

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031224\
 Data File : VN081383.D
 Acq On : 12 Mar 2024 19:25
 Operator : JC\MD
 Sample : P1734-05 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1342

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\82N030524W.M

Title : SW846 8260

Signal : TIC: VN081383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.659	110	120	140	rBV	11325070	19663989	100.00%	54.947%
2	3.789	303	312	324	rBV	96547	258984	1.32%	0.724%
3	7.224	884	896	915	rBV	546873	1492442	7.59%	4.170%
4	8.171	1045	1057	1061	rBV	262279	627483	3.19%	1.753%
5	8.224	1061	1066	1079	rVB	476846	1072990	5.46%	2.998%
6	8.582	1111	1127	1139	rBV	297473	723992	3.68%	2.023%
7	9.100	1206	1215	1228	rBV	678242	1430882	7.28%	3.998%
8	10.571	1456	1465	1474	rBV	1041677	1930111	9.82%	5.393%
9	11.865	1672	1685	1699	rBV	915036	1678329	8.54%	4.690%
10	12.853	1844	1853	1863	rBV	678443	1192529	6.06%	3.332%
11	13.341	1929	1936	1946	rBV	1780318	2674428	13.60%	7.473%
12	13.688	1988	1995	2005	rBV	437886	721221	3.67%	2.015%
13	13.794	2005	2013	2020	rVB	866532	1440674	7.33%	4.026%
14	13.876	2020	2027	2036	rBV	532621	879378	4.47%	2.457%

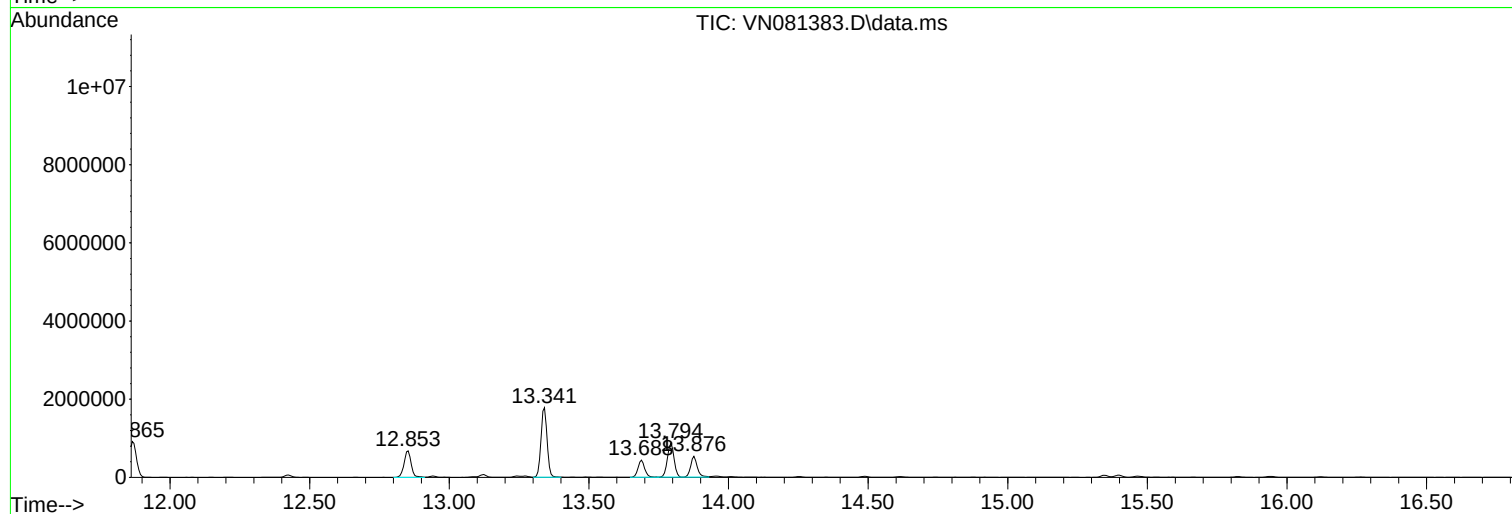
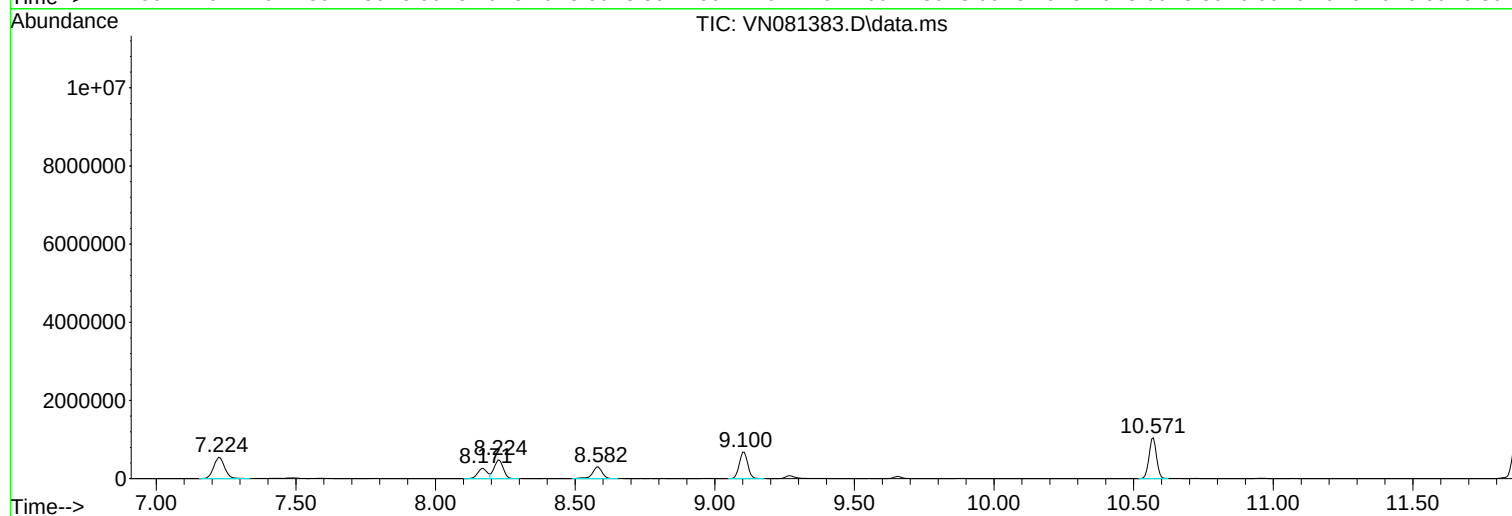
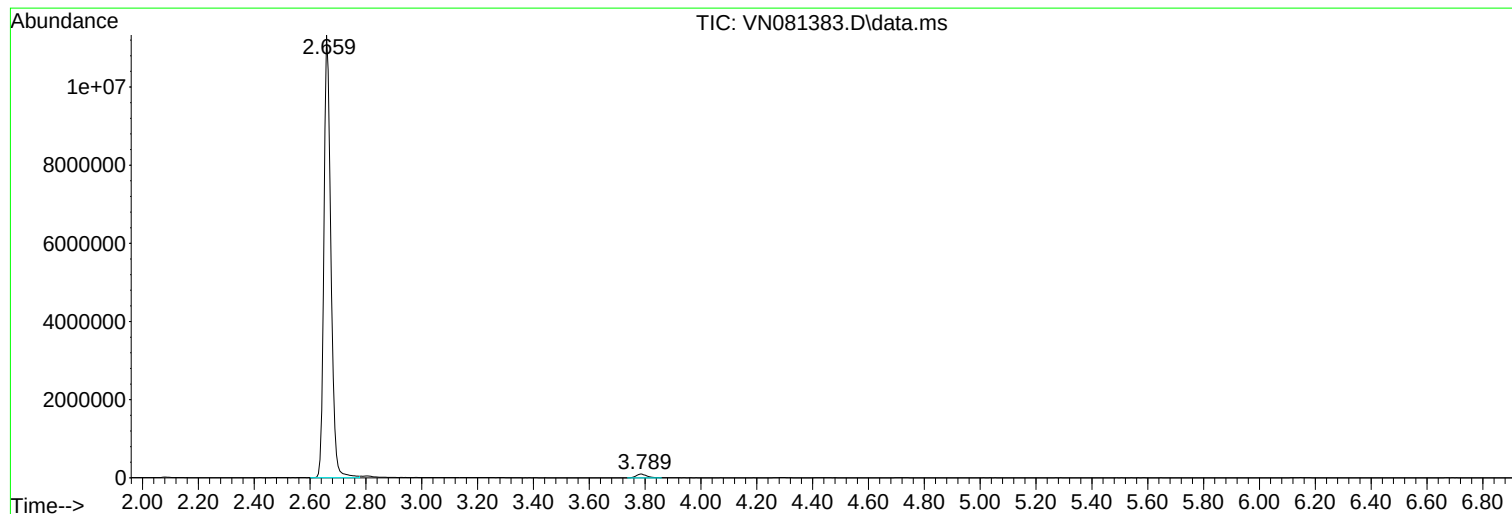
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



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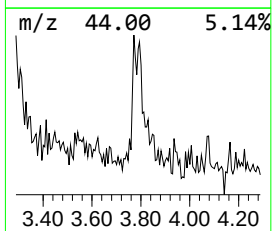
