

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
 Data File : VN080368.D
 Acq On : 05 Dec 2023 15:58
 Operator : JC\MD
 Sample : 05616-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1148

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\82N111623W.M

Title : SW846 8260

Signal : TIC: VN080368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.618	110	113	162	rBV2	36155283	85797760	100.00%	78.360%
2	3.783	301	311	327	rBV	1303009	3375765	3.93%	3.083%
3	4.283	383	396	409	rBV	643446	1869412	2.18%	1.707%
4	7.224	883	896	919	rBV	3130045	8678153	10.11%	7.926%
5	9.100	1207	1215	1226	rVB	423233	858012	1.00%	0.784%
6	10.565	1456	1464	1473	rBV	648654	1243783	1.45%	1.136%
7	11.865	1670	1685	1694	rBV	623091	1187633	1.38%	1.085%
8	11.976	1694	1704	1717	rVV	585326	973840	1.14%	0.889%
9	12.847	1846	1852	1862	rVB	542446	961041	1.12%	0.878%
10	13.794	2005	2013	2020	rBV	614863	1053387	1.23%	0.962%
11	13.876	2020	2027	2036	rBV	2121779	3493638	4.07%	3.191%

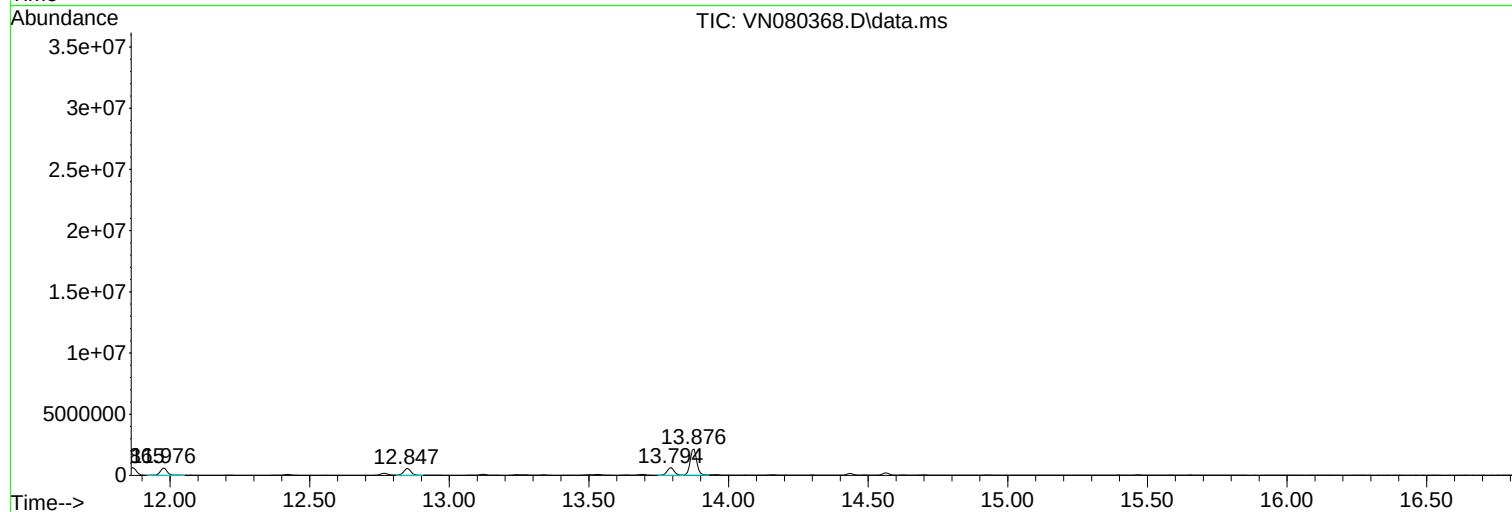
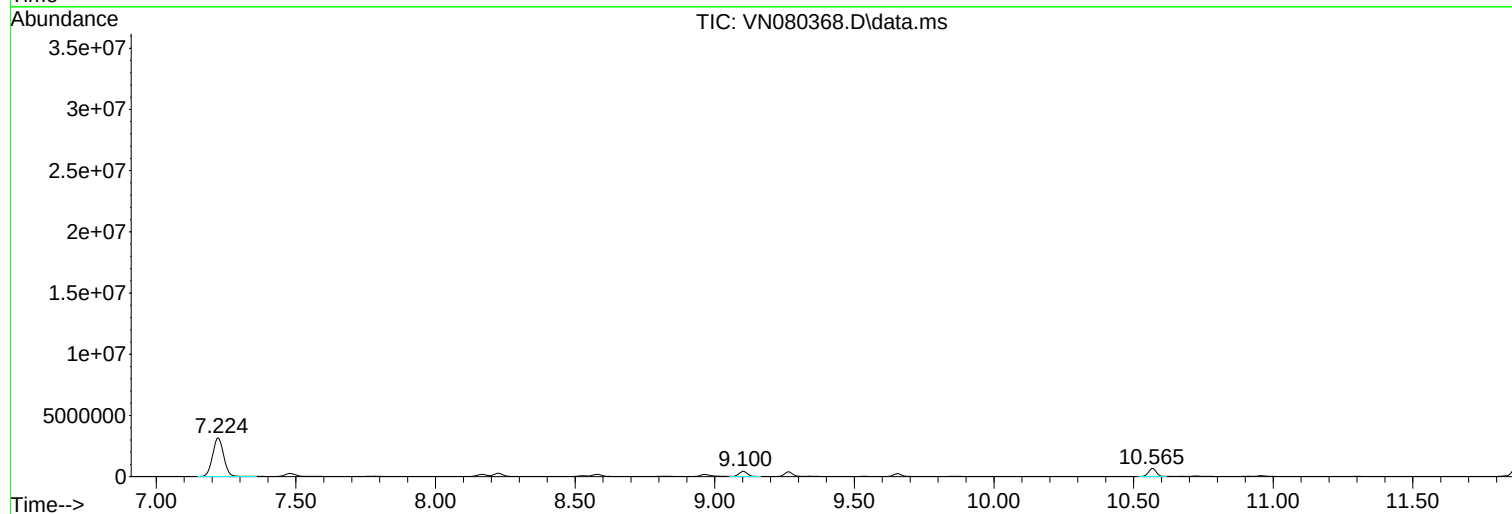
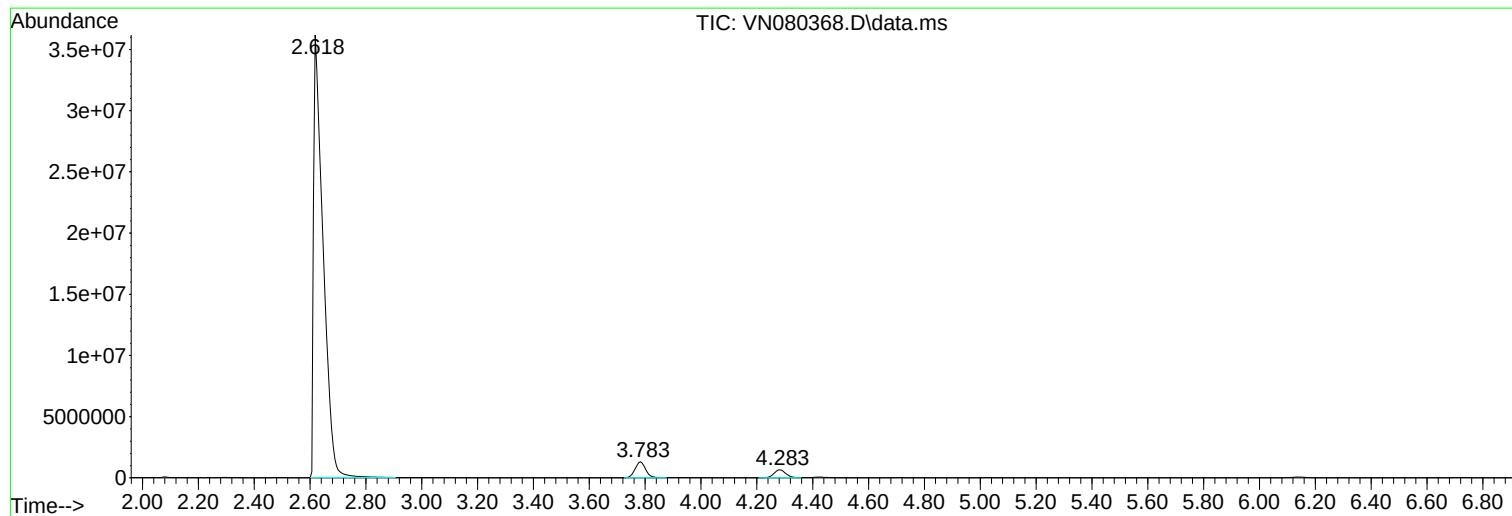
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



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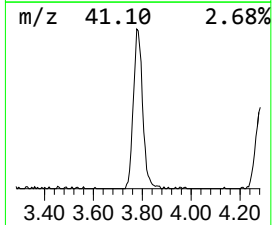
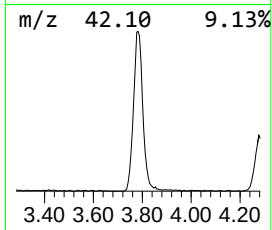
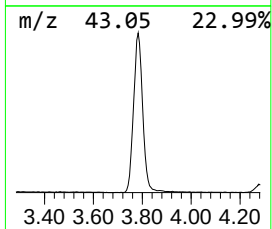
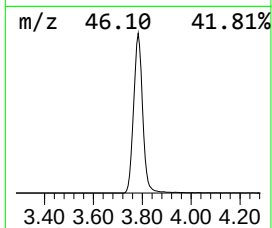
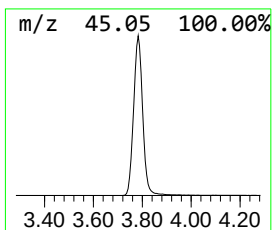
