

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081855.D
Acq On : 25 Apr 2024 17:04
Operator : JC\MD
Sample : P2257-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41C

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M

Title : SW846 8260

Signal : TIC: VN081855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.642	112	117	142	rBV	17421478	36538344	100.00%	58.586%
2	3.789	301	312	340	rBV	1901913	5154082	14.11%	8.264%
3	7.224	883	896	907	rBV	535724	1496654	4.10%	2.400%
4	7.482	929	940	949	rBV	660999	1723175	4.72%	2.763%
5	8.171	1048	1057	1060	rBV	169798	388553	1.06%	0.623%
6	8.224	1060	1066	1080	rVB	329391	753612	2.06%	1.208%
7	8.577	1121	1126	1134	rVB2	190763	400803	1.10%	0.643%
8	9.100	1206	1215	1231	rVB	510599	1045521	2.86%	1.676%
9	9.265	1235	1243	1257	rBV	225266	476762	1.30%	0.764%
10	10.565	1456	1464	1472	rBV	787378	1480278	4.05%	2.374%
11	11.865	1671	1685	1697	rBV	697871	1367899	3.74%	2.193%
12	12.417	1767	1779	1787	rBV	319760	571336	1.56%	0.916%
13	12.847	1844	1852	1862	rBV	536943	968456	2.65%	1.553%
14	13.335	1929	1935	1943	rVB	1552737	2403147	6.58%	3.853%
15	13.682	1988	1994	2005	rVB	340604	576012	1.58%	0.924%
16	13.794	2005	2013	2019	rBV	619354	1044794	2.86%	1.675%
17	13.870	2019	2026	2035	rBV	3668173	5977265	16.36%	9.584%

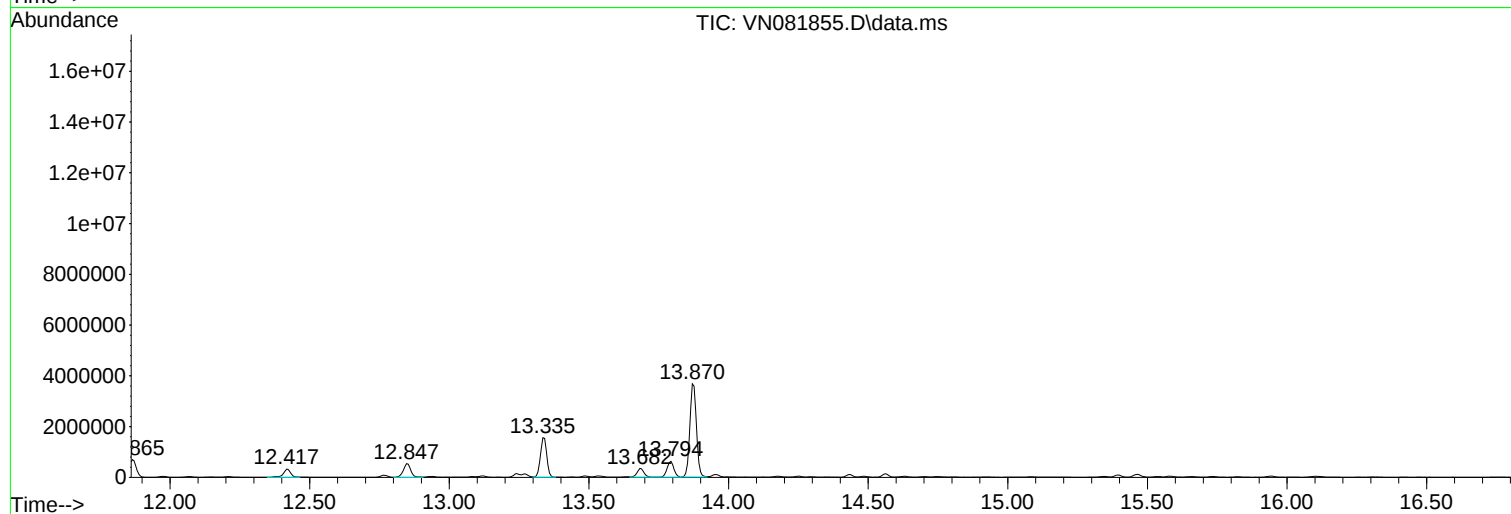
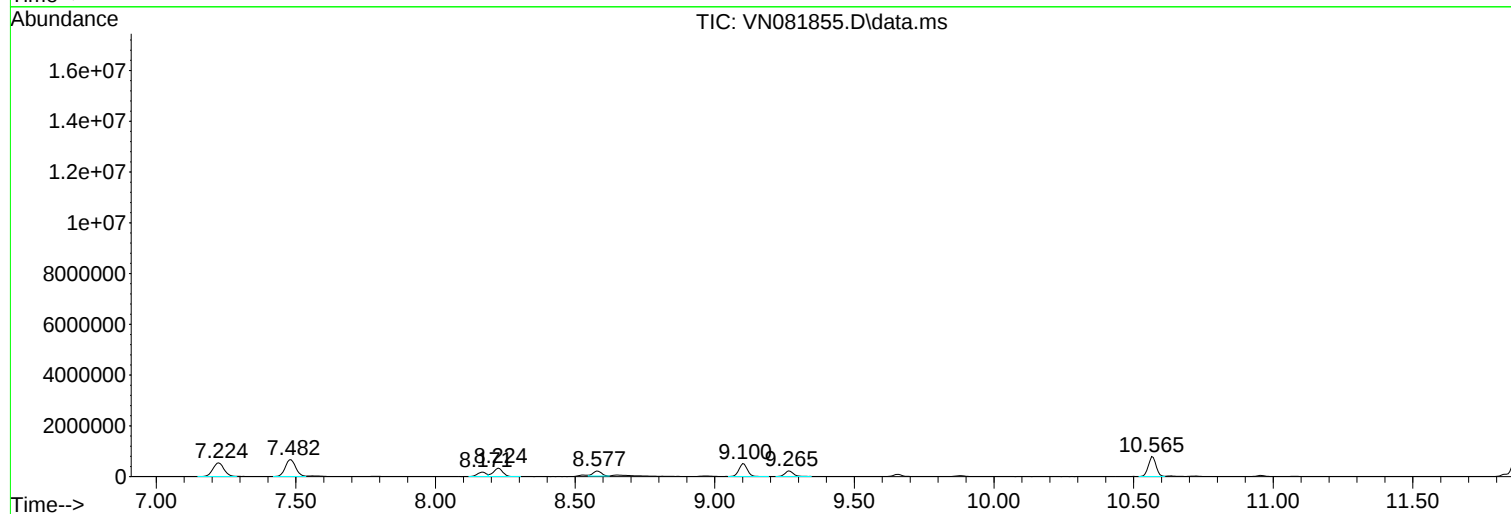
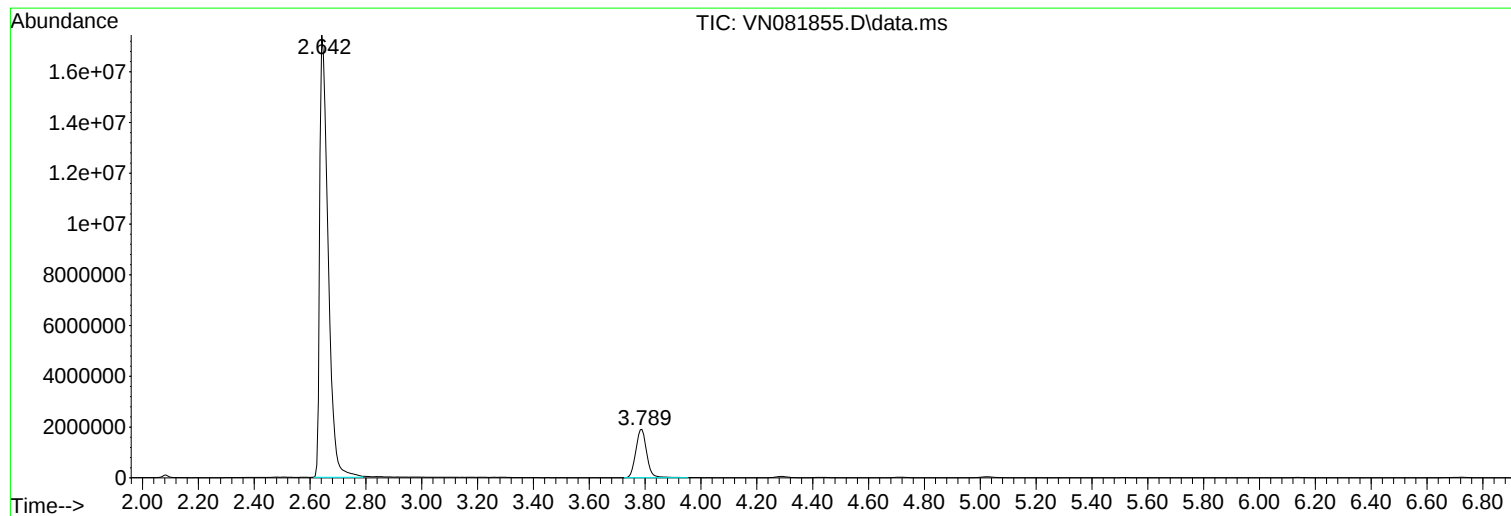
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Quant Title : SW846 8260

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



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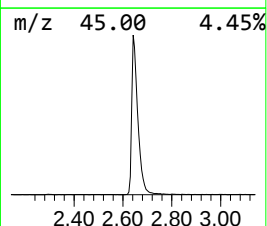
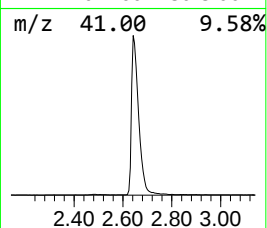
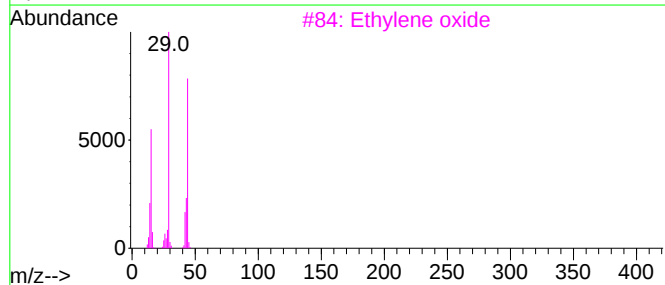
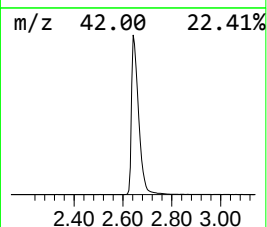
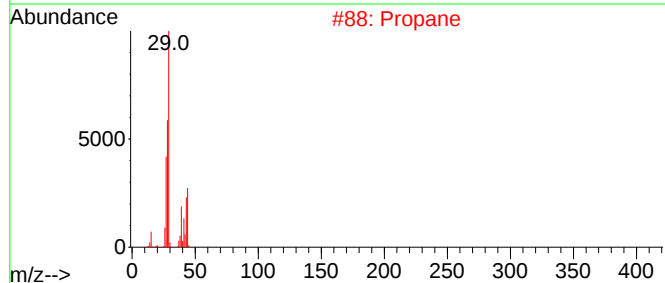
