

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
 Data File : VX021786.D
 Acq On : 21 Apr 2021 12:47
 Operator : JC/MD
 Sample : M2101-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31056

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\82X042021W.M
 Title : SW846 8260

Signal : TIC: VX021786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	74	rBV	899186	1042271	100.00%	15.398%
2	2.093	159	165	178	rBV	682265	1036713	99.47%	15.316%
3	2.331	199	204	213	rVB	31603	50758	4.87%	0.750%
4	2.422	213	219	228	rVB	25623	43053	4.13%	0.636%
5	3.008	309	315	324	rVB2	6329	13829	1.33%	0.204%
6	3.385	367	377	384	rBV	8516	20018	1.92%	0.296%
7	4.300	516	527	538	rBV2	43958	120601	11.57%	1.782%
8	4.635	573	582	596	rBV2	24614	73159	7.02%	1.081%
9	5.086	649	656	666	rBV4	4200	13048	1.25%	0.193%
10	5.464	706	718	731	rBV2	95806	277532	26.63%	4.100%
11	5.629	733	745	758	rBV	160512	447643	42.95%	6.613%
12	6.031	797	811	824	rBV	97128	255666	24.53%	3.777%
13	6.678	908	917	928	rVB6	5426	17637	1.69%	0.261%
14	6.830	931	942	955	rBV	250105	587444	56.36%	8.678%
15	7.269	1006	1014	1024	rBV	21399	48661	4.67%	0.719%
16	8.104	1144	1151	1157	rBV	7126	11645	1.12%	0.172%
17	8.696	1240	1248	1256	rBV	519722	815934	78.28%	12.054%
18	10.098	1471	1478	1489	rBV	477118	691266	66.32%	10.212%
19	11.122	1640	1646	1655	rBV	399556	528108	50.67%	7.802%
20	12.061	1795	1800	1806	rBV	536563	651285	62.49%	9.622%
21	12.256	1827	1832	1838	rBV	14475	22716	2.18%	0.336%