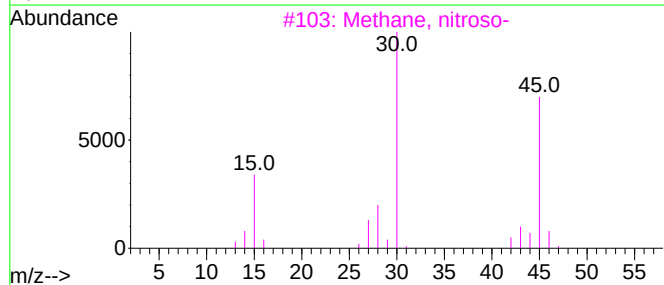
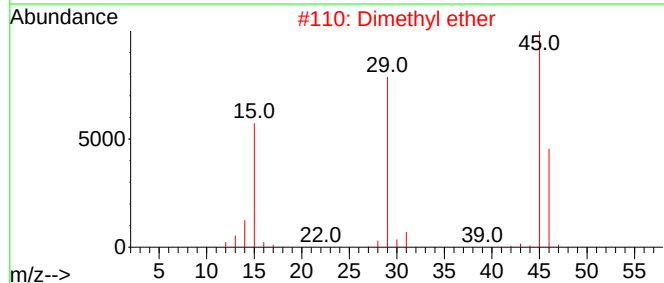
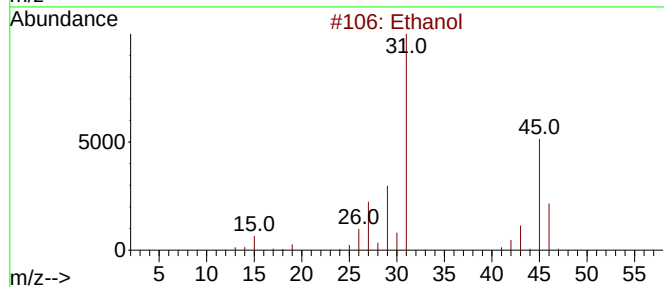
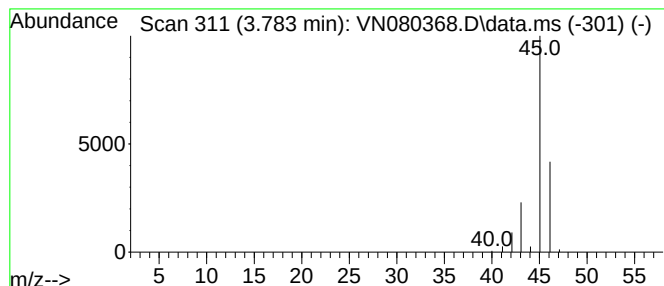
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	196.72 ug/l	3375770	Pentafluorobenzene	8.224

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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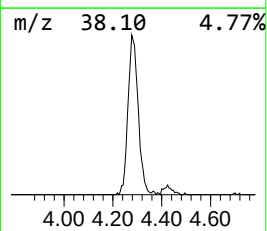
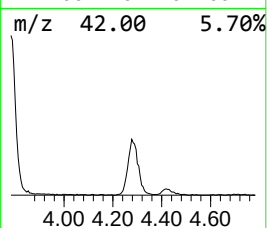
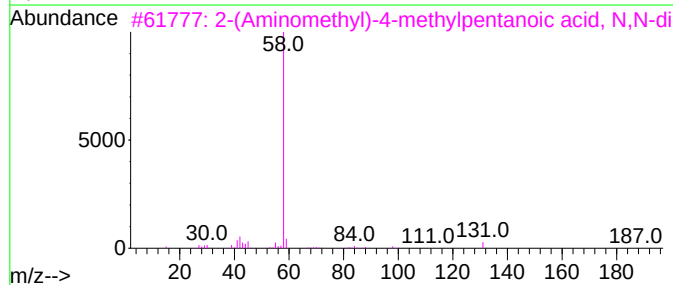
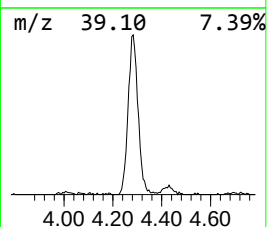
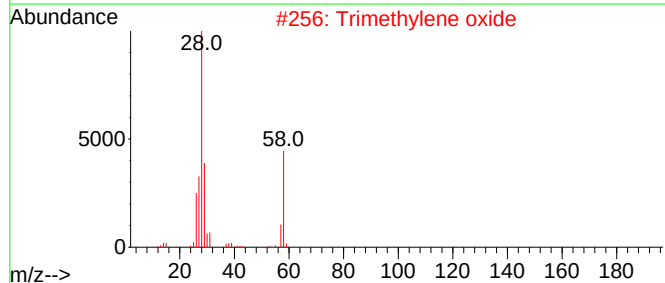
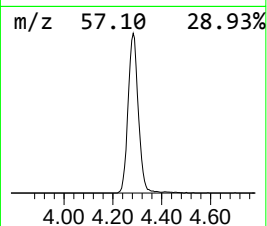
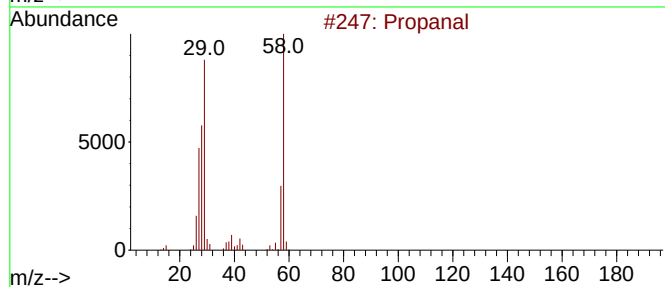
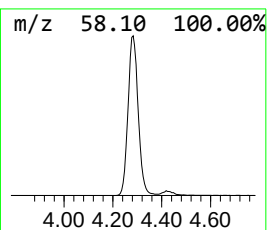