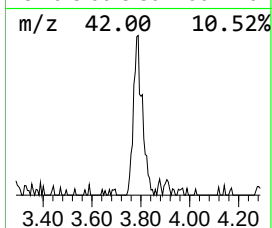
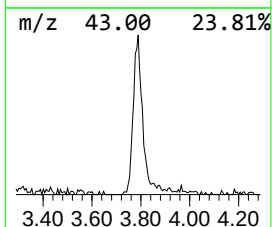
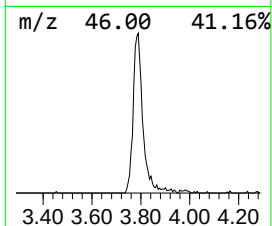
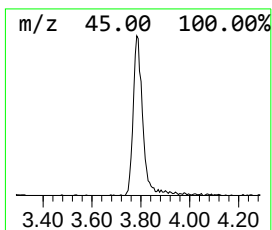
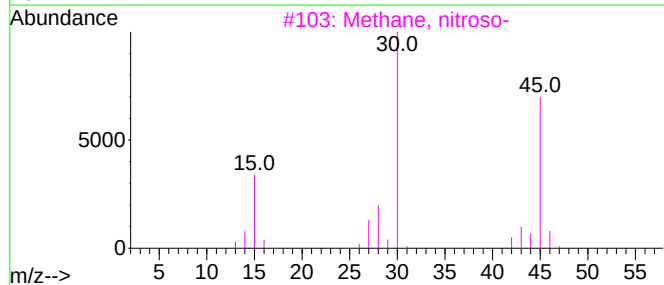
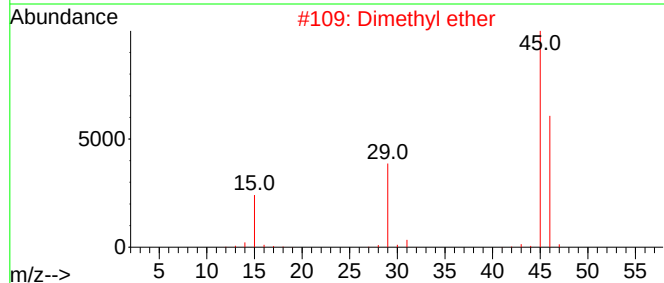
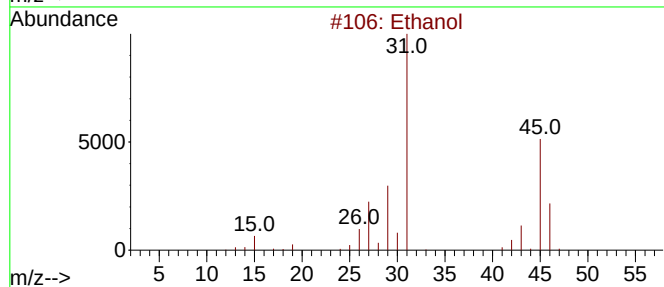
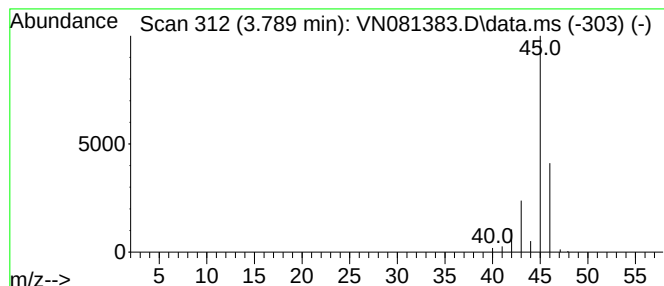
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	12.07 ug/l	258984	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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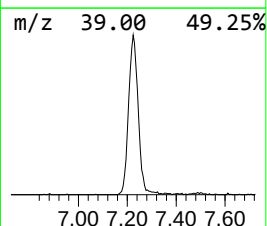
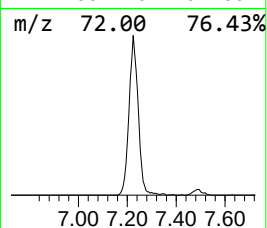
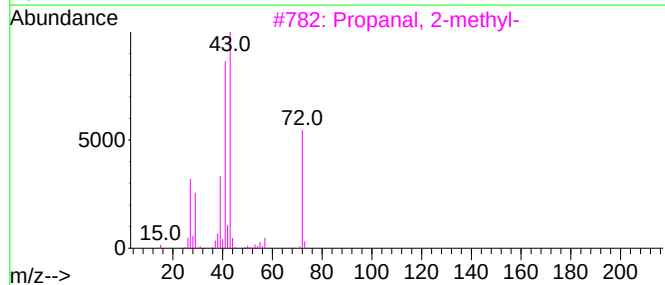
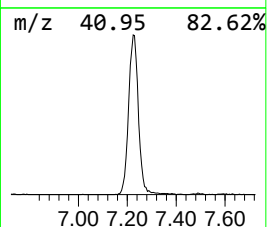