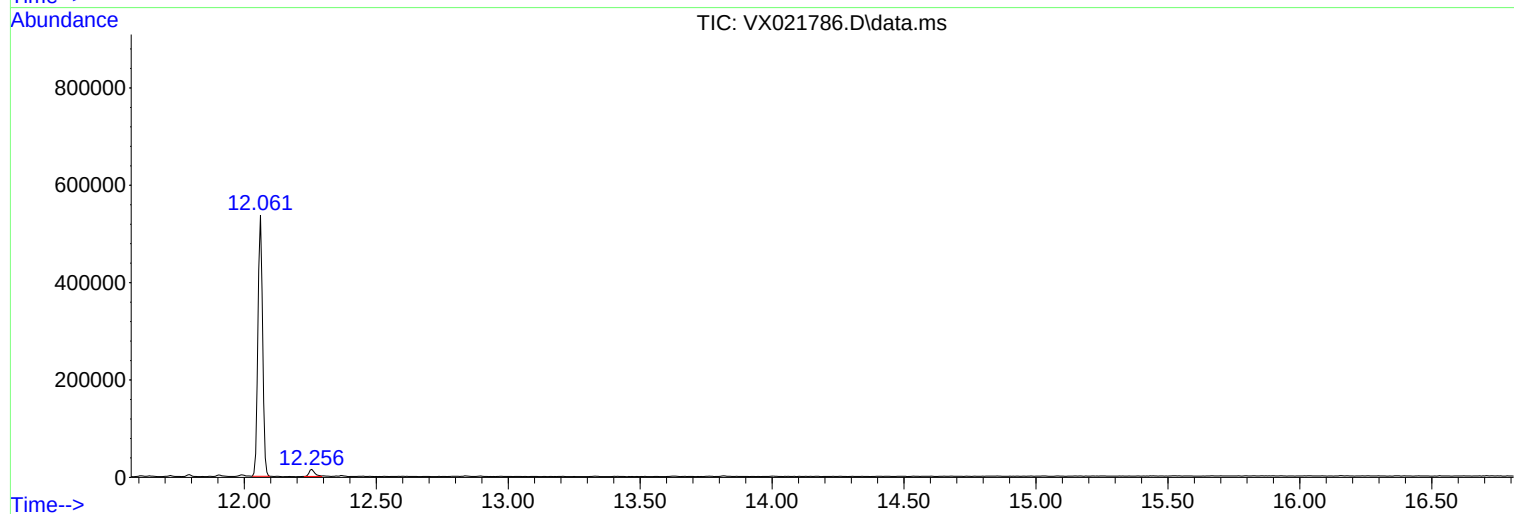
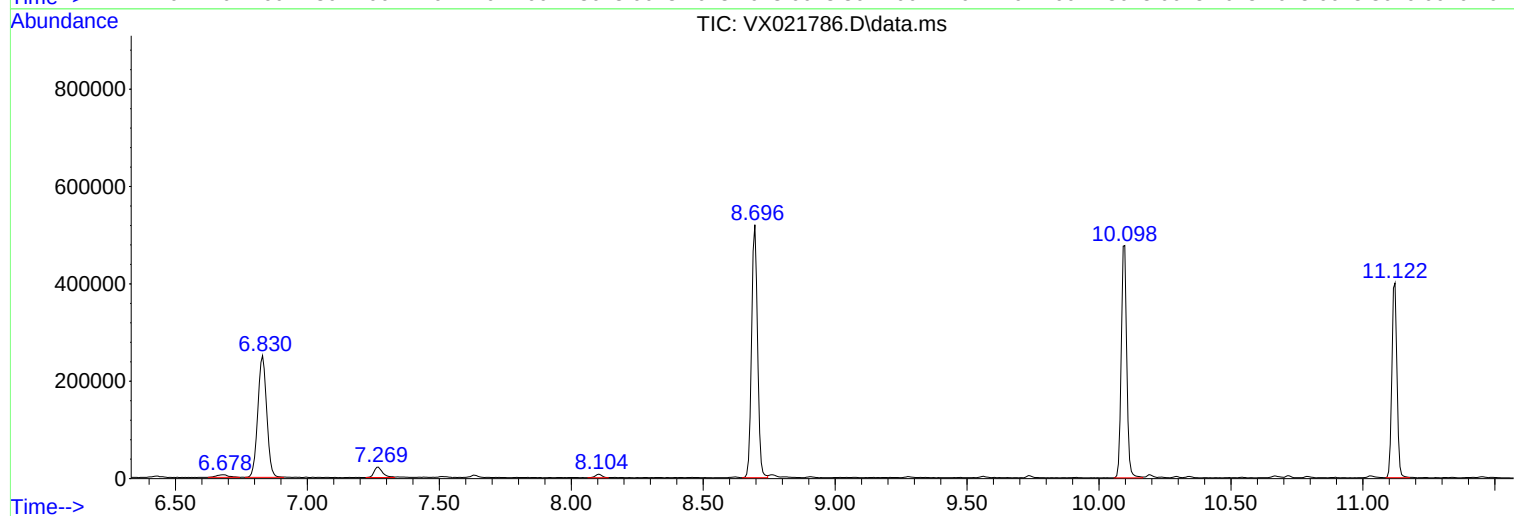
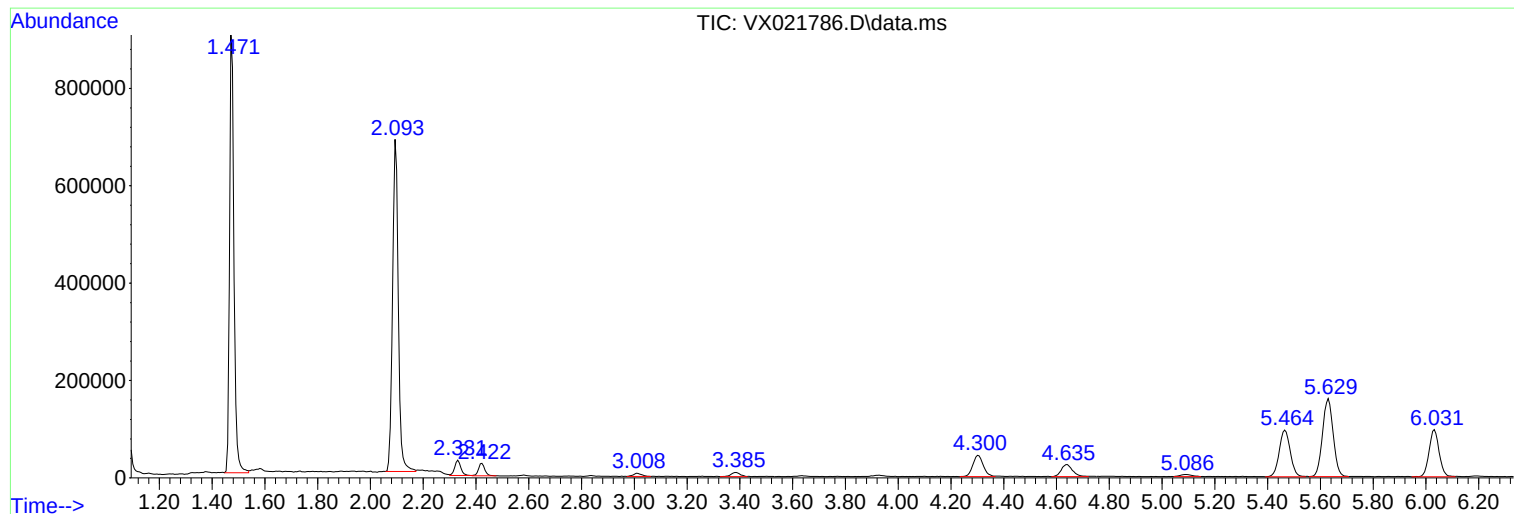
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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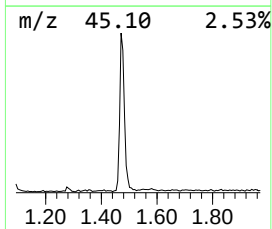
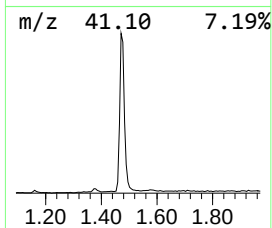
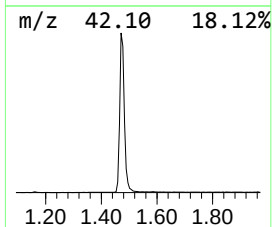
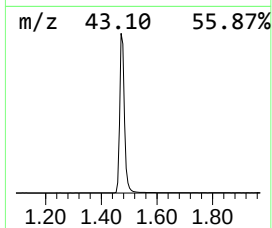
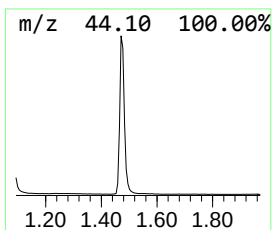
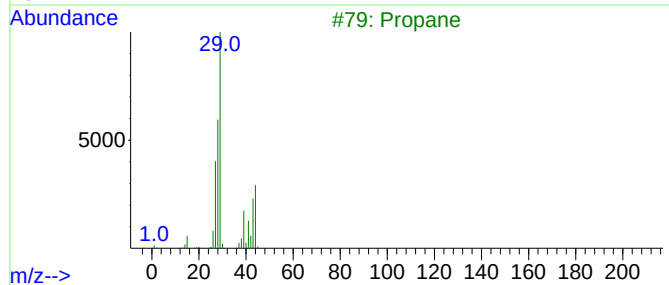
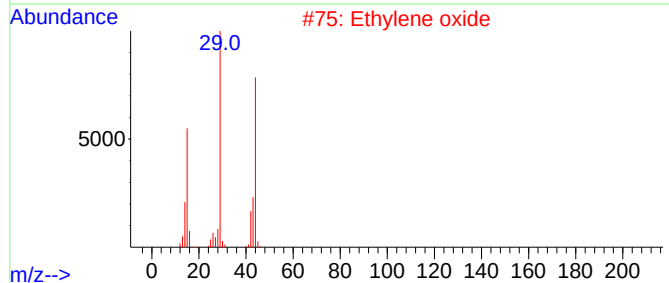
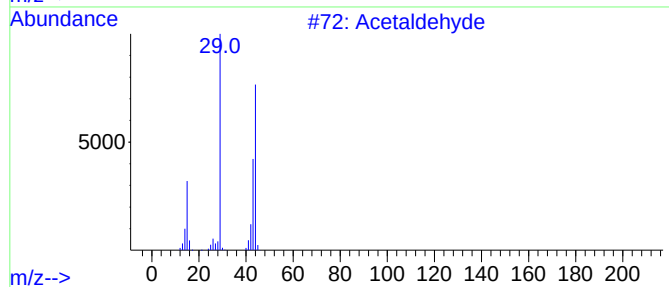
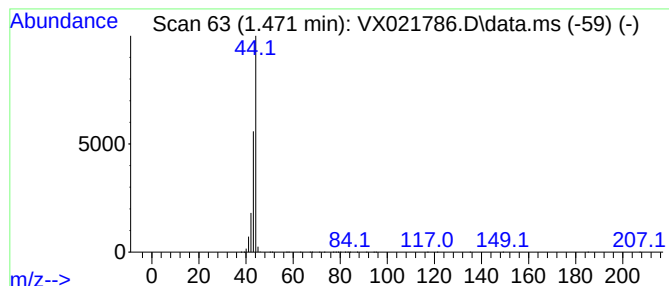
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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.