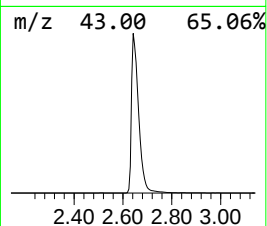
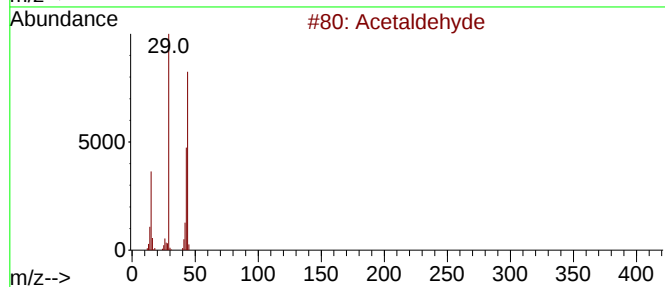
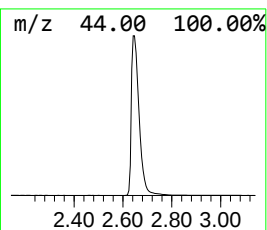
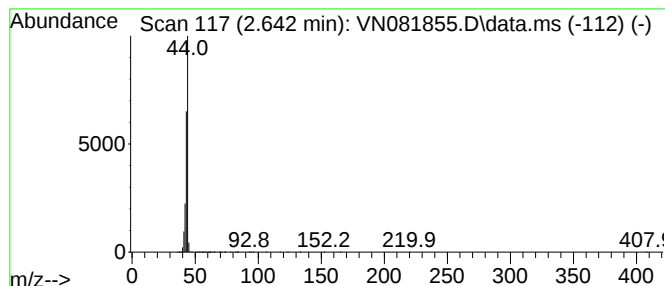
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.642	2424.21 ug/l	36538300	Pentafluorobenzene	8.224

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			1-(Methylamino)propan-2-ol	89	C4H11NO	1000486-79-1	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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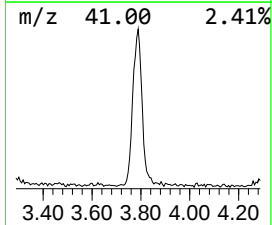
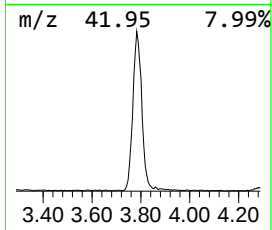
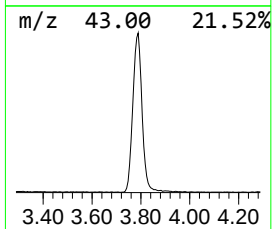
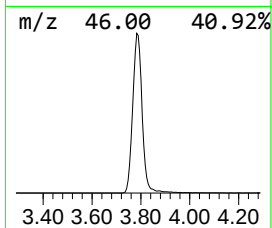
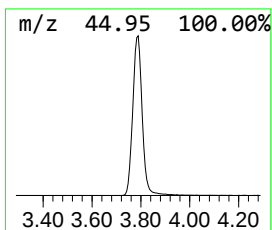
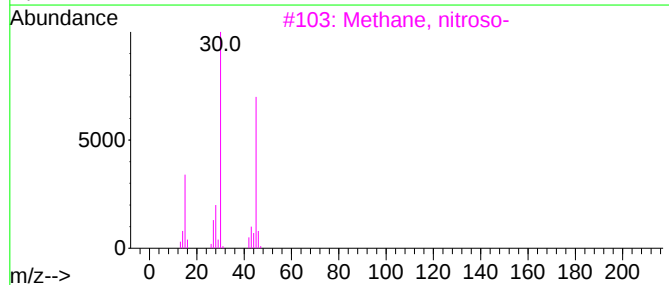
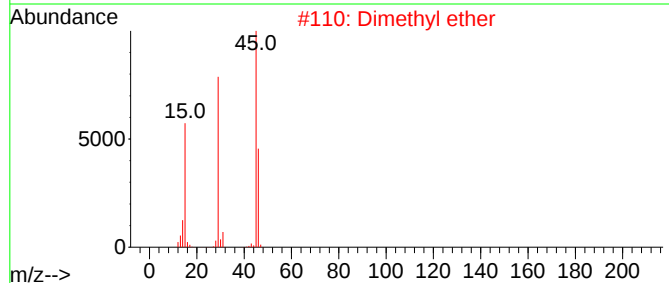
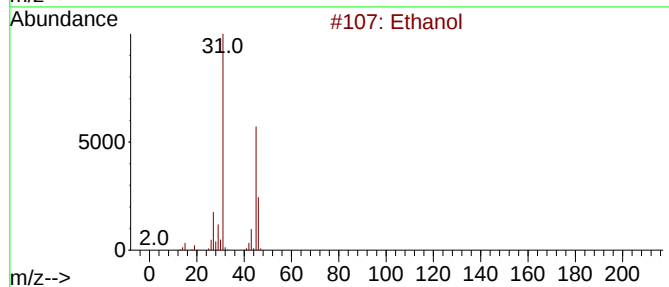
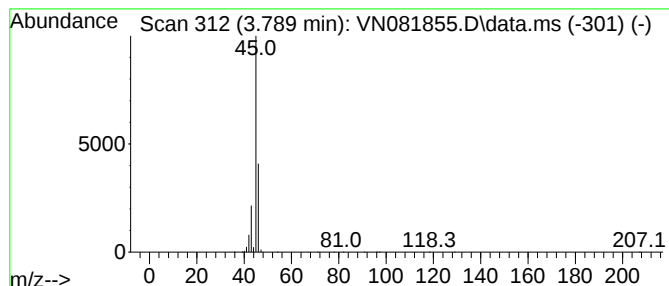