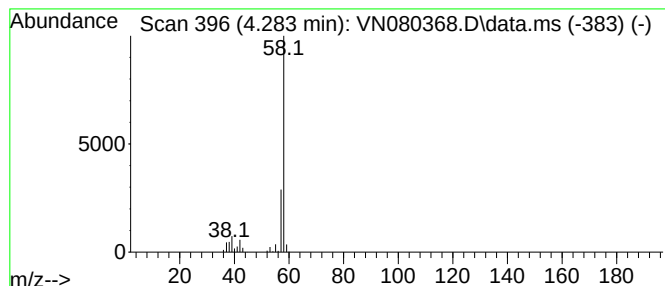
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	108.94 ug/l	1869410	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4			Propylene oxide	58	C3H6O	000075-56-9	7
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5



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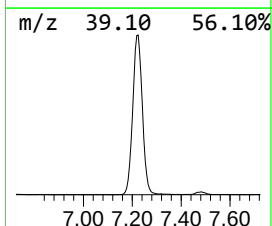
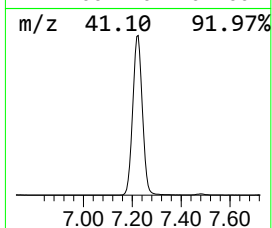
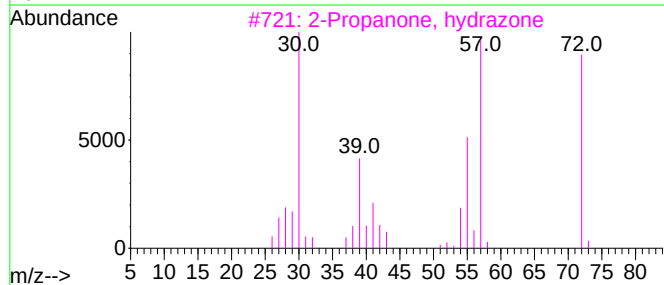
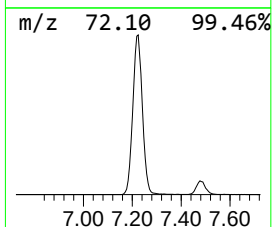
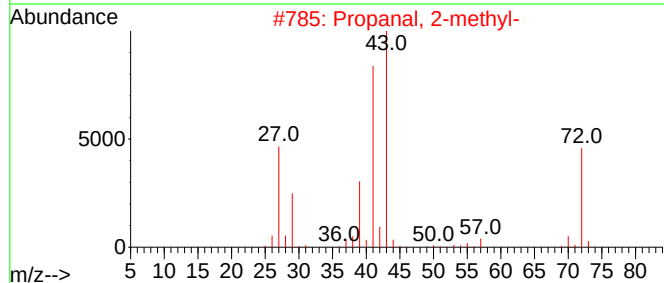
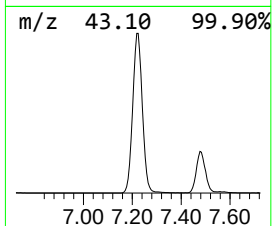
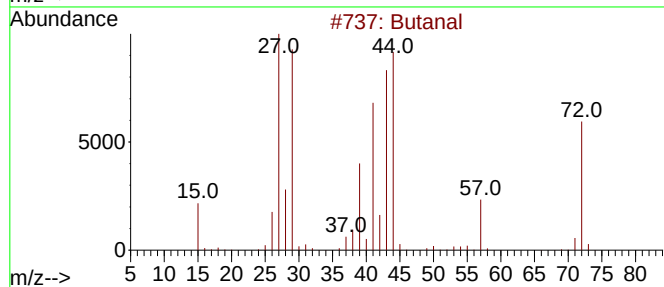
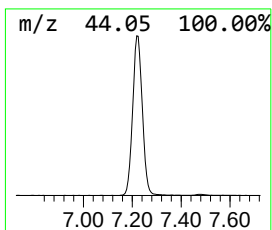
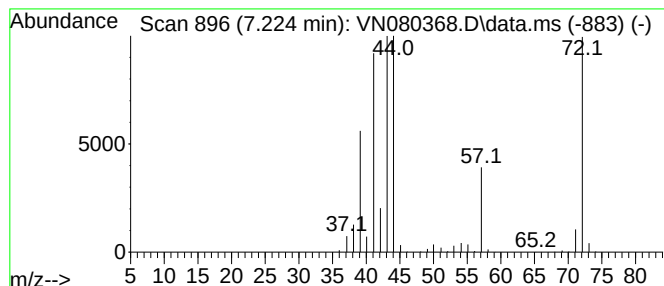