1.471	116.42 ug/l	1042270	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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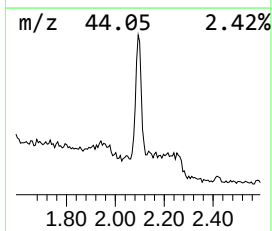
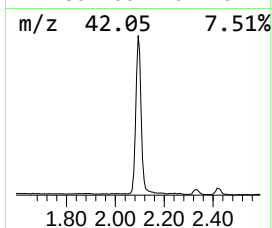
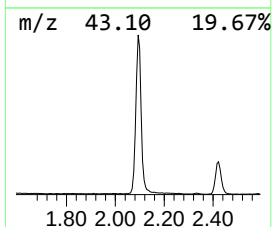
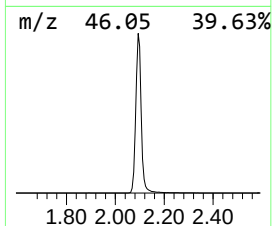
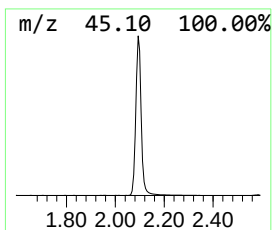
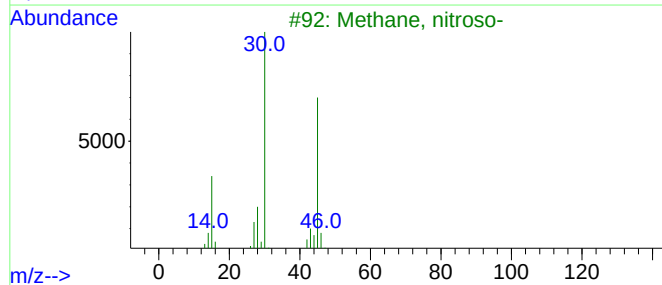
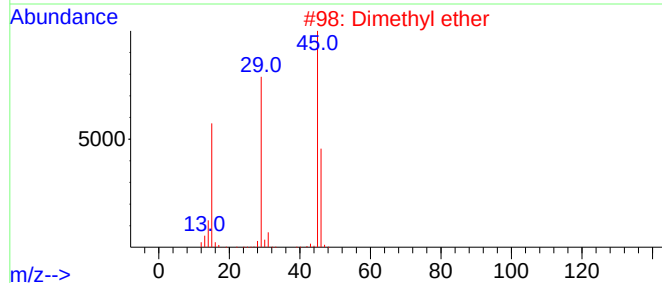
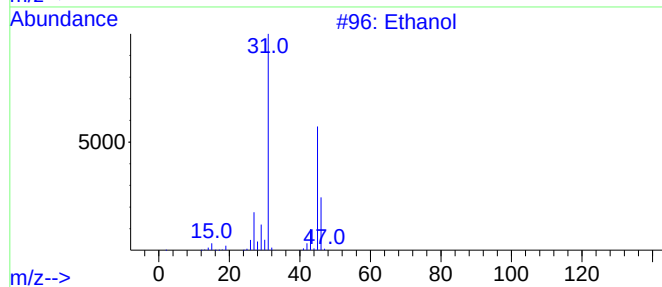
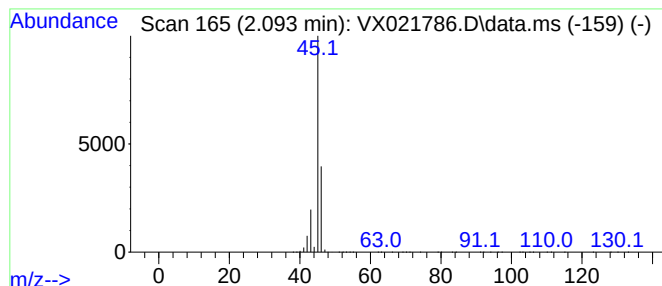
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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.