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	341.96 ug/l	5154080	Pentafluorobenzene	8.224

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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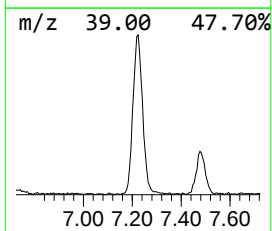
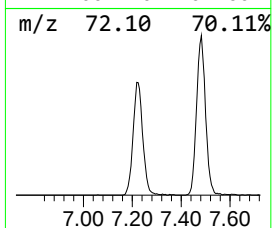
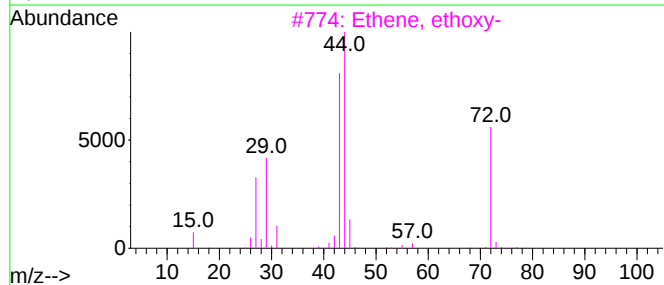
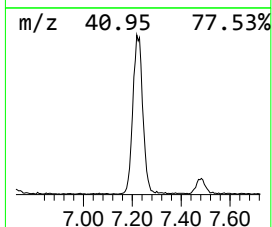
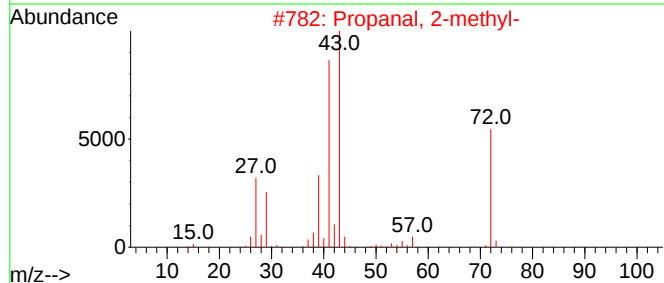
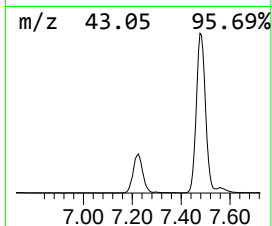
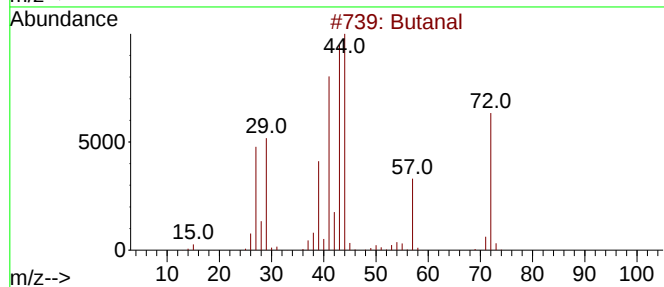
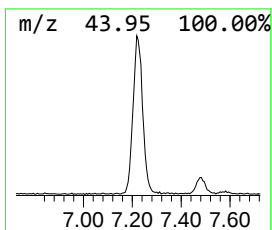
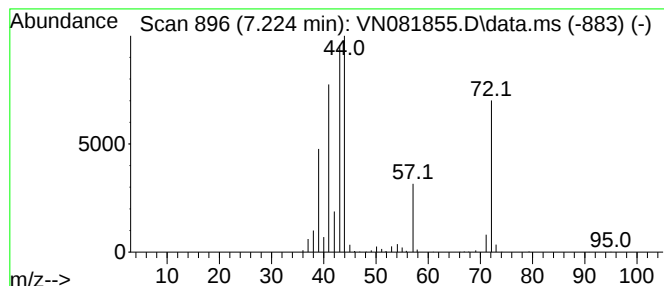
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Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.224	99.30 ug/l	1496650	Pentafluorobenzene	8.224	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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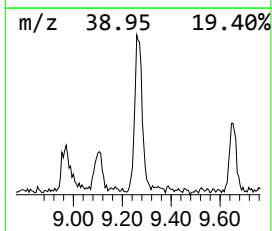
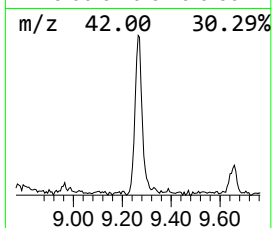
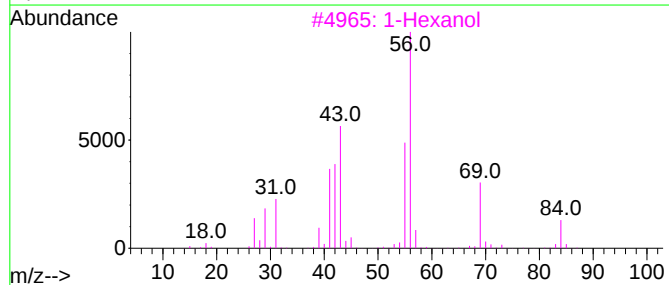
