

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021499.D
Acq On : 25 Mar 2021 20:13
Operator : JC/MD
Sample : M1774-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41736

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\82X032421W.M
Title : SW846 8260

Signal : TIC: VX021499.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.452	59	62	116	rBV	15144171	35297798	100.00%	93.137%
2	2.093	165	171	184	rBV	303799	496943	1.41%	1.311%
3	4.299	534	546	562	rBV	164838	440765	1.25%	1.163%
4	8.694	1286	1293	1300	rBV	263828	405784	1.15%	1.071%
5	10.094	1522	1531	1542	rBV	285381	393372	1.11%	1.038%
6	12.253	1893	1898	1910	rBV	659511	864216	2.45%	2.280%

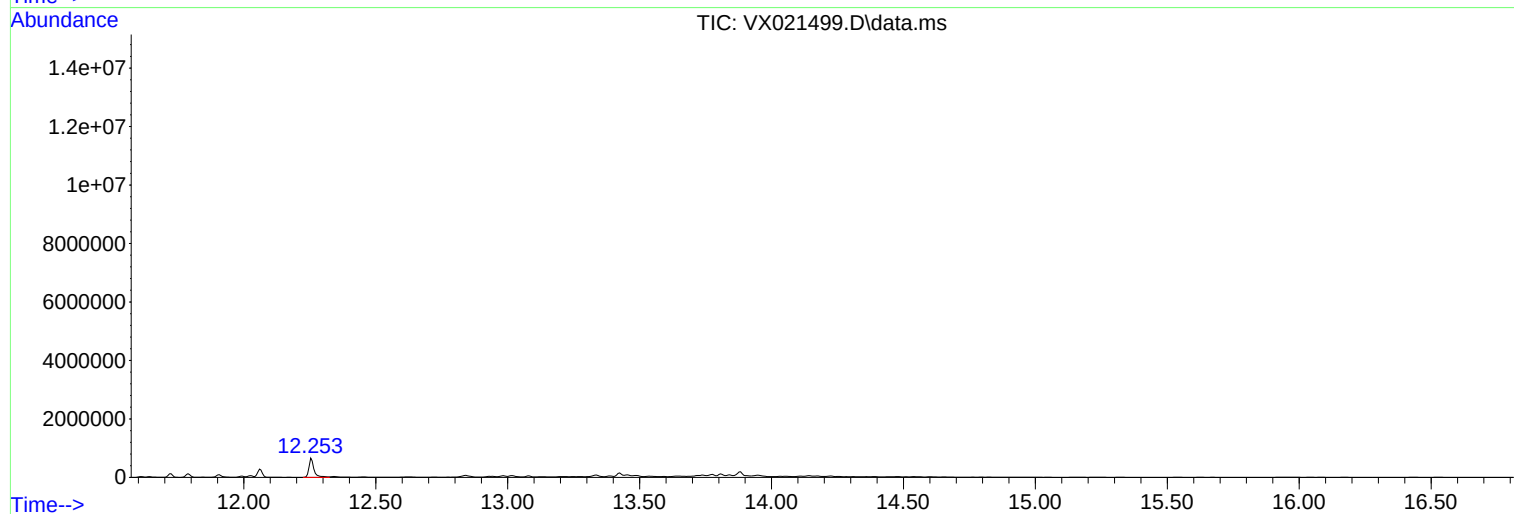
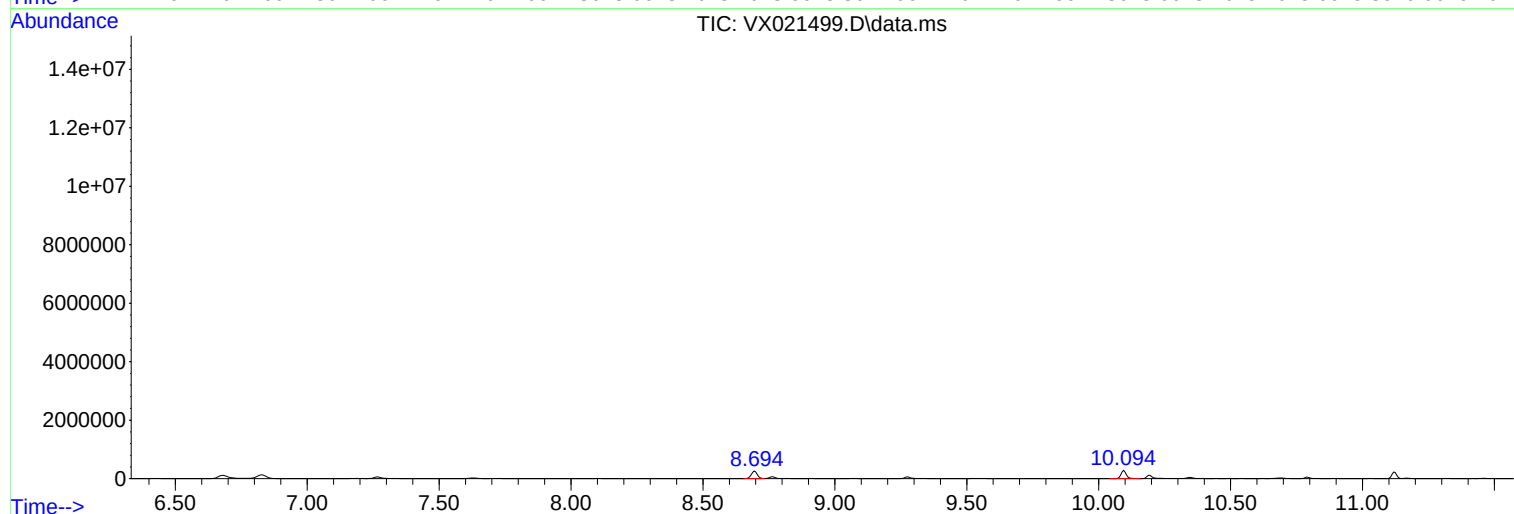
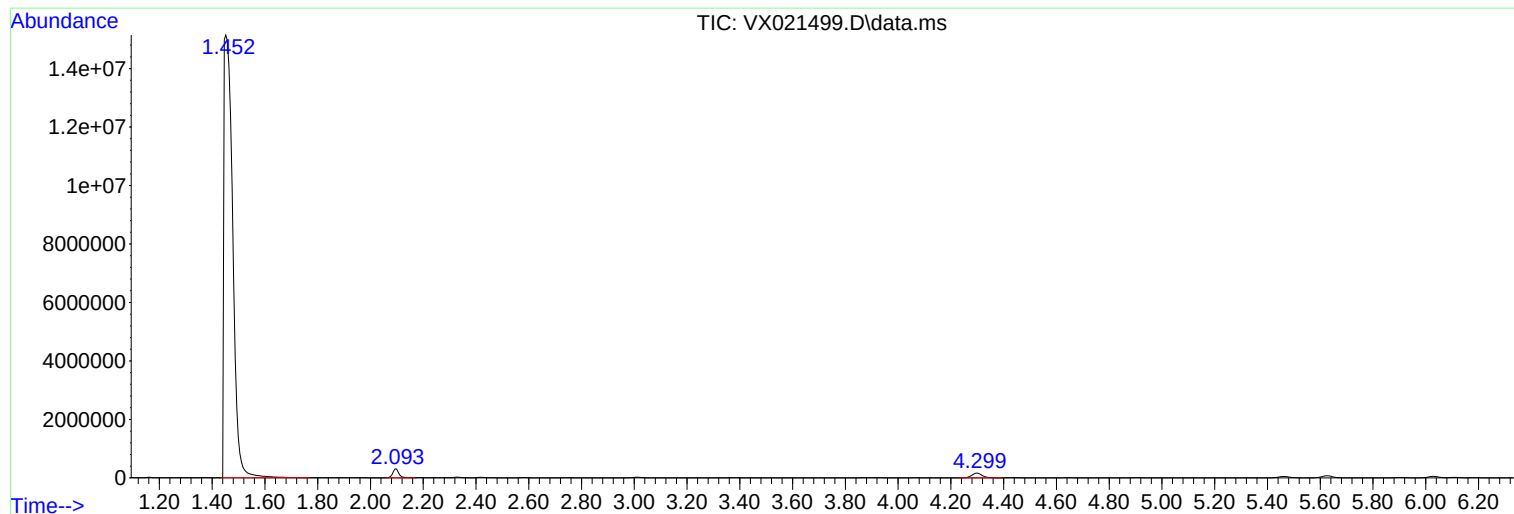
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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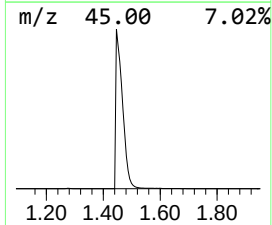