2.093	115.80 ug/l	1036710	Pentafluorobenzene	5.629

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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Instrument :
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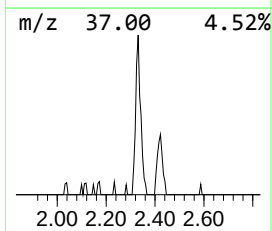
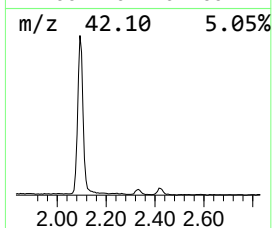
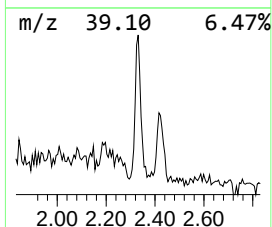
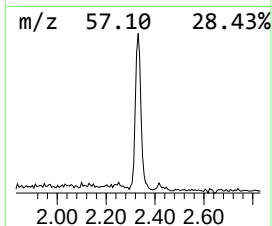
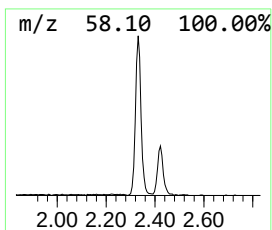
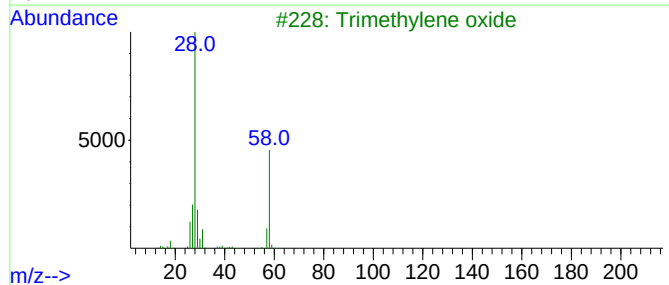
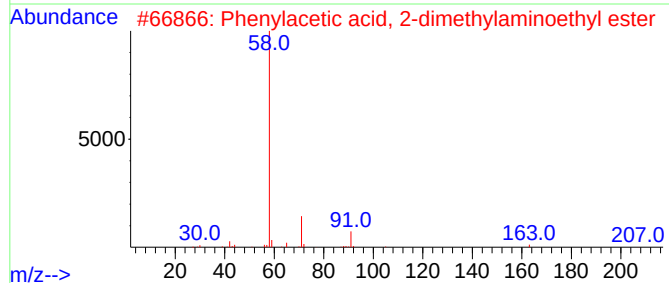
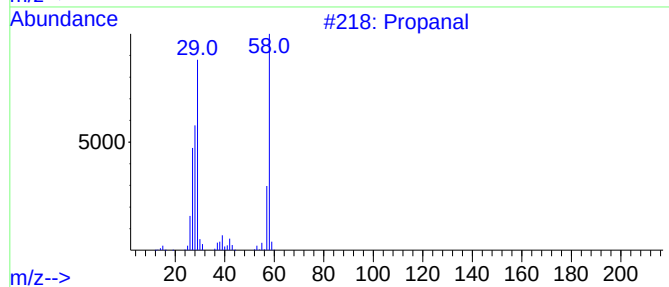
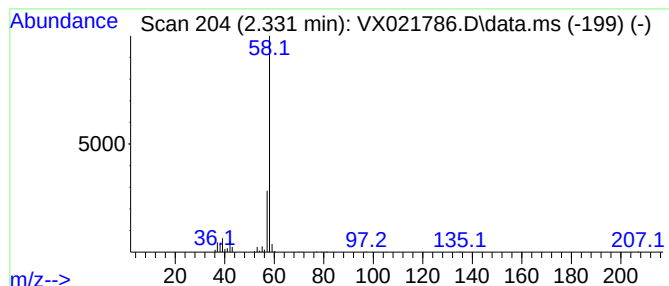
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.331	5.67 ug/l	50758	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	64
2			Phenylacetic acid, 2-dimethylami...	207	C12H17NO2	1000331-13-5	9
3			Trimethylene oxide	58	C3H6O	000503-30-0	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			N,N-Dimethyl-3-methoxypropylamine	117	C6H15NO	020650-07-1	9