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Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	505.71 ug/l	8678150	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	80
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
4		Propane	44	C3H8	000074-98-6	35
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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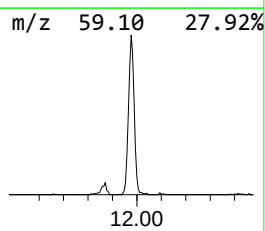
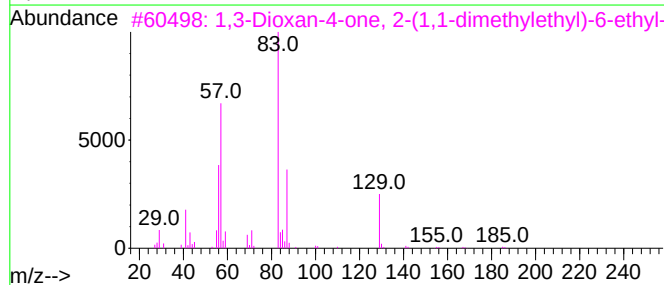
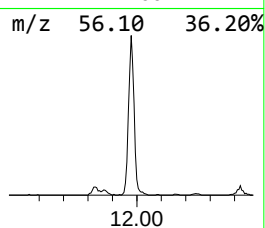
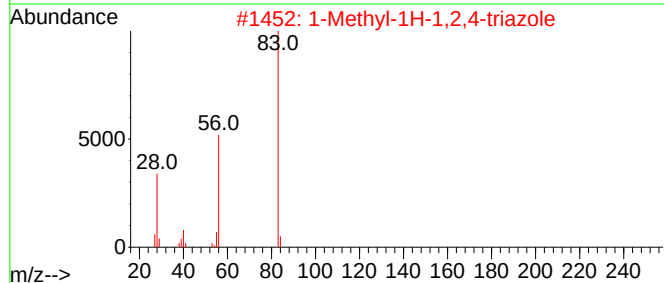
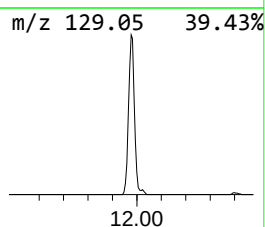
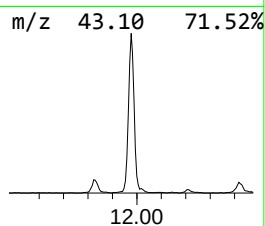
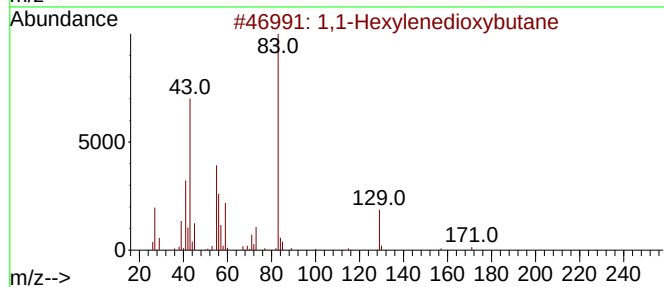
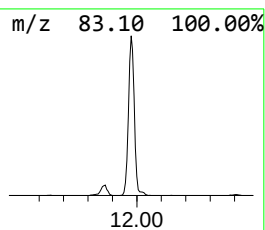