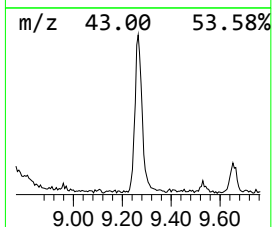
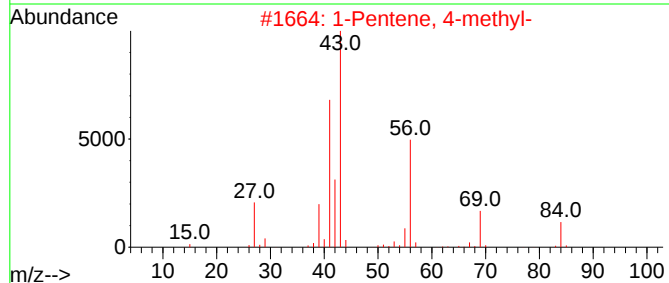
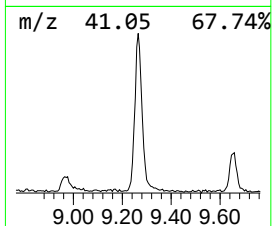
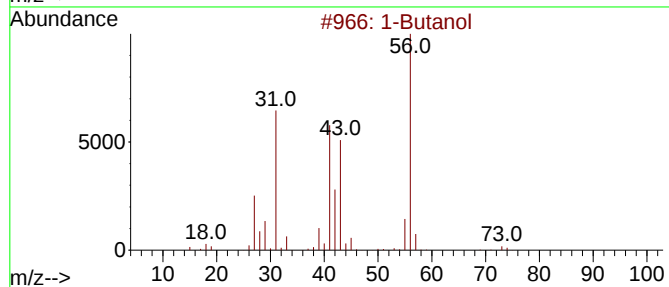
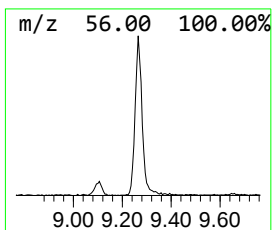
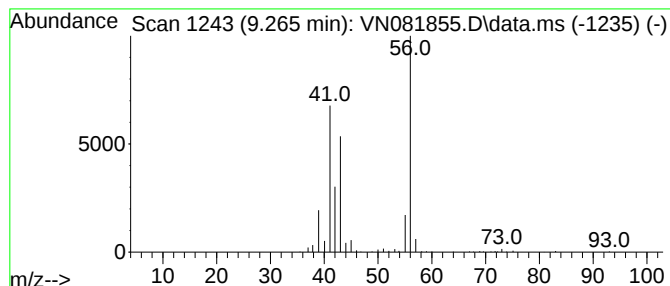
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Peak Number 4 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	22.80 ug/l	476762	1,4-Difluorobenzene	9.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	83
2	1-Pentene, 4-methyl-		84	C6H12	000691-37-2	40
3	1-Hexanol		102	C6H14O	000111-27-3	40
4	1-Pentanol, 4-methyl-		102	C6H14O	000626-89-1	40
5	2H-Pyran-2-one, tetrahydro-5,6-d...		128	C7H12O2	024405-16-1	38



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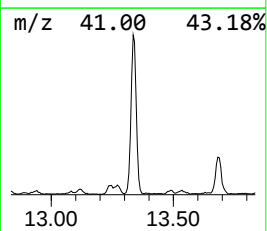
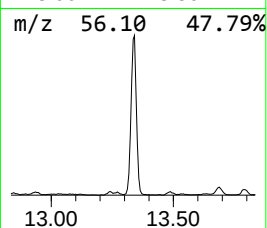
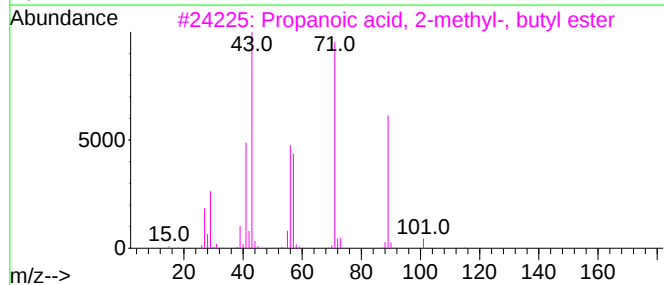
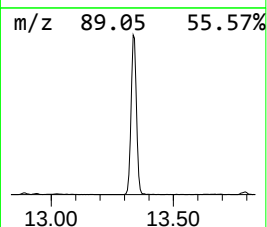
