

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061623\
 Data File : VX036195.D
 Acq On : 16 Jun 2023 20:45
 Operator : JC/MD
 Sample : 03301-01 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1619

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\82X061623W.M

Title : SW846 8260

Signal : TIC: VX036195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	88	rBV	3980871	5193989	100.00%	46.979%
2	2.111	157	168	193	rVB	47272	218829	4.21%	1.979%
3	4.233	507	516	532	rBV2	19756	56536	1.09%	0.511%
4	5.385	694	705	721	rBV	117277	345627	6.65%	3.126%
5	5.550	721	732	748	rVB	197345	562999	10.84%	5.092%
6	5.952	789	798	817	rVB	154760	410088	7.90%	3.709%
7	6.757	920	930	946	rBV	323447	769802	14.82%	6.963%
8	8.647	1233	1240	1249	rBV	645607	1002543	19.30%	9.068%
9	10.055	1465	1471	1480	rBV	662176	899788	17.32%	8.138%
10	10.311	1507	1513	1523	rVB	74818	102651	1.98%	0.928%
11	11.079	1634	1639	1653	rBV	527746	662989	12.76%	5.997%
12	12.018	1788	1793	1802	rVB	652228	830167	15.98%	7.509%

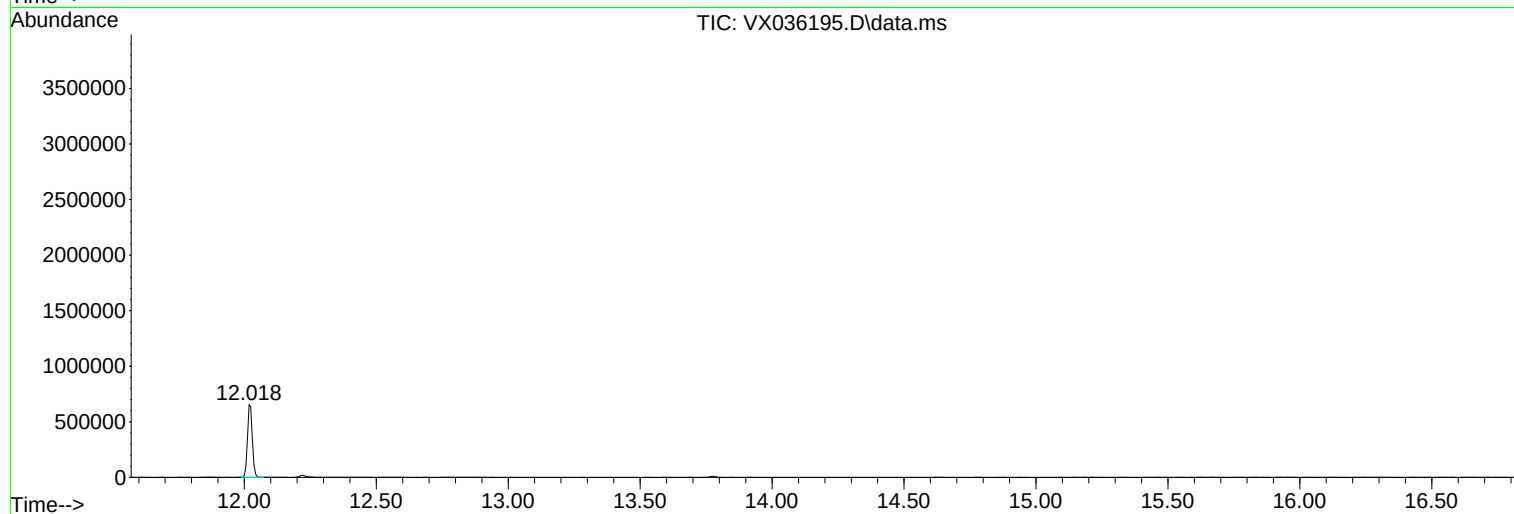
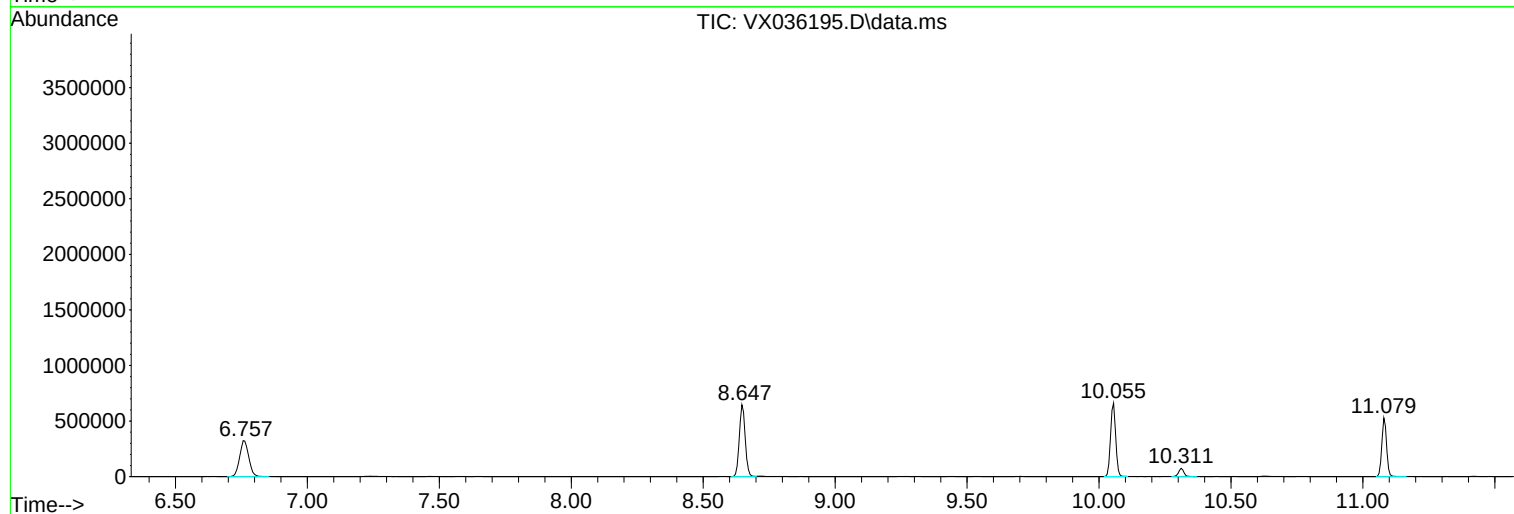
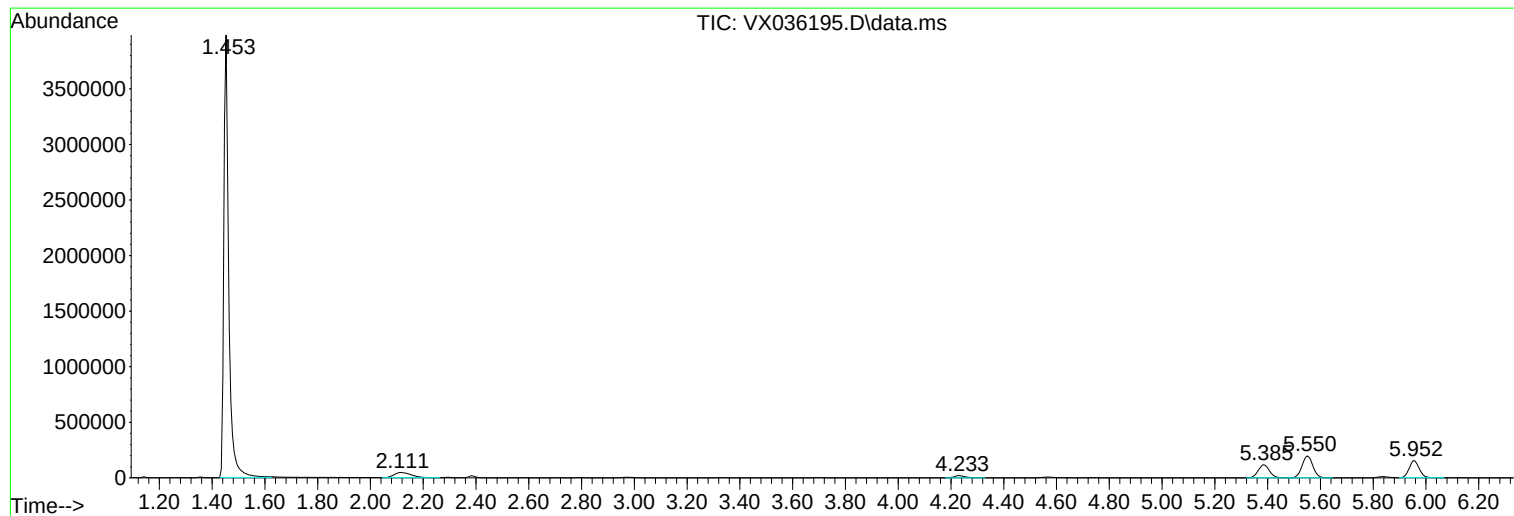
Sum of corrected areas: 11056008

