

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
 Data File : VX020754.D
 Acq On : 26 Jan 2021 15:31
 Operator : JC/SP
 Sample : M1189-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41091

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\82X012521W.M

Title : SW846 8260

Signal : TIC: VX020754.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	57	59	83	rBV	34639851	81207040	100.00%	72.495%
2	2.093	158	165	177	rBV	668370	1146608	1.41%	1.024%
3	2.416	212	218	236	rVB	729663	1220994	1.50%	1.090%
4	3.751	426	437	452	rBV	583131	1621381	2.00%	1.447%
5	4.300	512	527	542	rBV	372559	1057267	1.30%	0.944%
6	5.623	732	744	757	rVB	385195	1074242	1.32%	0.959%
7	6.824	931	941	953	rVB	602861	1443539	1.78%	1.289%
8	8.696	1241	1248	1254	rBV	1275904	1996650	2.46%	1.782%
9	10.092	1469	1477	1489	rBV	1290814	1779785	2.19%	1.589%
10	10.348	1514	1519	1529	rVB	9483407	13052826	16.07%	11.652%
11	11.122	1640	1646	1650	rBV	1116143	1445239	1.78%	1.290%
12	12.061	1797	1800	1807	rVB	1325439	1603542	1.97%	1.432%
13	12.256	1824	1832	1843	rBV	2283510	3368430	4.15%	3.007%

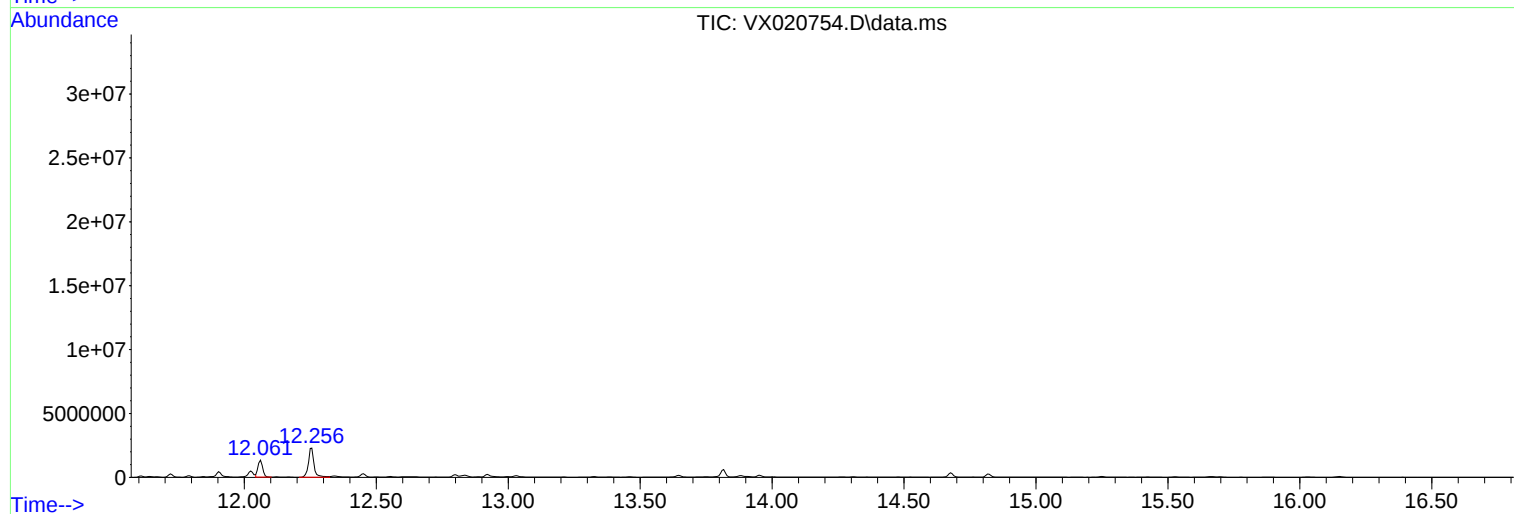
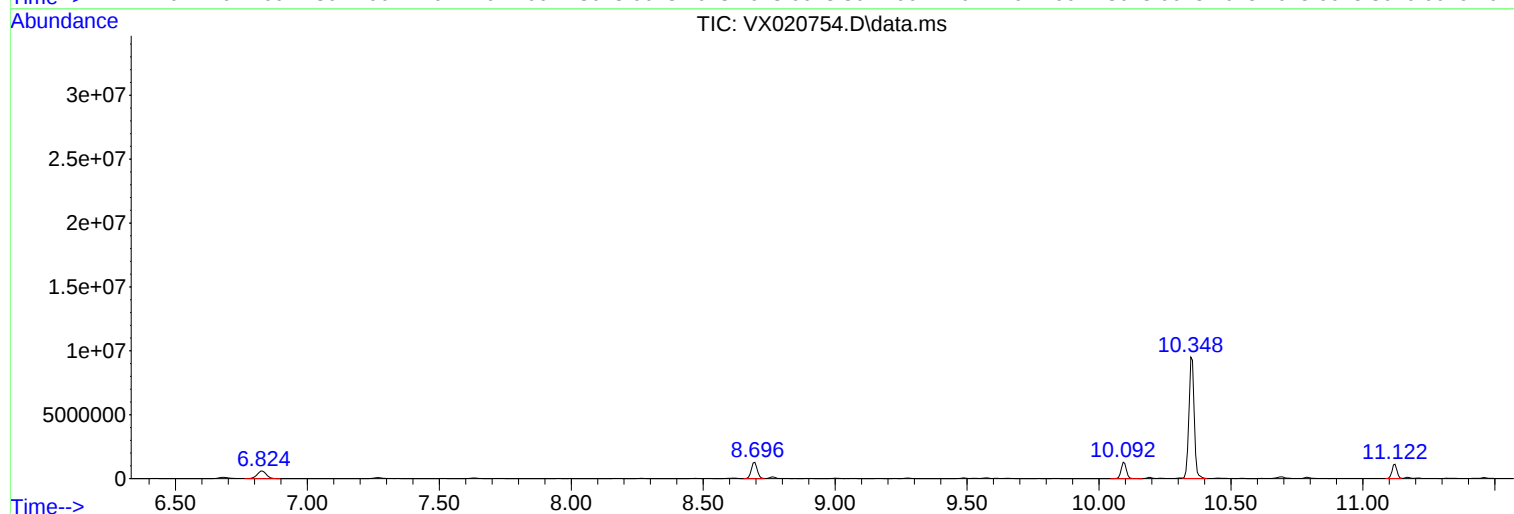
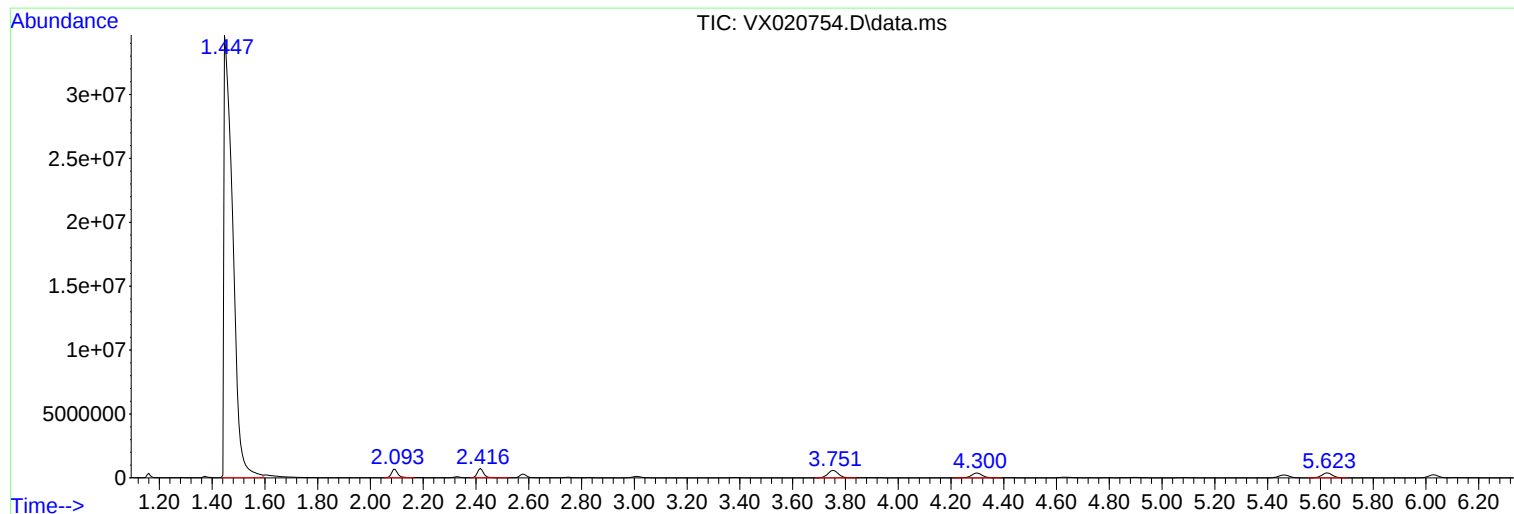
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



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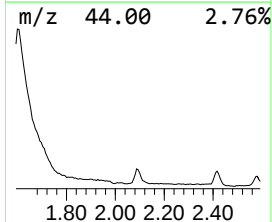