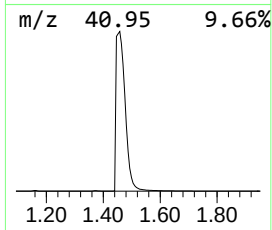
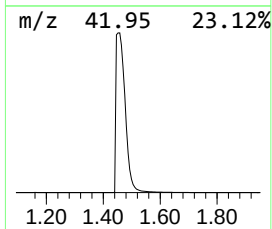
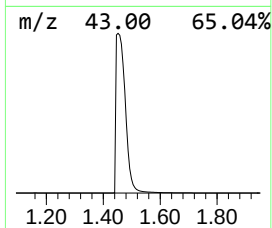
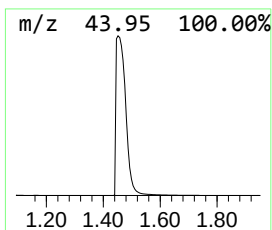
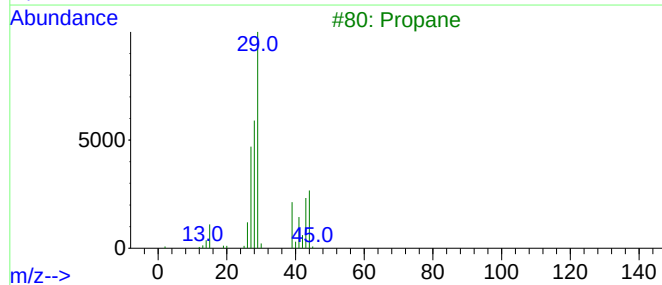
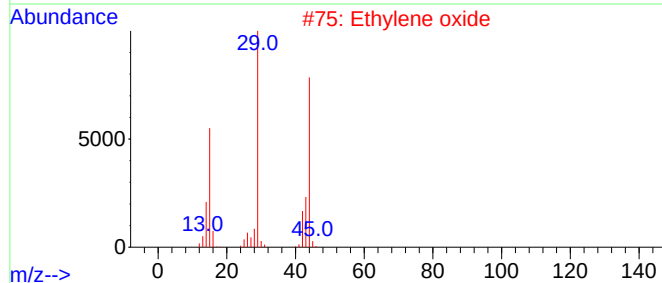
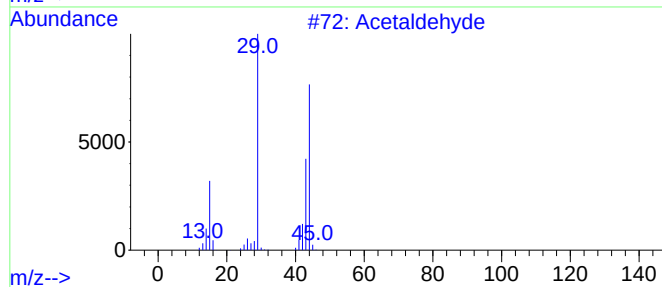
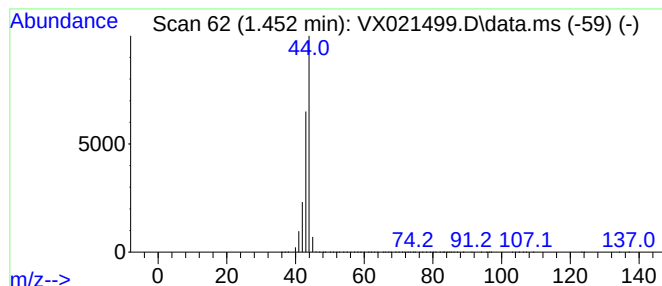
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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.