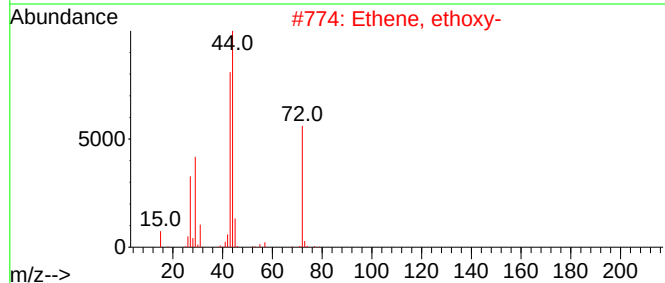
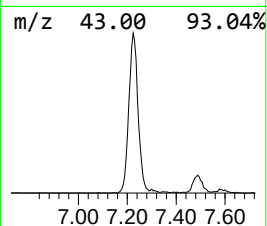
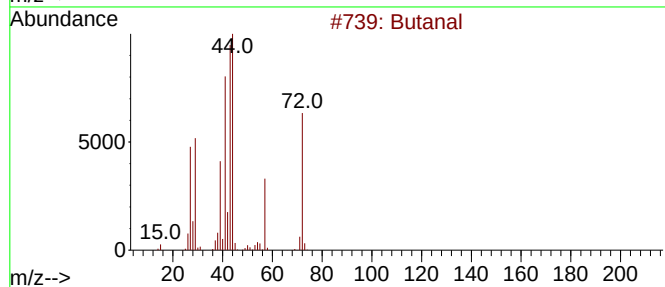
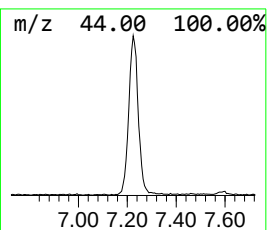
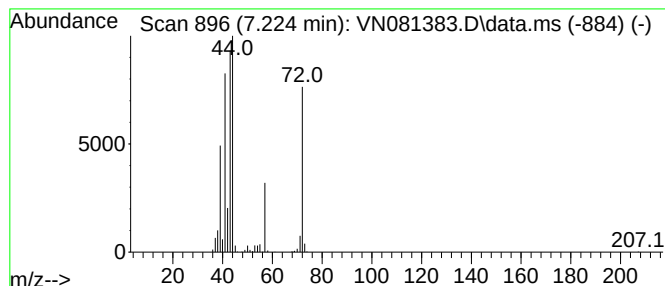
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	69.55 ug/l	1492440	Pentafluorobenzene	8.224

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	52
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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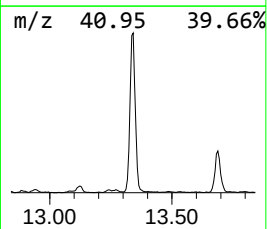
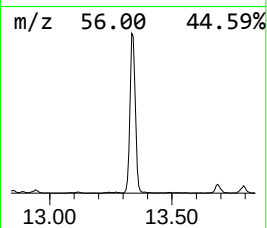
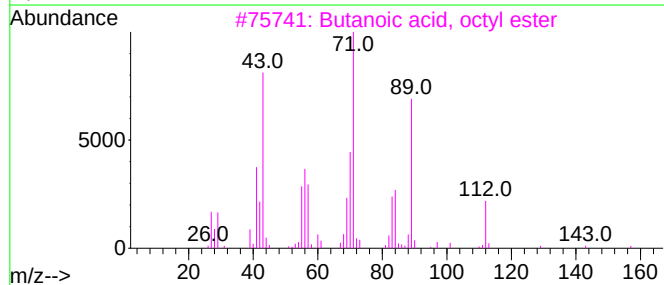
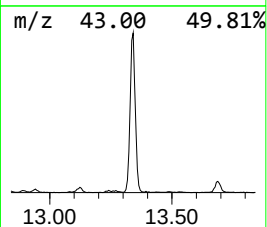
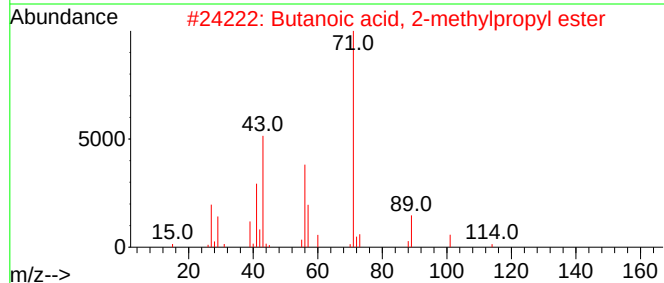