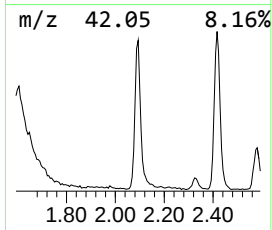
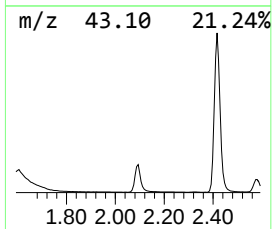
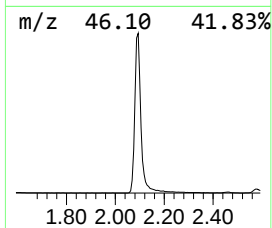
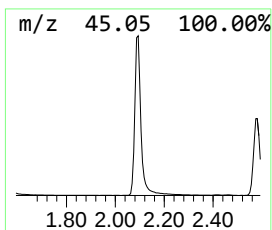
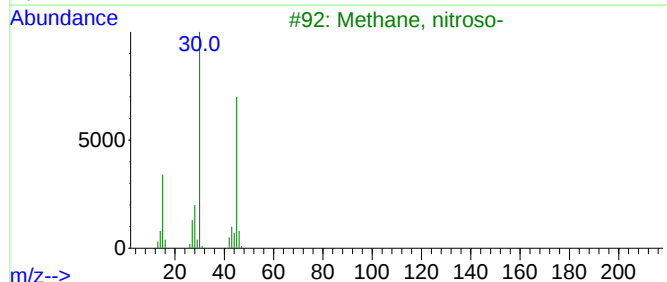
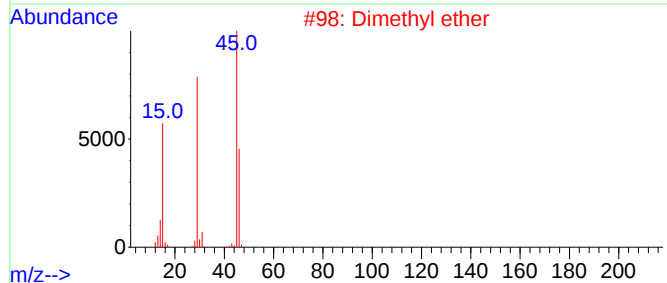
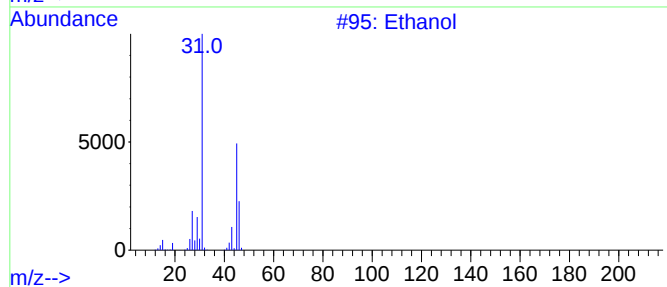
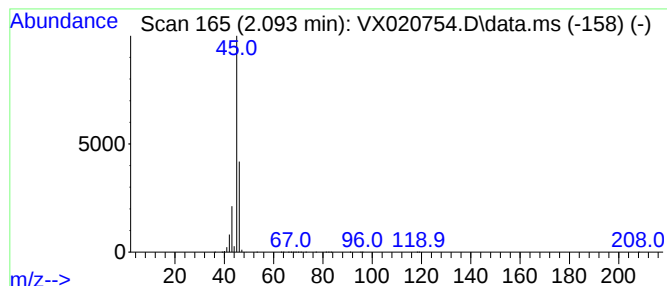
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.093	53.37 ug/l	1146610	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	78
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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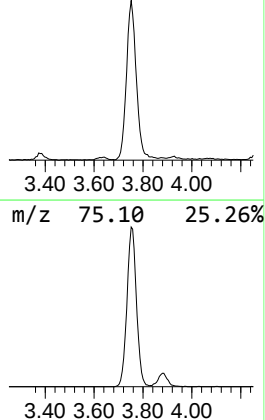
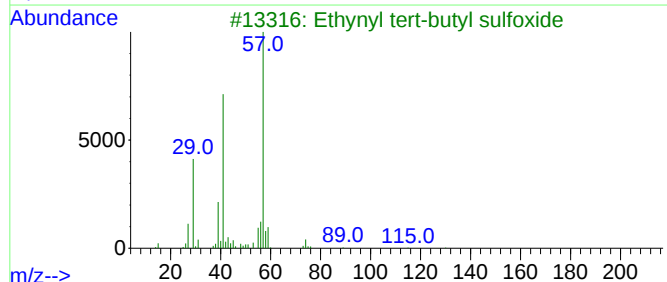
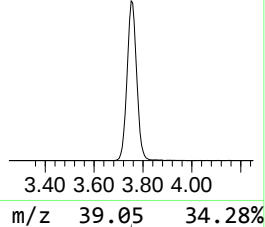