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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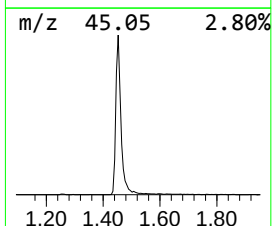
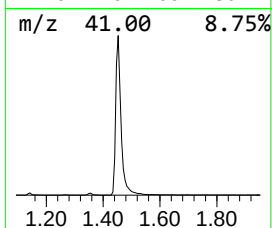
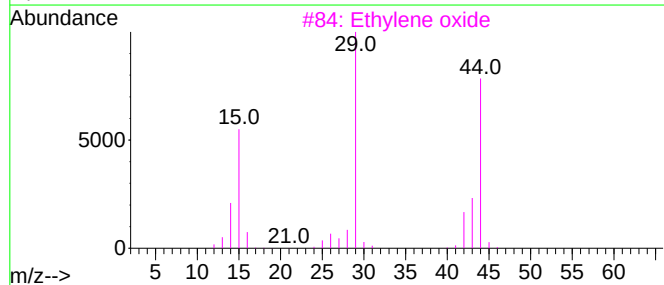
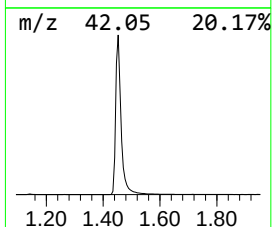
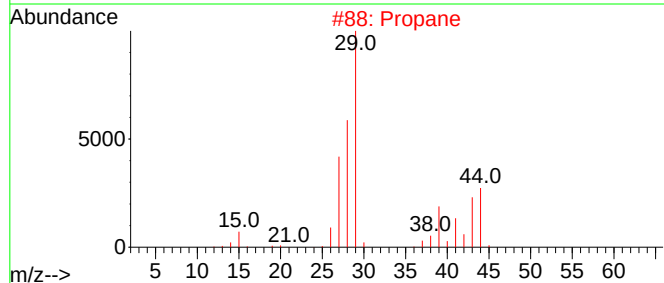
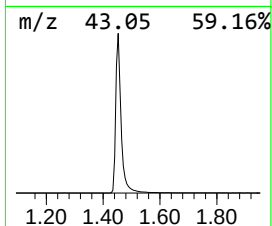
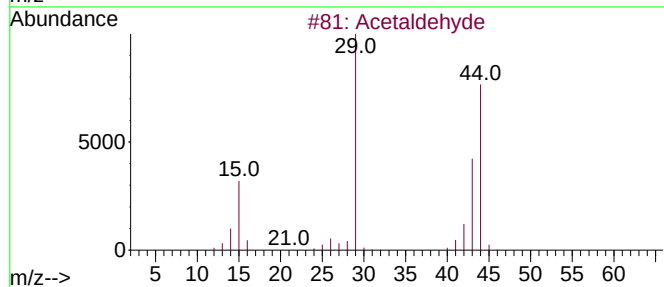
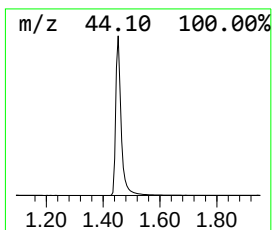
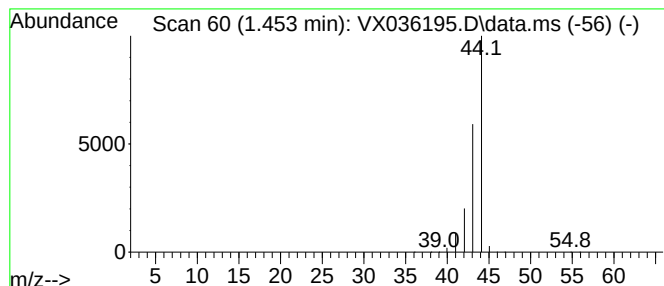
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	461.28 ug/l	5193990	Pentafluorobenzene	5.550