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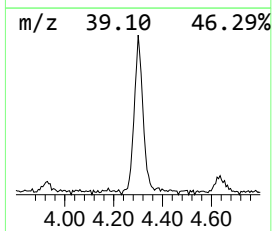
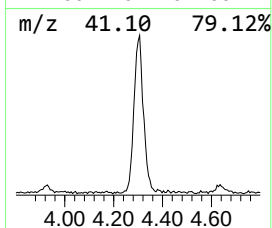
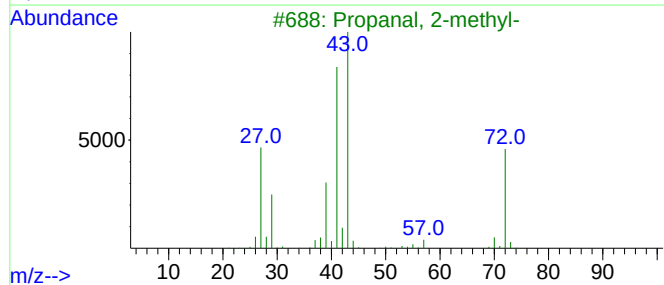
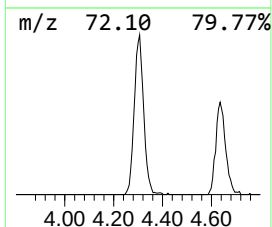
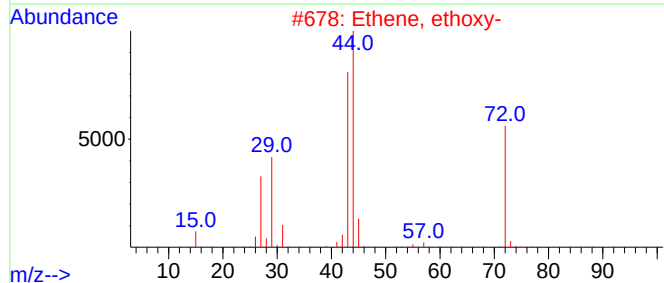
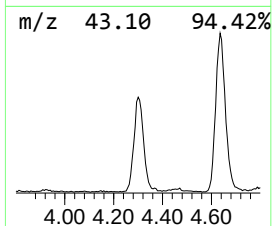
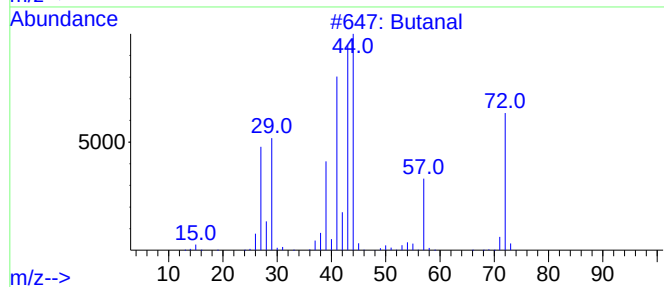
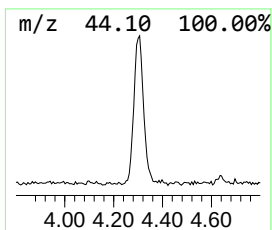
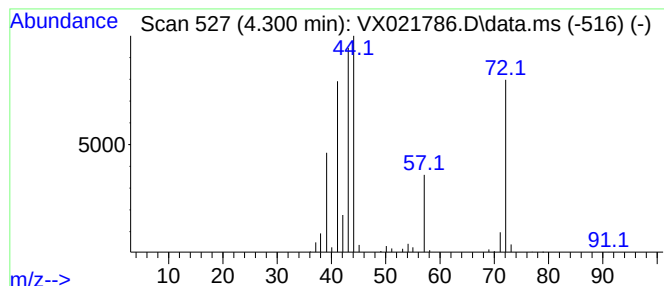
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	13.47 ug/l	120601	Pentafluorobenzene	5.629

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			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
5			Isobutylene epoxide	72	C4H8O	000558-30-5	27



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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	1.471	116.4	ug/l	1042270	1	5.629	447643	50.0
Ethanol	2.093	115.8	ug/l	1036710	1	5.629	447643	50.0
Propanal	2.331	5.7	ug/l	50758	1	5.629	447643	50.0
Butanal	4.300	13.5	ug/l	120601	1	5.629	447643	50.0