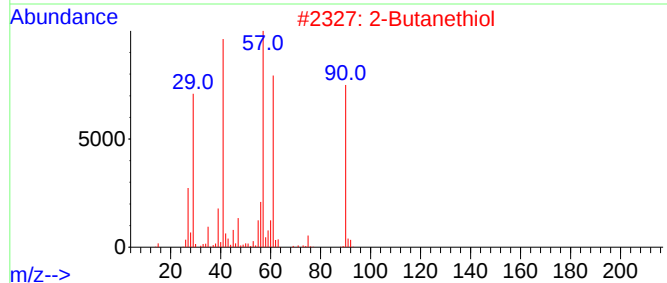
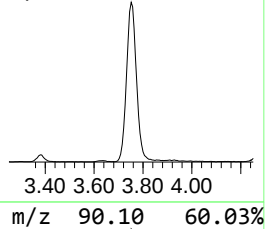
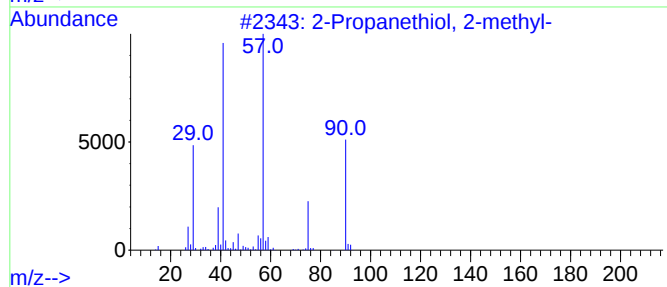
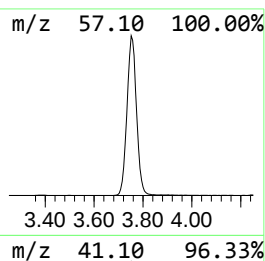
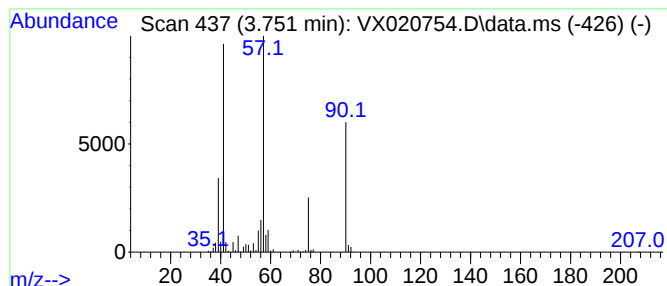
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.751	75.47 ug/l	1621380	Pentafluorobenzene	5.623

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	45
3			Ethynyl tert-butyl sulfoxide	130	C6H10OOS	041463-34-7	35
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	12



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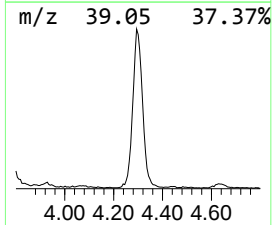
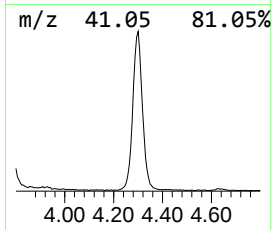
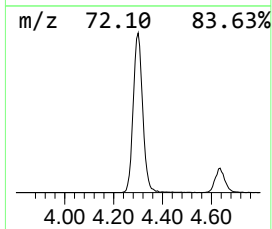
