

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030321\
 Data File : VN066124.D
 Acq On : 3 Mar 2021 15:02
 Operator : JC/MD
 Sample : M1507-09
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30769

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: VN066124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.274	159	166	219	rBV	8540161	21690287	100.00%	79.122%
2	3.251	449	470	508	rBV	326937	803484	3.70%	2.931%
3	5.962	1290	1313	1350	rBV2	70123	238108	1.10%	0.869%
4	6.499	1458	1480	1504	rBV2	257496	775717	3.58%	2.830%
5	7.627	1819	1831	1853	rVB3	93987	223551	1.03%	0.815%
6	7.991	1920	1944	1970	rBV4	103303	301084	1.39%	1.098%
7	8.550	2101	2118	2134	rVB	156043	322677	1.49%	1.177%
8	10.058	2573	2587	2598	rBV	249865	465296	2.15%	1.697%
9	11.376	2984	2997	3021	rBV2	299818	575110	2.65%	2.098%
10	12.373	3294	3307	3324	rBV	199421	357169	1.65%	1.303%
11	13.312	3588	3599	3619	rVB	238202	434216	2.00%	1.584%
12	13.418	3619	3632	3651	rBV	699690	1227081	5.66%	4.476%

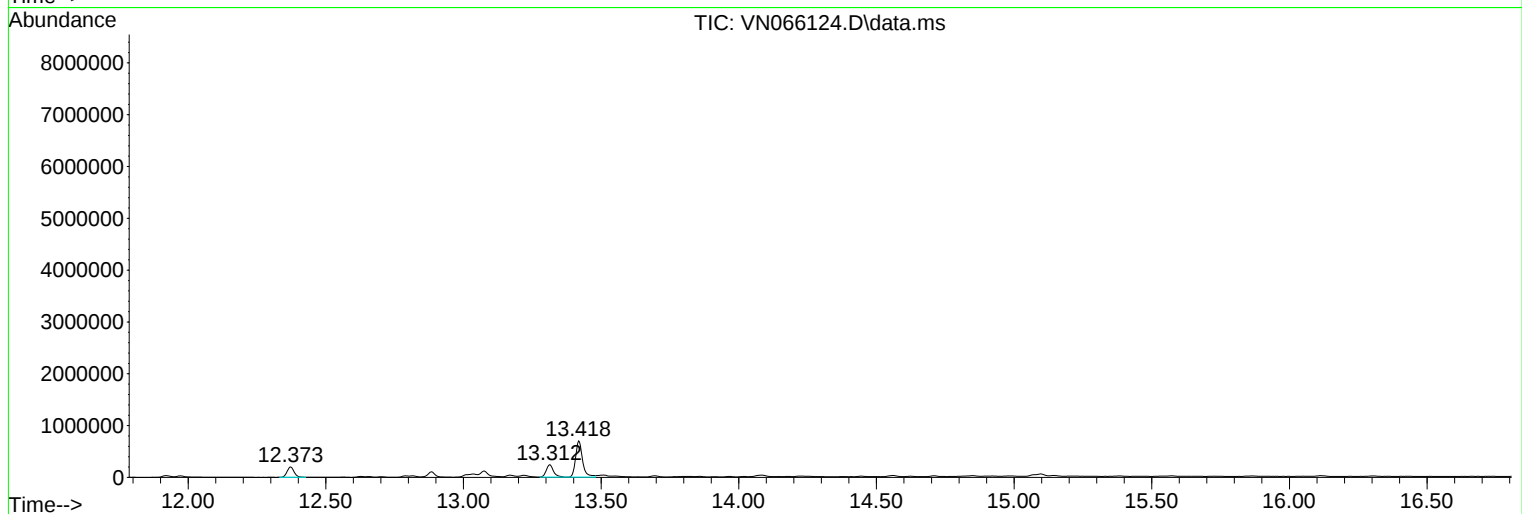
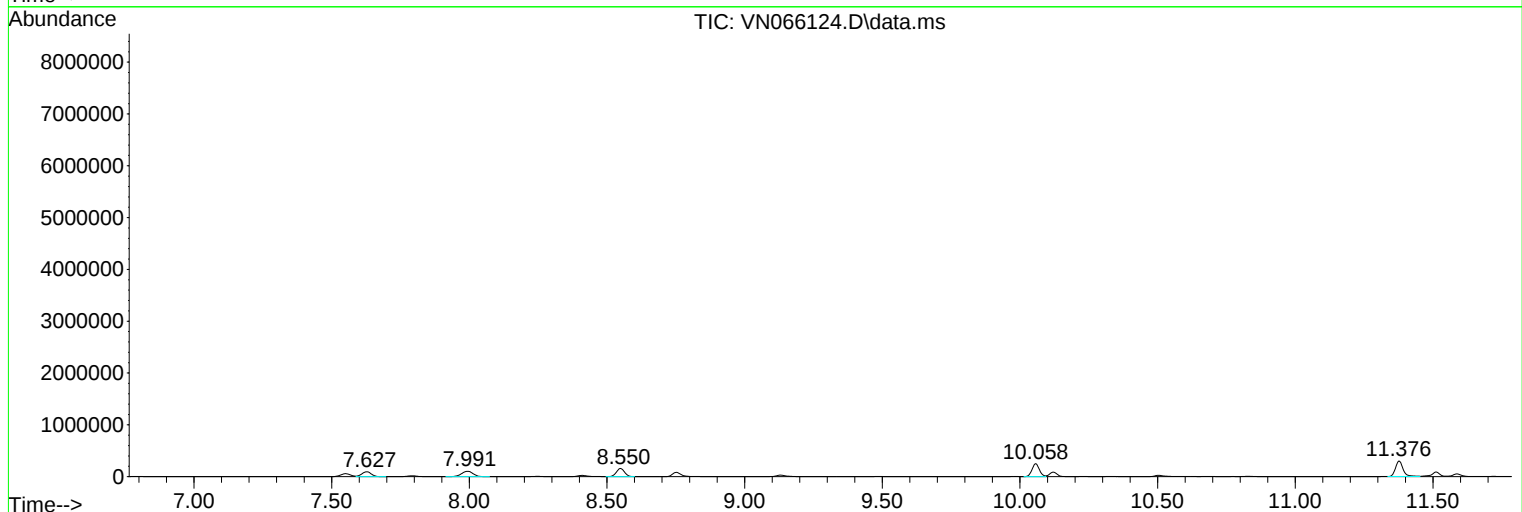
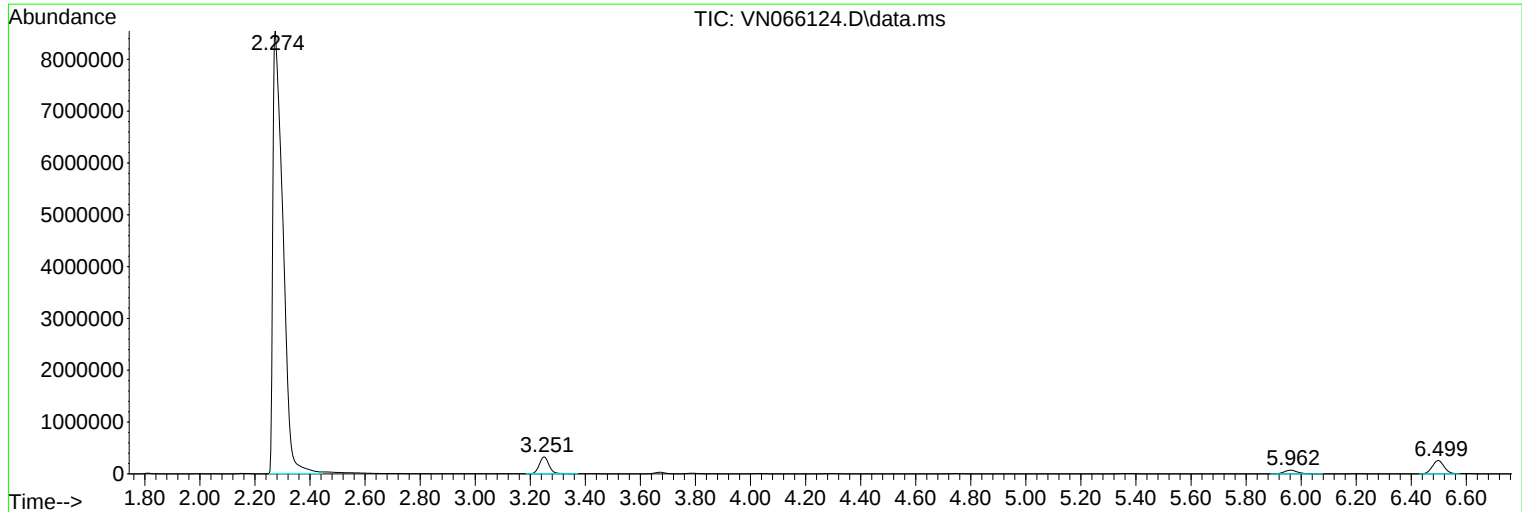
Sum of corrected areas: 27413780

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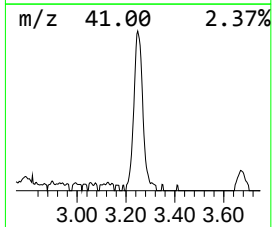
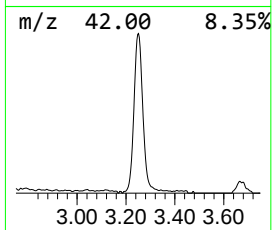
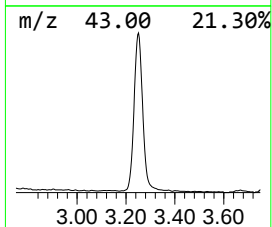
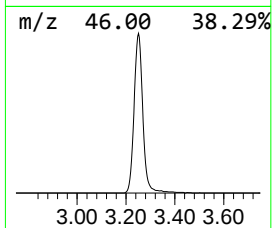
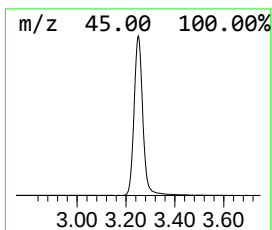
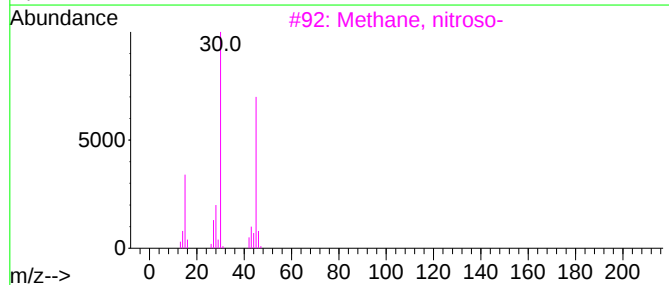
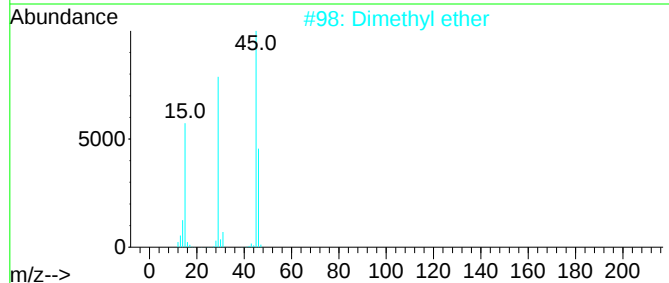