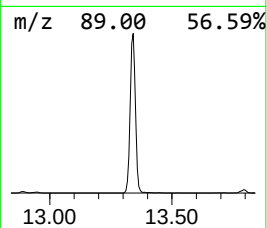
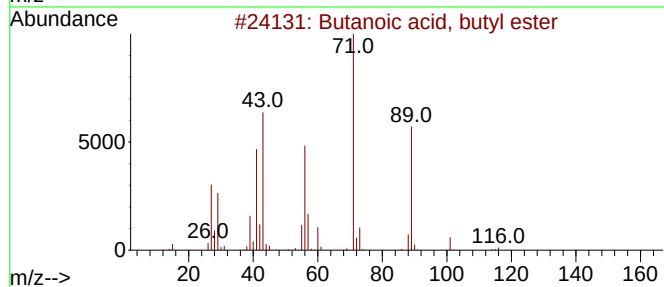
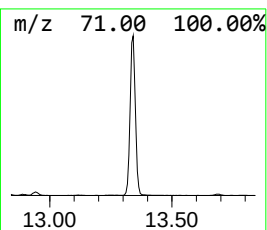
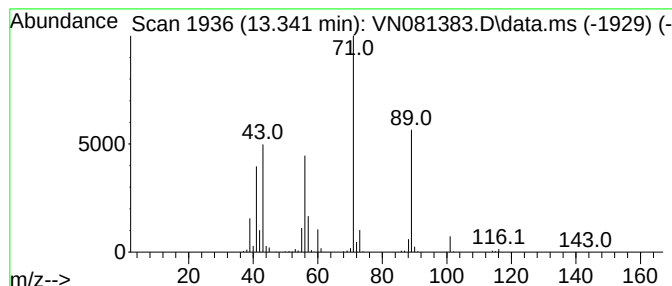
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Peak Number 4 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	92.82 ug/l	2674430	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50



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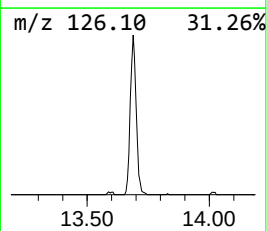
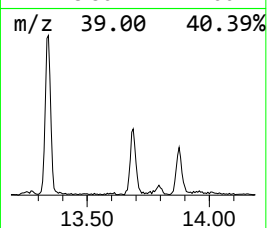
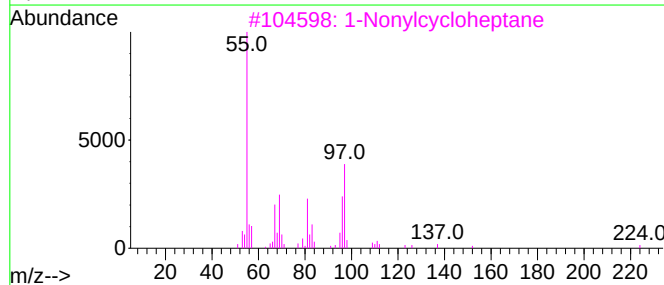
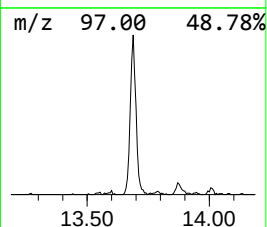
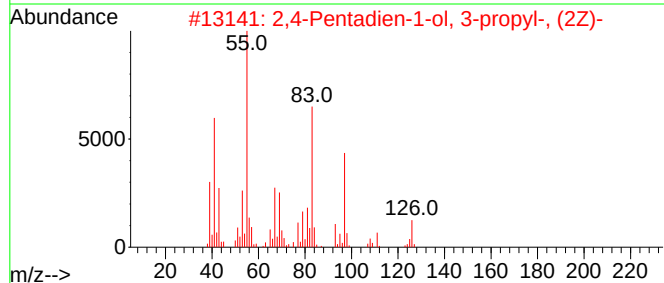
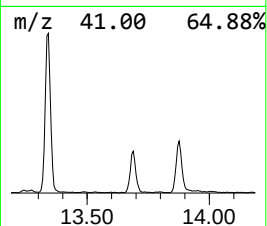
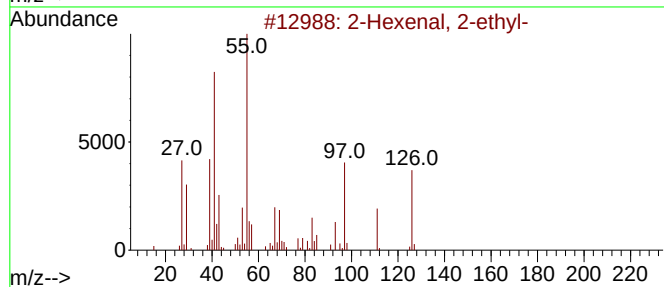