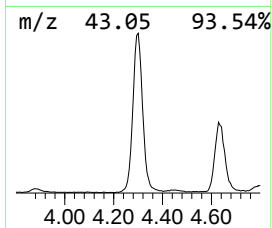
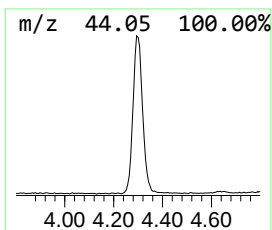
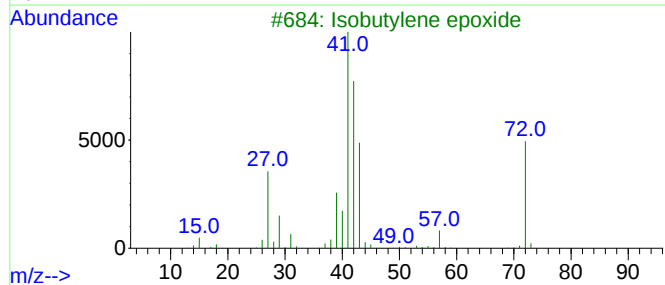
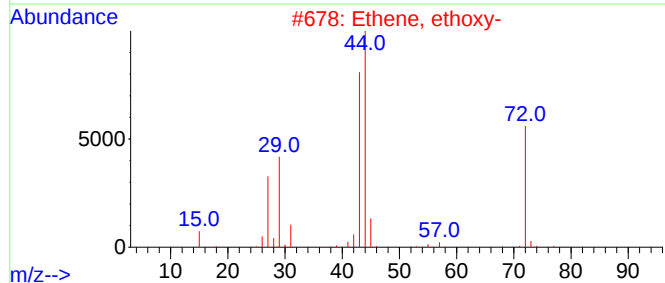
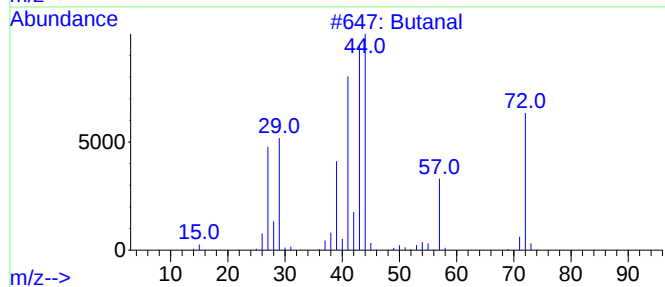
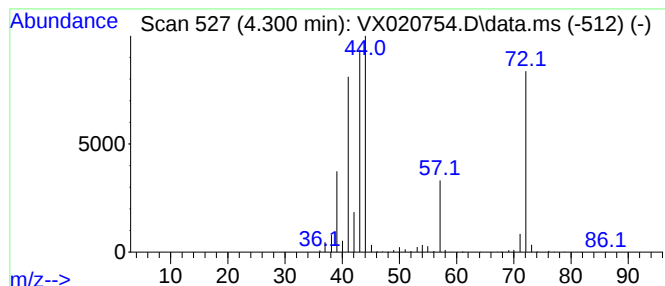
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Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	49.21 ug/l	1057270	Pentafluorobenzene	5.623

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	64
3			Isobutylene epoxide	72	C4H8O	000558-30-5	38
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38



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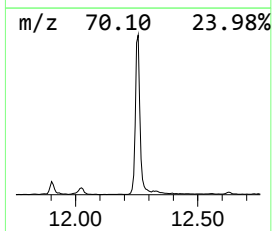