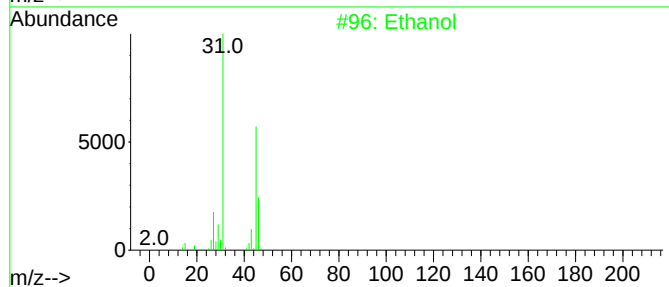
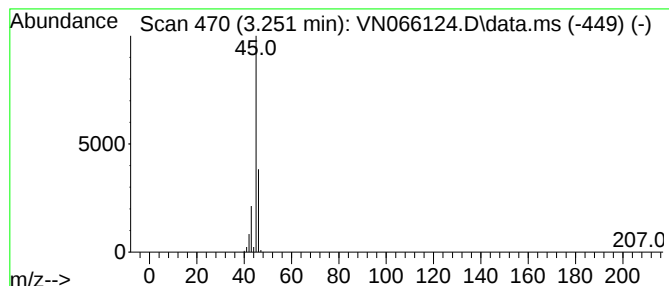
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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	179.71 ug/l	803484	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			L-Lactic acid	90	C3H6O3	000079-33-4	2



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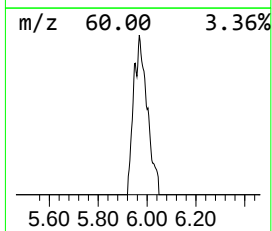
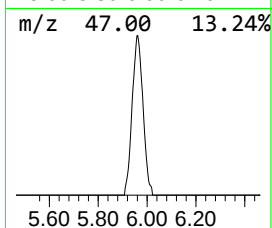
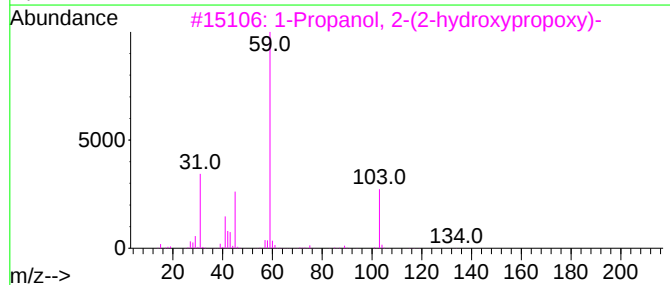
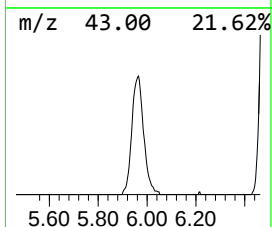
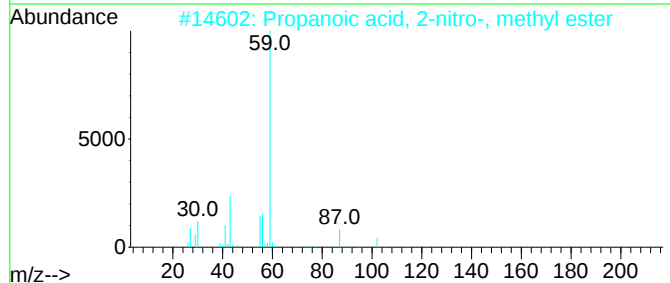
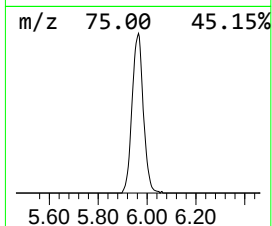
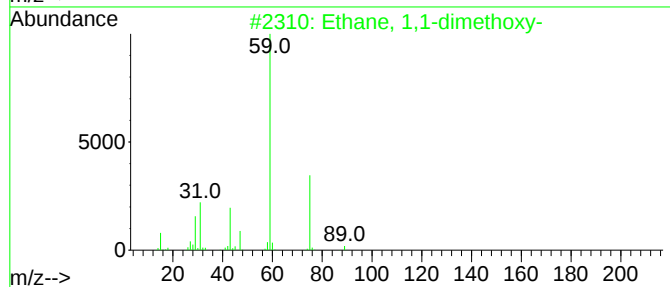
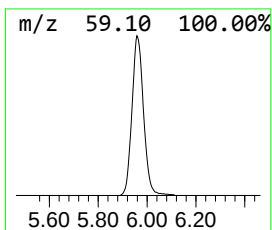
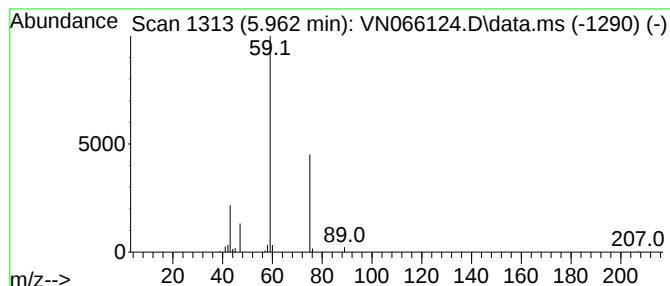
