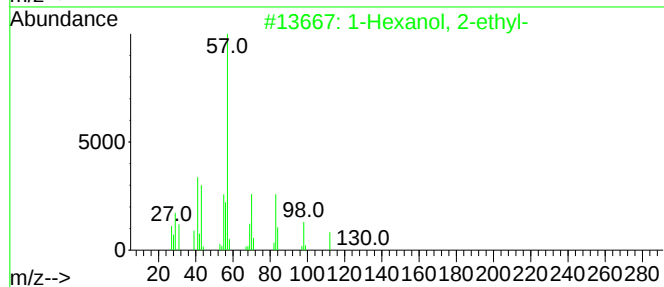
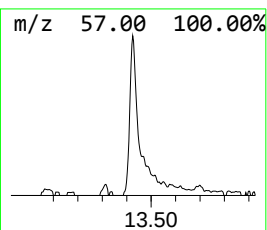
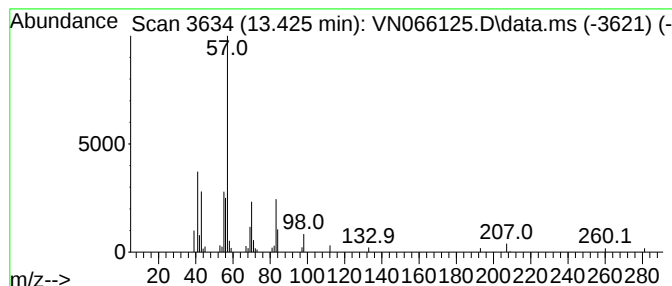
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.425	8.50 ug/l	64140	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	78
2			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45
5			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	43



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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	2.306	336.3	ug/l	1505450	1	7.627	223819	50.0
Ethanol	3.251	102.0	ug/l	456591	1	7.627	223819	50.0
Butanal	6.505	8.4	ug/l	37499	1	7.627	223819	50.0
unknown11.512	11.512	12.2	ug/l	105995	3	11.376	434954	50.0
1-Hexanol, 2-et...	13.425	8.5	ug/l	64140	4	13.315	377343	50.0