1.452	4004.15 ug/l	35297800	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Glycidol	74	C3H6O2	000556-52-5	4
5			D-Alanine	89	C3H7NO2	000338-69-2	4



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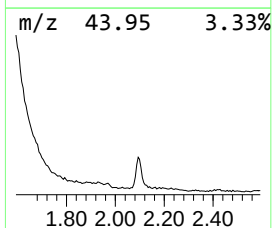
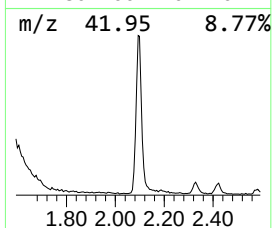
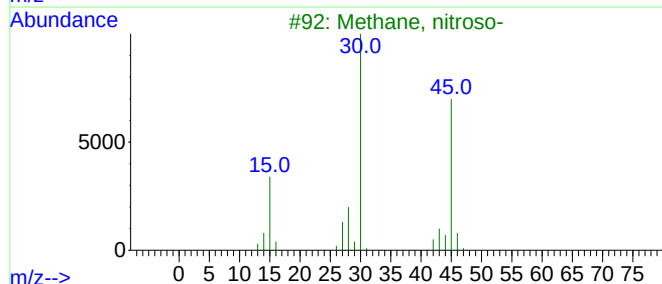
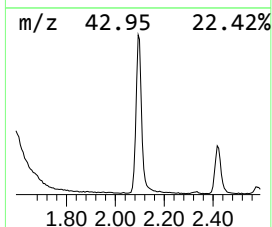
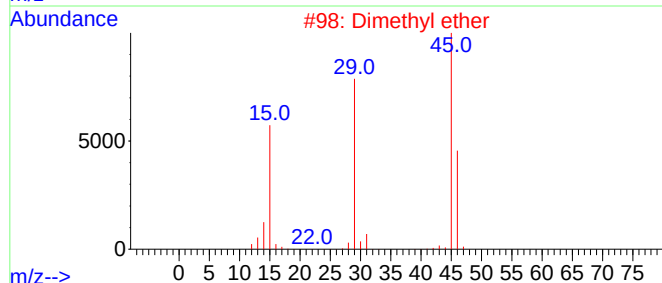
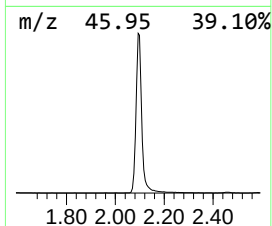
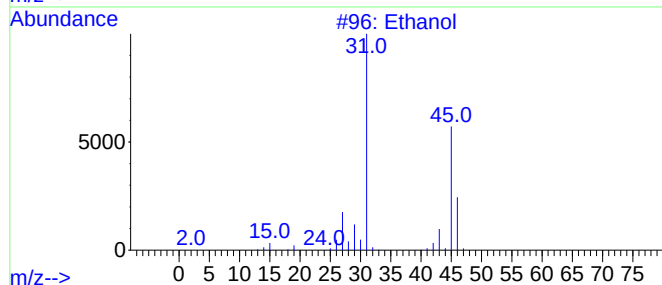
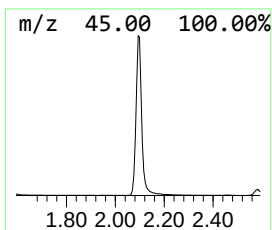
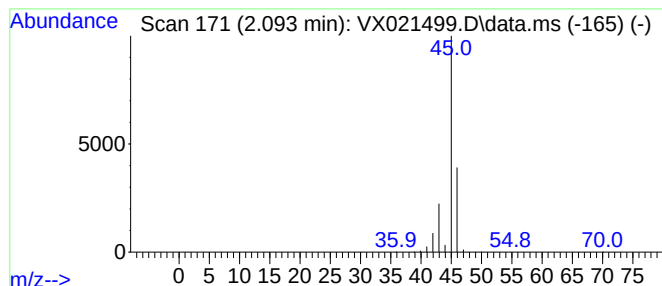
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Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.093	56.37 ug/l	496943	Pentafluorobenzene	5.629