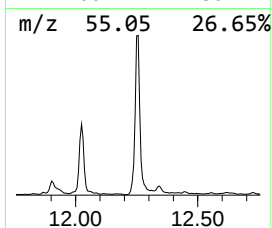
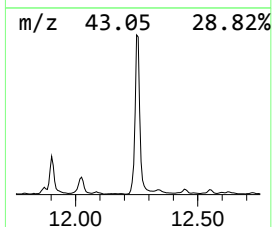
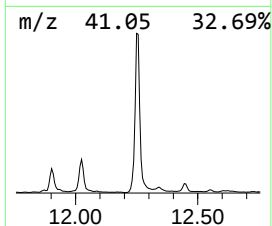
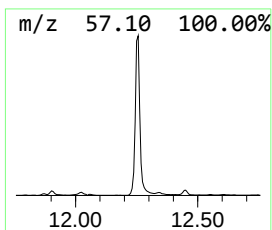
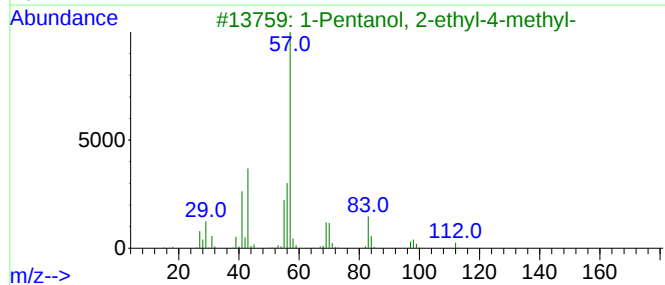
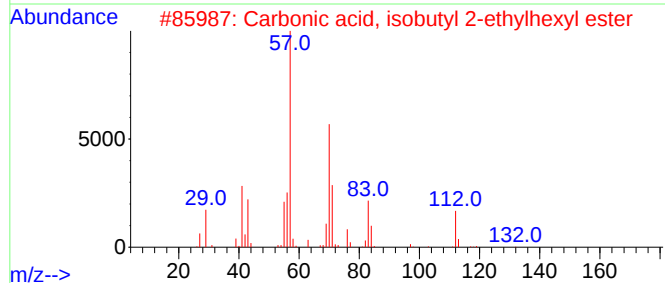
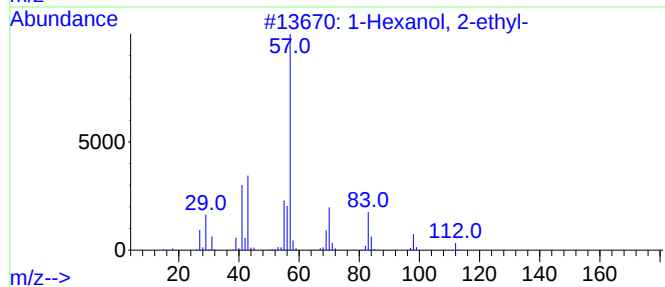
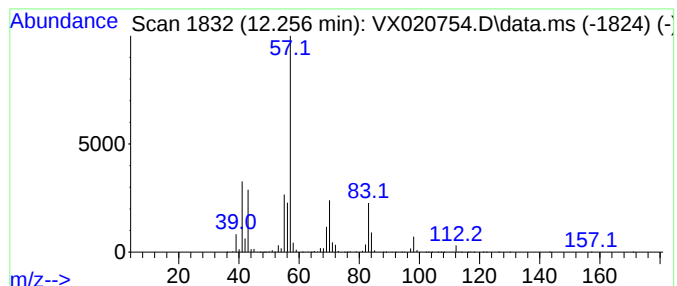
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	105.03 ug/l	3368430	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.093	53.4	ug/l	1146610	1	5.623	1074240	50.0
2-Propanethiol,...	3.751	75.5	ug/l	1621380	1	5.623	1074240	50.0
Butanal	4.300	49.2	ug/l	1057270	1	5.623	1074240	50.0
1-Hexanol, 2-et...	12.256	105.0	ug/l	3368430	4	12.061	1603540	50.0