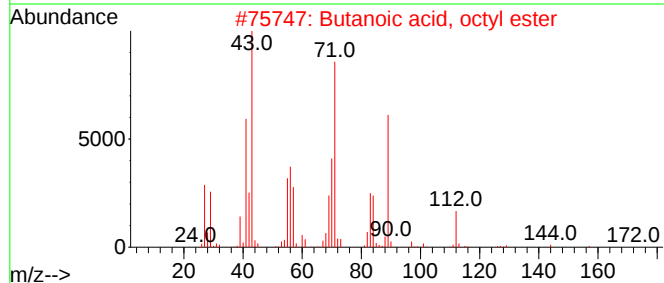
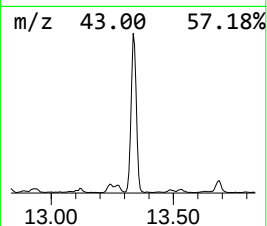
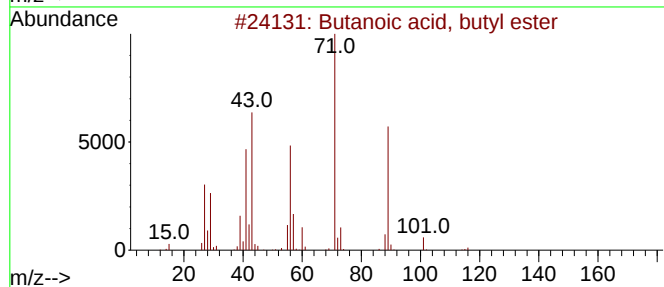
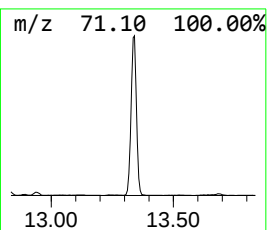
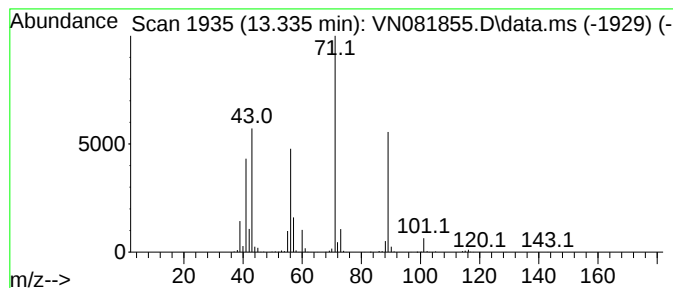
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	115.01 ug/l	2403150	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	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	72
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53



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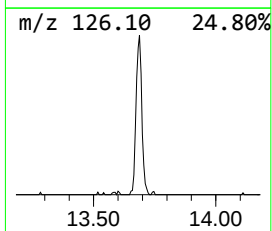
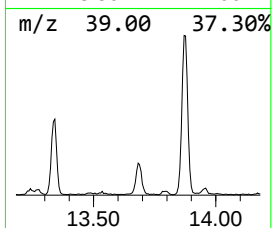
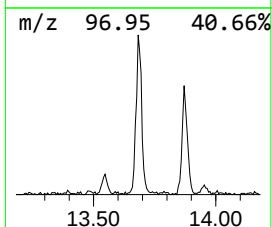
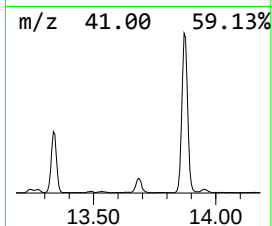
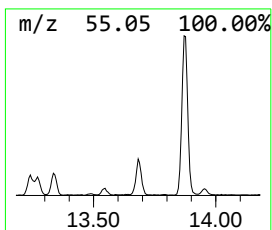
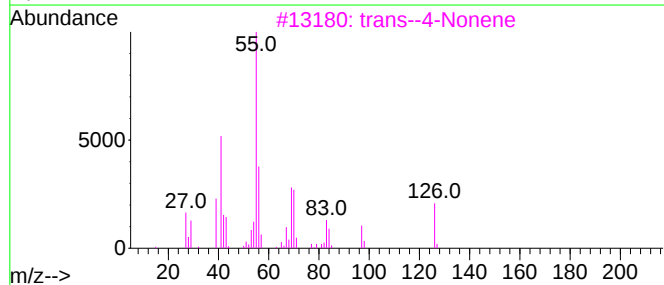
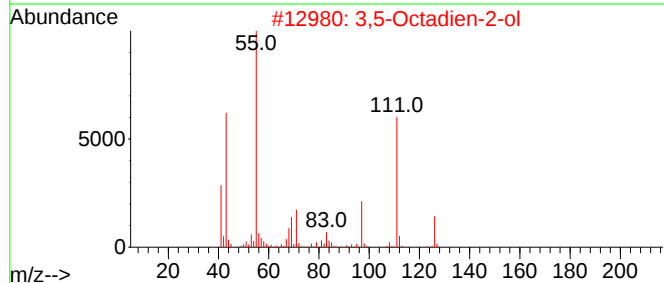
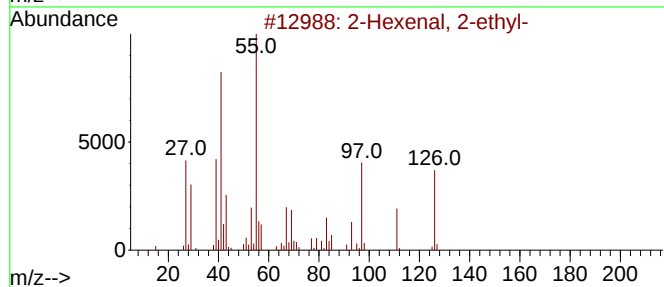
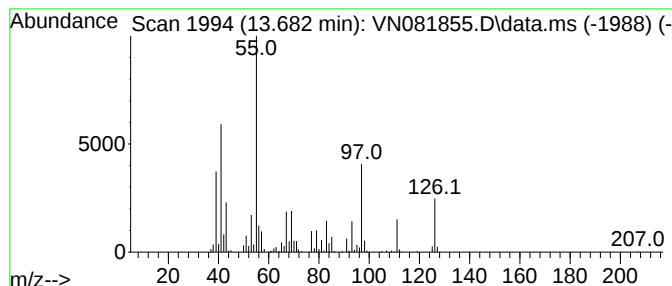