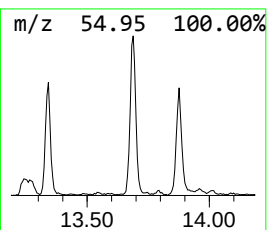
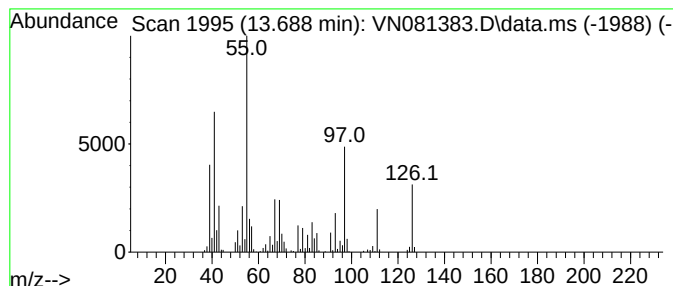
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Hexenal, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	25.03 ug/l	721221	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	97
2			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	53
3			1-Nonylcycloheptane	224	C16H32	1000371-47-7	43
4			cis-1-Methyl-2-(2'-propenyl)cycl...	96	C7H12	076588-97-1	38
5			Acetamide, N-2-propynyl-	97	C5H7NO	065881-41-6	38



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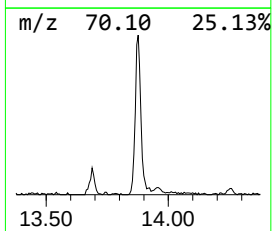
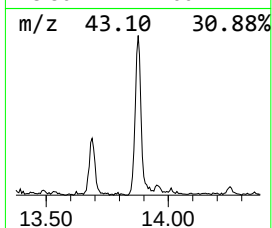
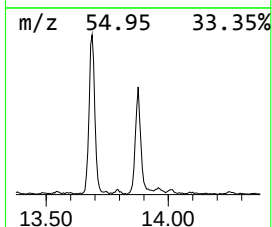
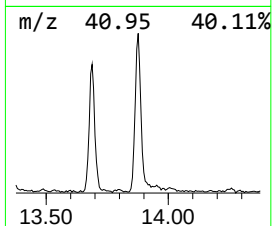