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Quant Title : SW846 8260

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Peak Number 3 Ethane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.962	53.26 ug/l	238108	Pentafluorobenzene	7.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	83
2			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	9
4			Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
5			Methane, diethoxy-	104	C5H12O2	000462-95-3	9



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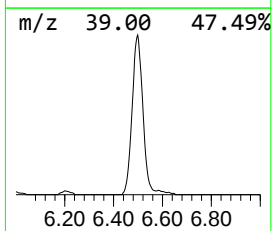
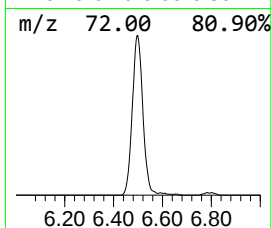
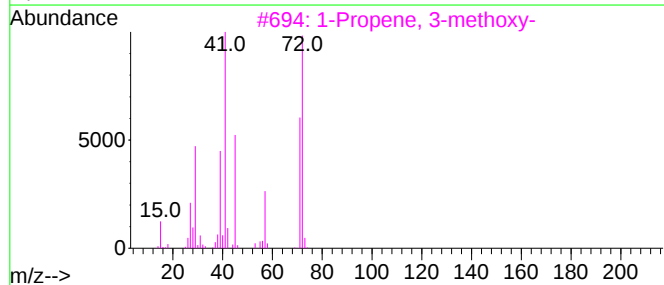
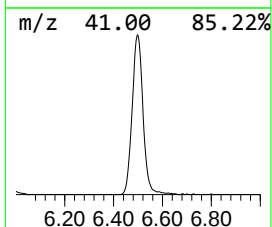
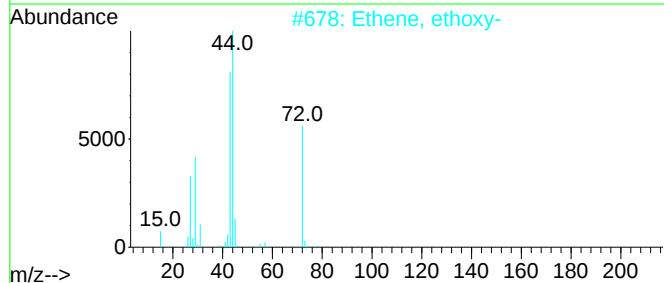