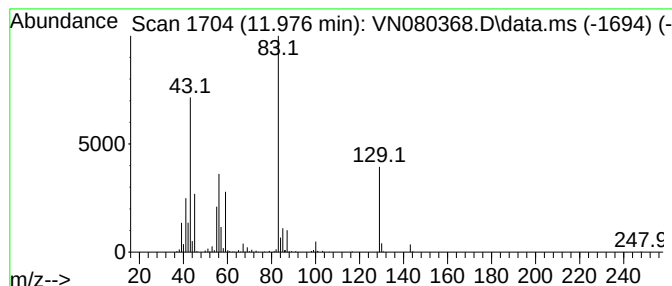
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown11.977 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.977	41.00 ug/l	973840	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	42
2			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	35
3			1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	33
4			2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	25
5			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	25



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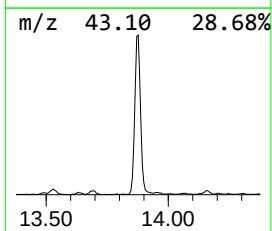
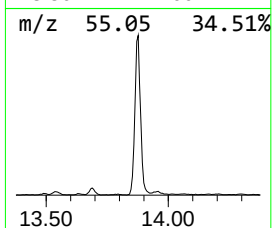
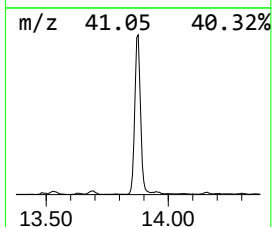
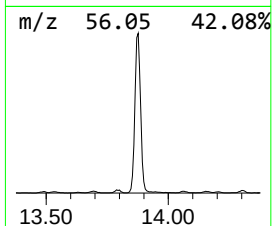