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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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Instrument :
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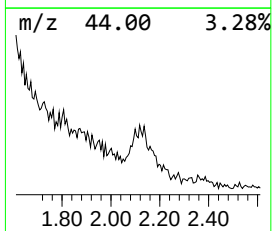
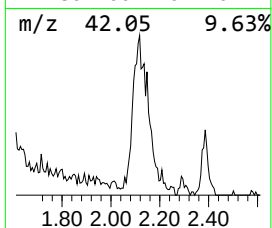
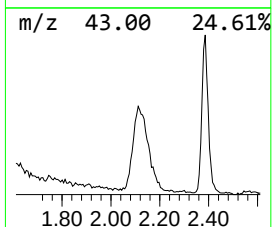
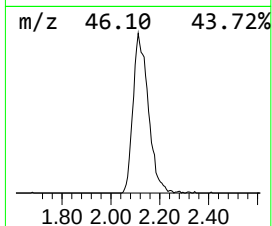
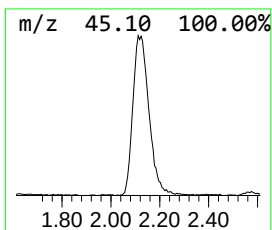
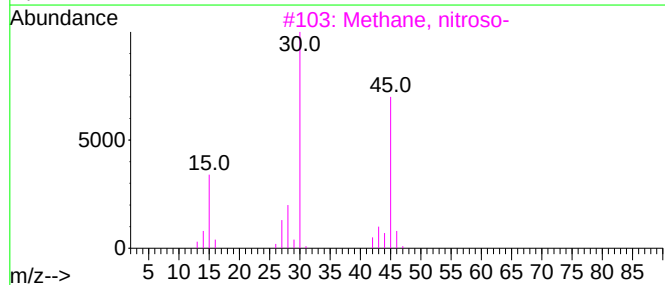
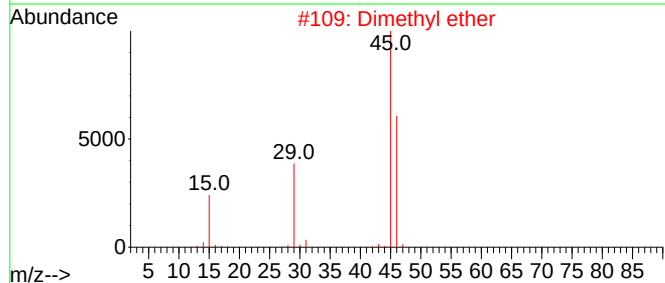
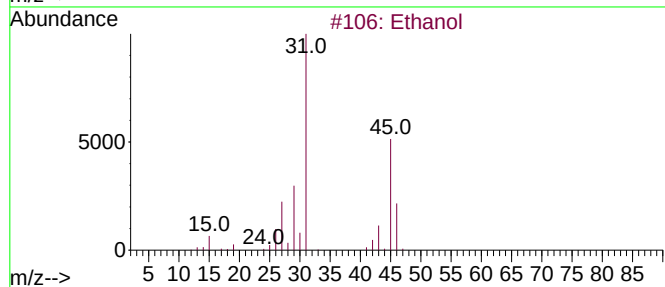
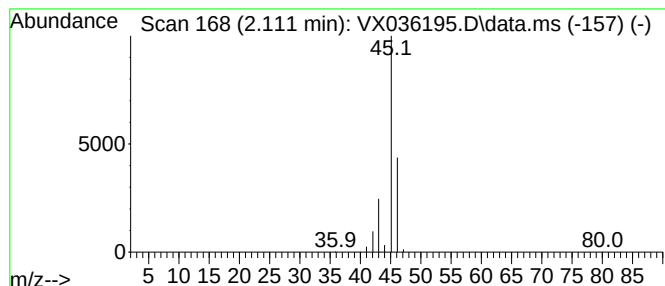
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.111	19.43 ug/l	218829	Pentafluorobenzene	5.550