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Quant Title : SW846 8260

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

Peak Number 6 2-Hexenal, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.682	27.57 ug/l	576012	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	96
2			3,5-Octadien-2-ol	126	C8H14O	069668-82-2	47
3			trans--4-Nonene	126	C9H18	010405-85-3	38
4			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	38
5			1-Decyn-4-ol	154	C10H18O	027907-00-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081855.D
Acq On : 25 Apr 2024 17:04
Operator : JC\MD
Sample : P2257-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41C

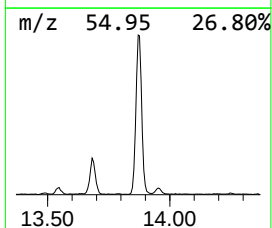
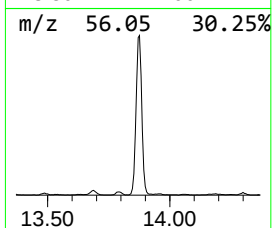
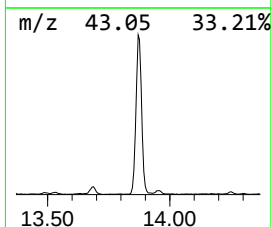
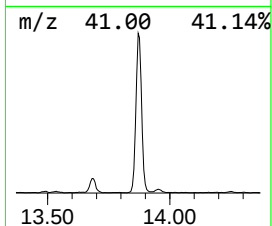
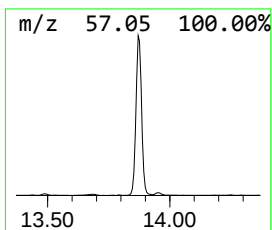
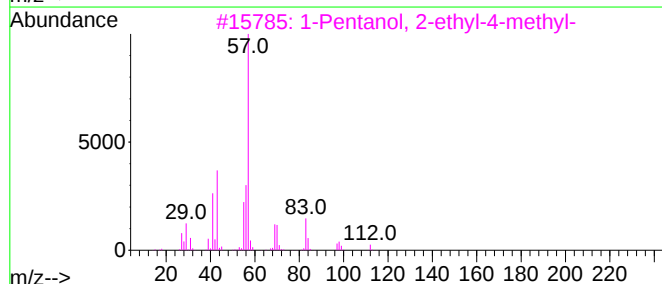