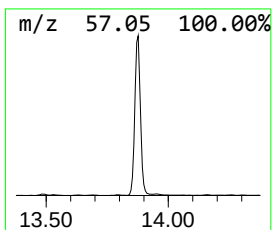
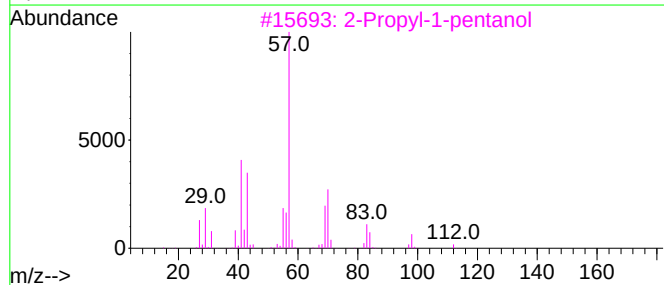
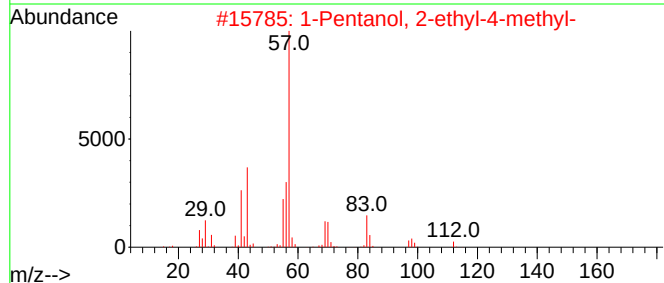
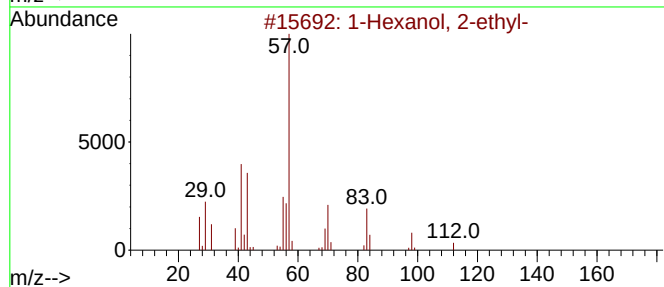
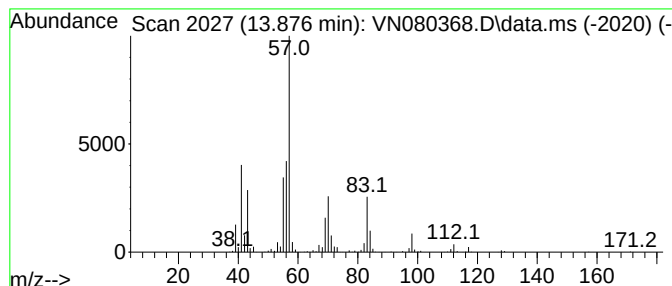
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	165.83 ug/l	3493640	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Isobutyl octyl carbonate	230	C13H26O3	1010372-74-6	45
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.783	196.7	ug/l	3375770	1	8.224	858012	50.0
Propanal	4.283	108.9	ug/l	1869410	1	8.224	858012	50.0
Butanal	7.224	505.7	ug/l	8678150	1	8.224	858012	50.0
unknown11.977	11.977	41.0	ug/l	973840	3	11.865	1187630	50.0
1-Hexanol, 2-et...	13.876	165.8	ug/l	3493640	4	13.794	1053390	50.0