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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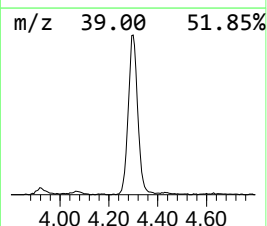
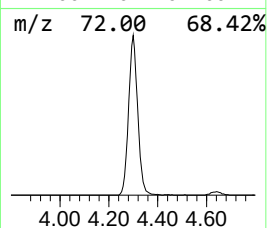
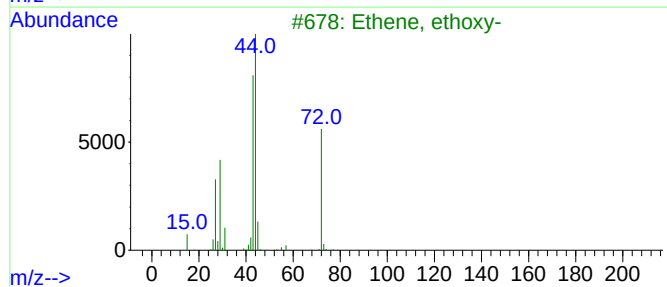
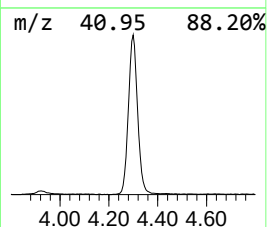
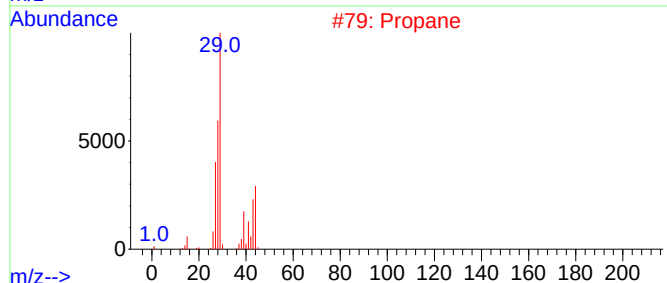
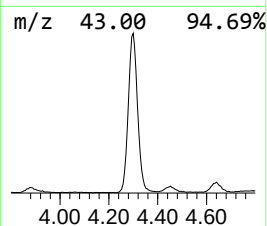
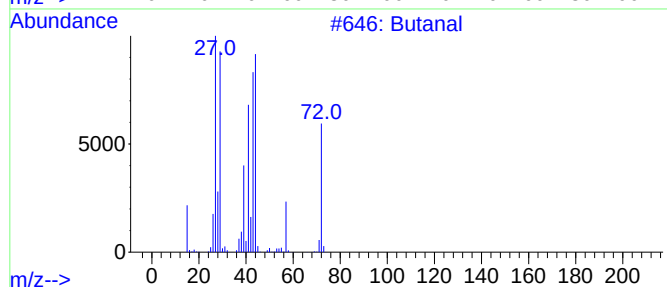
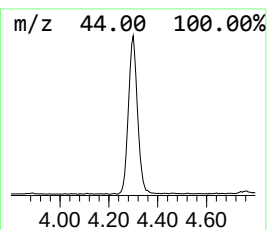
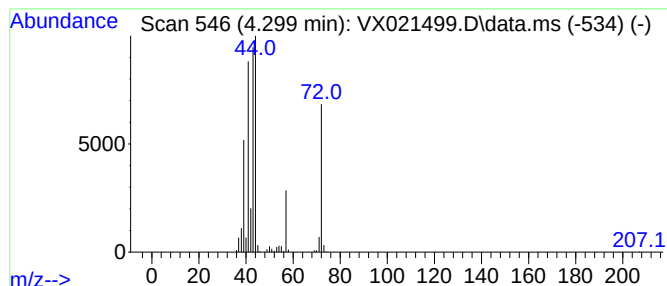
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Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	50.00 ug/l	440765	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	59
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	49
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			Methacrolein	70	C4H6O	000078-85-3	27