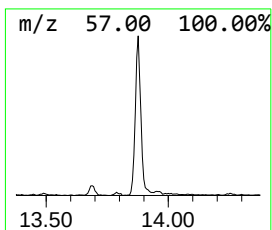
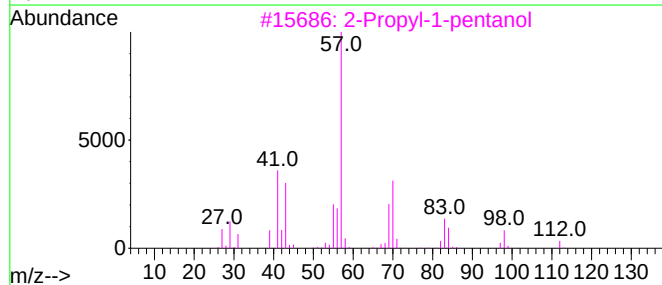
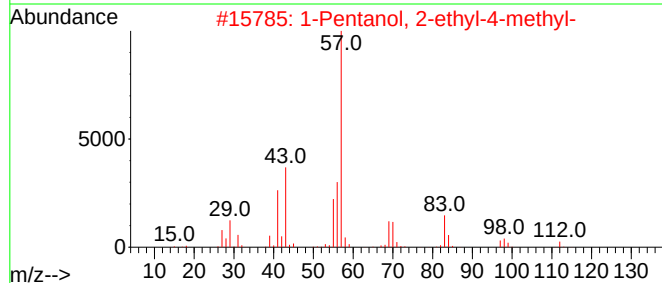
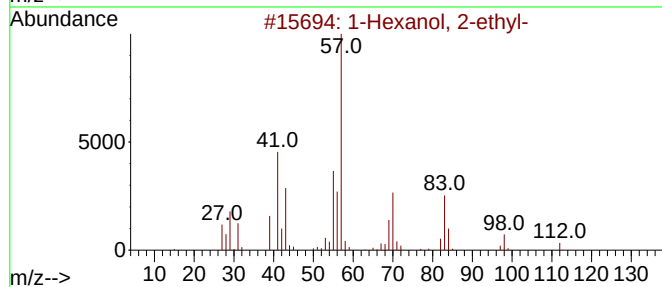
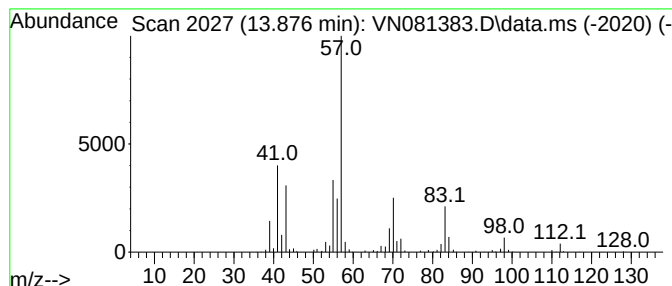
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	30.52 ug/l	879378	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	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.789	12.1	ug/l	258984	1	8.224	1072990	50.0
Butanal	7.224	69.5	ug/l	1492440	1	8.224	1072990	50.0
Butanoic acid, ...	13.341	92.8	ug/l	2674430	4	13.794	1440670	50.0
2-Hexenal, 2-et...	13.688	25.0	ug/l	721221	4	13.794	1440670	50.0
1-Hexanol, 2-et...	13.876	30.5	ug/l	879378	4	13.794	1440670	50.0