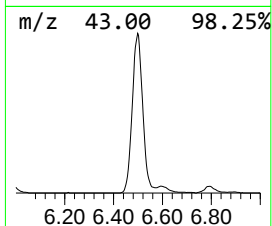
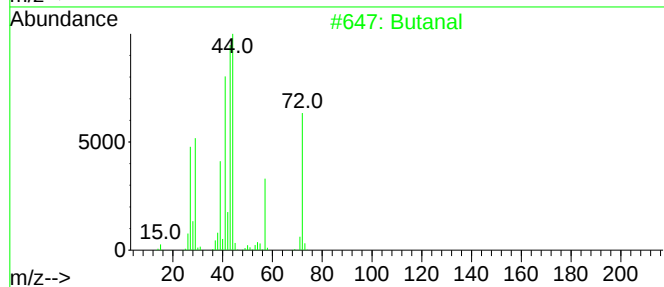
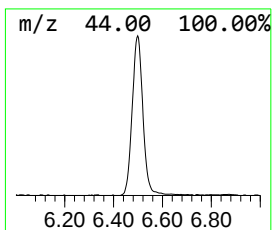
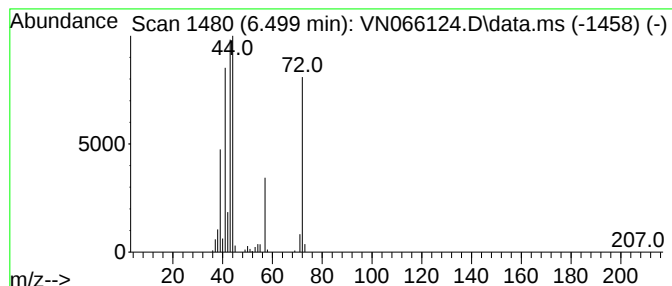
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Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.499	173.50 ug/l	775717	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	53
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
5			Isobutylene epoxide	72	C4H8O	000558-30-5	35



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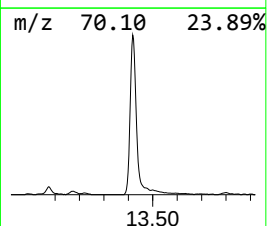
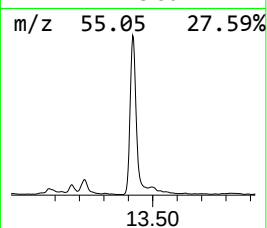
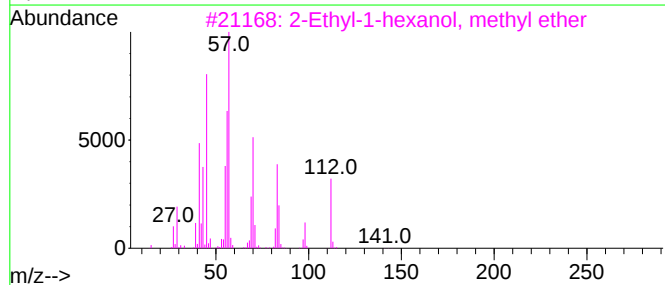
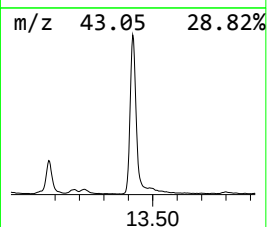
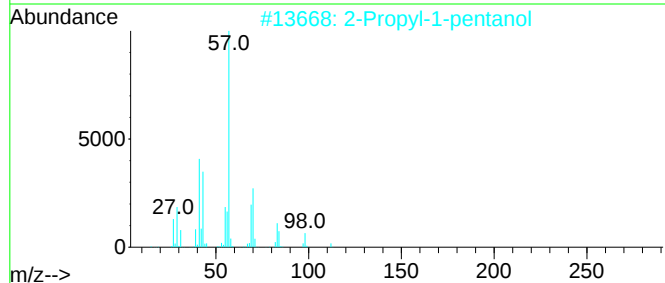