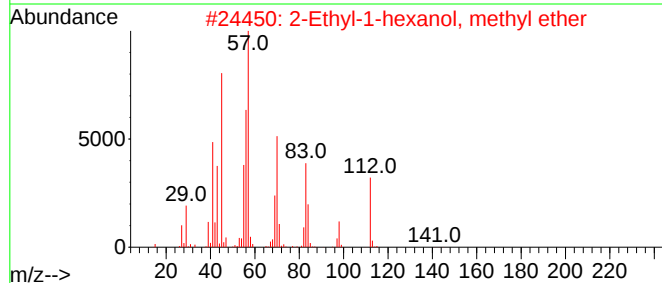
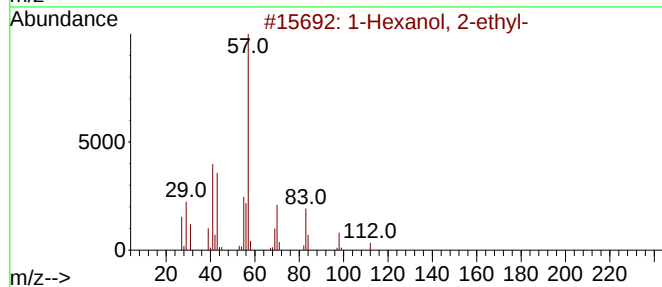
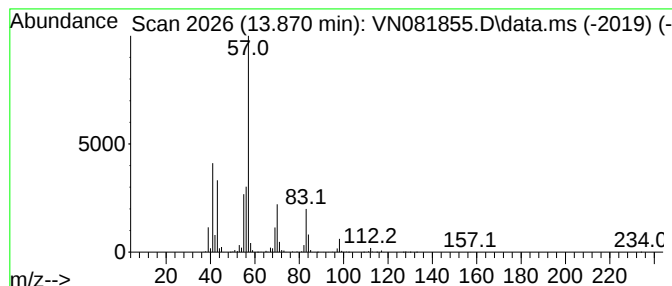
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	286.05 ug/l	5977270	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	83
2			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53
4			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081855.D
Acq On : 25 Apr 2024 17:04
Operator : JC\MD
Sample : P2257-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.642	2424.2	ug/l	36538300	1	8.224	753612	50.0
Ethanol	3.789	342.0	ug/l	5154080	1	8.224	753612	50.0
Butanal	7.224	99.3	ug/l	1496650	1	8.224	753612	50.0
1-Butanol	9.265	22.8	ug/l	476762	2	9.100	1045520	50.0
Butanoic acid, ...	13.335	115.0	ug/l	2403150	4	13.794	1044790	50.0
2-Hexenal, 2-et...	13.682	27.6	ug/l	576012	4	13.794	1044790	50.0
1-Hexanol, 2-et...	13.870	286.1	ug/l	5977270	4	13.794	1044790	50.0