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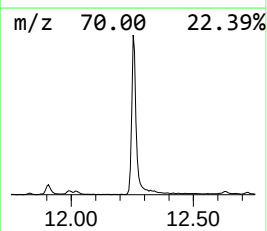
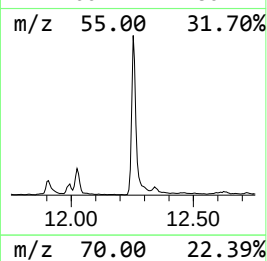
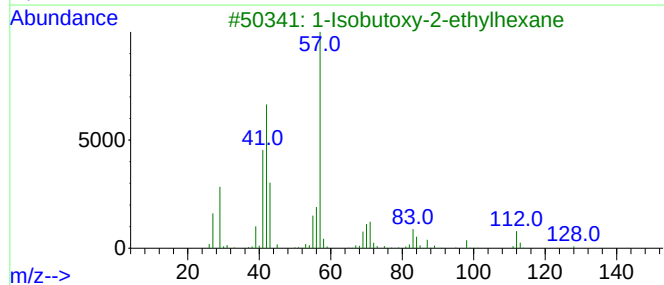
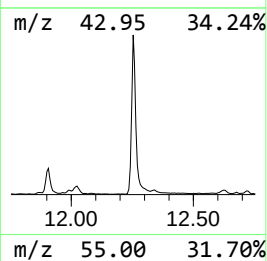
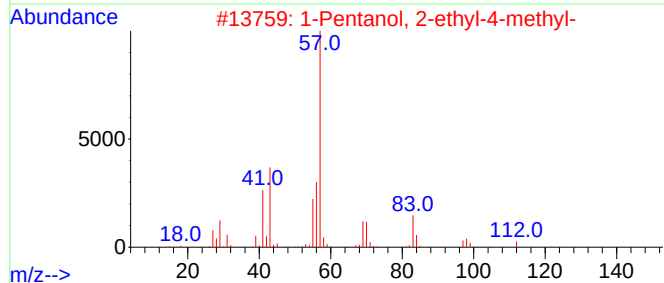
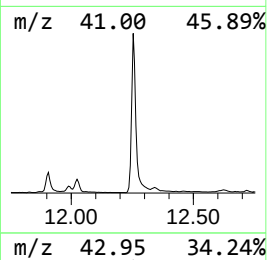
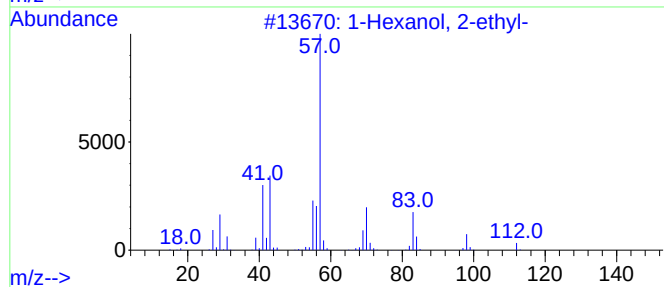
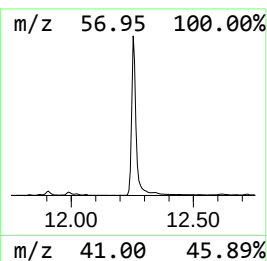
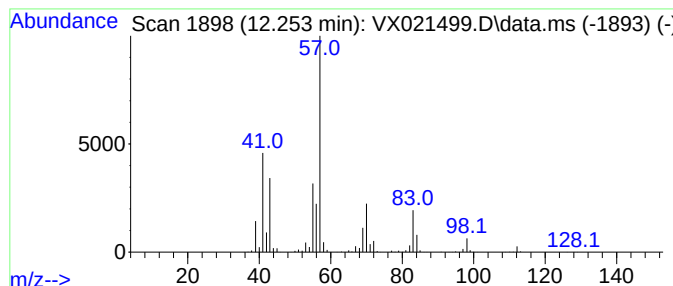
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	50.00 ug/l	864216	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.452	4004.2	ug/l	35297800	1	5.629	440765	50.0
Ethanol	2.093	56.4	ug/l	496943	1	5.629	440765	50.0
Butanal	4.299	50.0	ug/l	440765	1	5.629	440765	50.0
1-Hexanol, 2-et...	12.253	50.0	ug/l	864216	4	12.059	864216	50.0