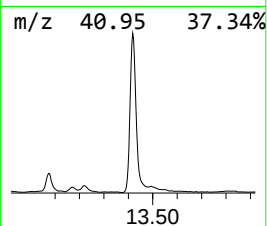
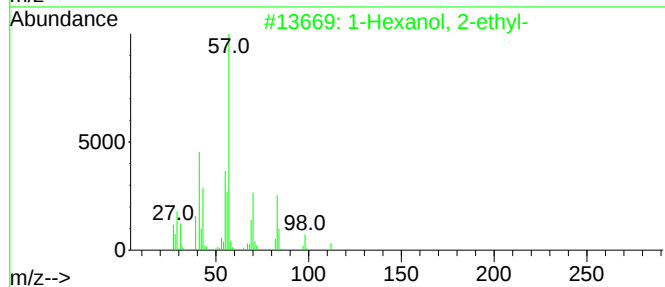
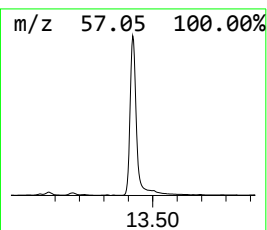
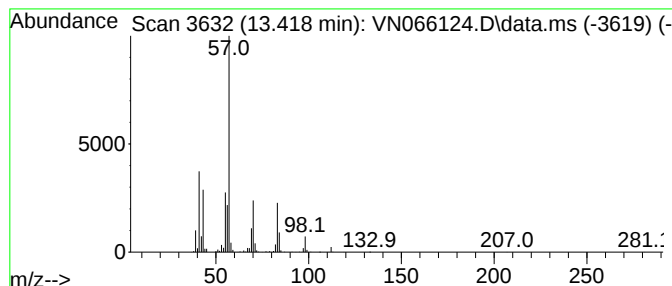
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	141.30 ug/l	1227080	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53
3	2-Ethyl-1-hexanol, methyl ether			144	C9H20O	1000365-10-2	50
4	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	50
5	3-Undecene, 6-methyl-, (E)-			168	C12H24	074630-52-7	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.251	179.7	ug/l	803484	1	7.627	223551	50.0
Ethane, 1,1-dim...	5.962	53.3	ug/l	238108	1	7.627	223551	50.0
Butanal	6.499	173.5	ug/l	775717	1	7.627	223551	50.0
1-Hexanol, 2-et...	13.418	141.3	ug/l	1227080	4	13.312	434216	50.0