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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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1619

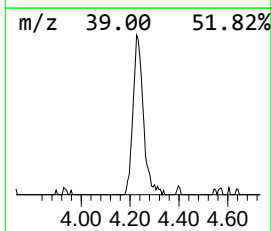
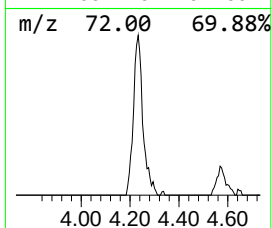
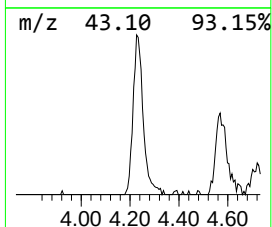
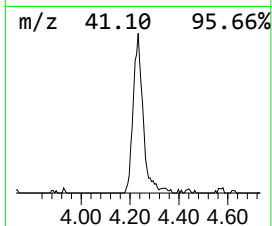
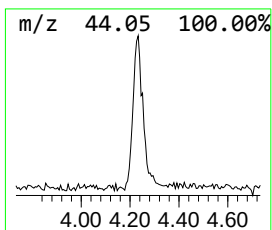
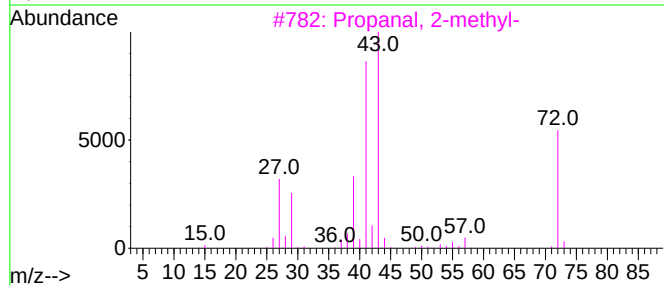
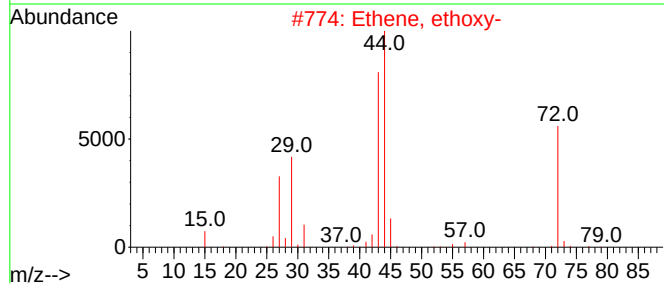
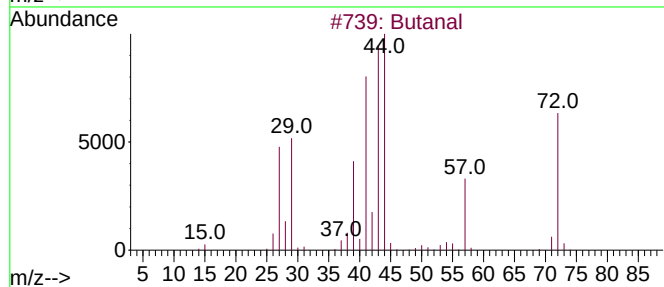
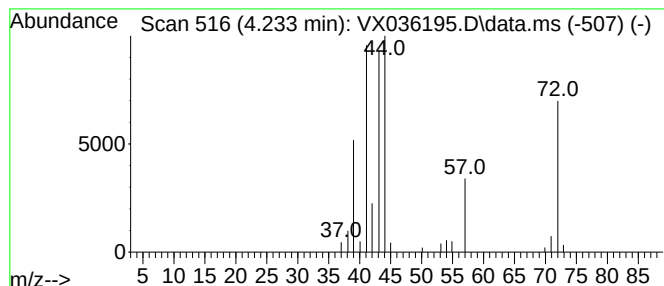
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Quant Title : SW846 8260

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Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	5.02 ug/l	56536	Pentafluorobenzene	5.550

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	38
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	32
5			(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	27



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ClientSampleId :
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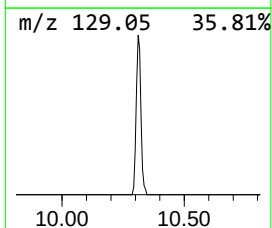
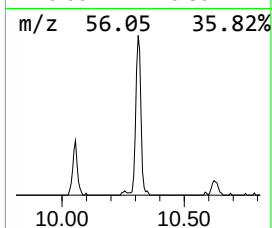
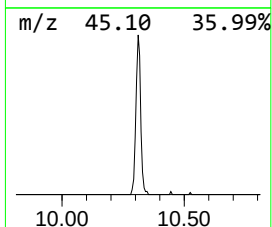
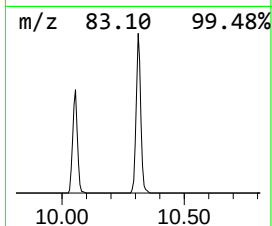
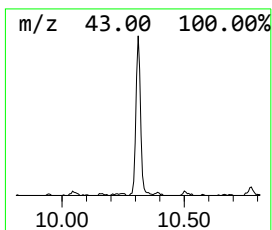
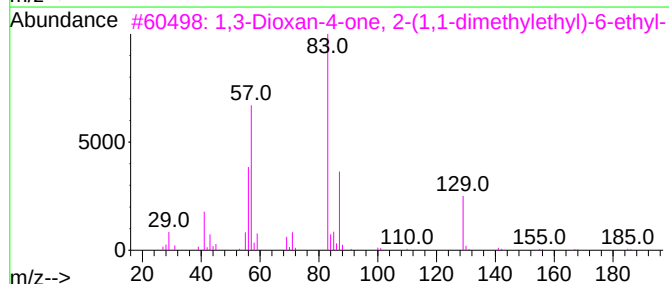
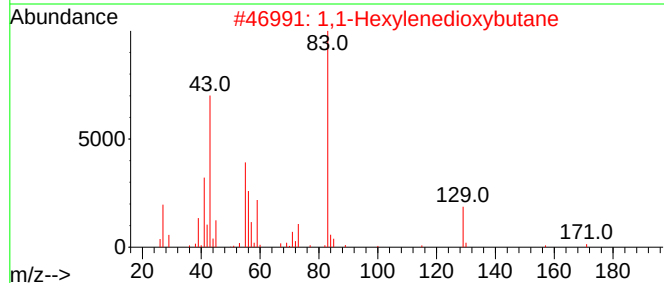
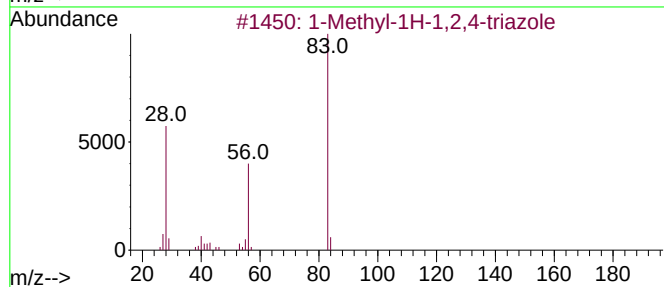
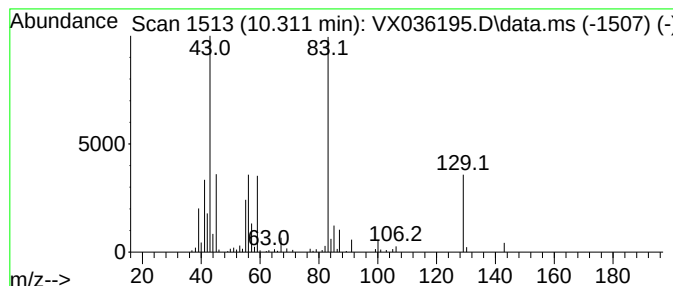
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.311 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.311	5.70 ug/l	102651	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	43
2			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	38
3			1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
4			2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	33
5			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	461.3	ug/l	5193990	1	5.550	562999	50.0
Ethanol	2.111	19.4	ug/l	218829	1	5.550	562999	50.0
Butanal	4.233	5.0	ug/l	56536	1	5.550	562999	50.0
unknown10.311	10.311	5.7	ug/l	102651	3	10.055	899788	50.0