

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081853.D
 Acq On : 25 Apr 2024 16:17
 Operator : JC\MD
 Sample : P2257-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41A

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\82N042524W.M
 Title : SW846 8260

Signal : TIC: VN081853.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	148	rBV	18441571	39411706	100.00%	65.598%
2	3.783	302	311	326	rBV	530627	1400586	3.55%	2.331%
3	7.224	883	896	912	rBV2	722912	2018594	5.12%	3.360%
4	8.224	1061	1066	1078	rVB	301734	671339	1.70%	1.117%
5	8.576	1121	1126	1138	rVB	200861	456756	1.16%	0.760%
6	9.100	1207	1215	1225	rBV	459263	952810	2.42%	1.586%
7	9.265	1236	1243	1257	rBV	295059	604407	1.53%	1.006%
8	10.565	1456	1464	1472	rBV	735729	1384654	3.51%	2.305%
9	11.865	1680	1685	1696	rVB	610407	1118878	2.84%	1.862%
10	12.417	1774	1779	1794	rVB	354242	599284	1.52%	0.997%
11	12.847	1844	1852	1862	rBV	463547	868634	2.20%	1.446%
12	13.335	1929	1935	1943	rVB	2050794	3156101	8.01%	5.253%
13	13.682	1989	1994	2002	rVB	310796	523718	1.33%	0.872%
14	13.794	2006	2013	2019	rBV	520033	878997	2.23%	1.463%
15	13.870	2019	2026	2035	rVV	3713402	6034029	15.31%	10.043%

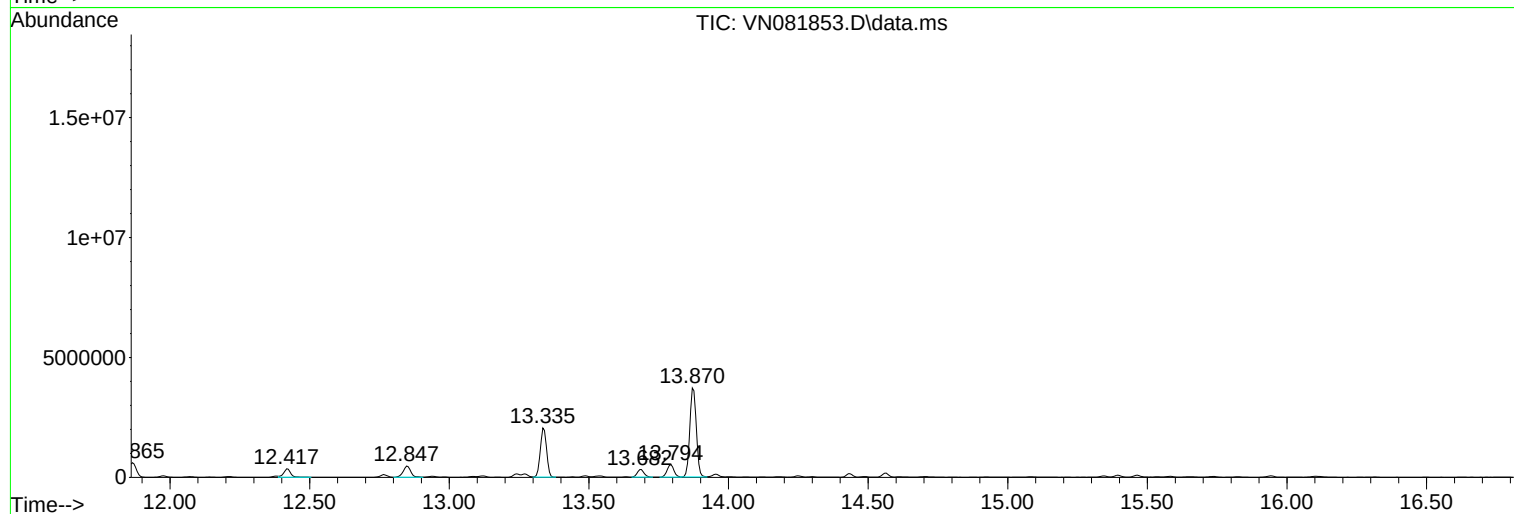
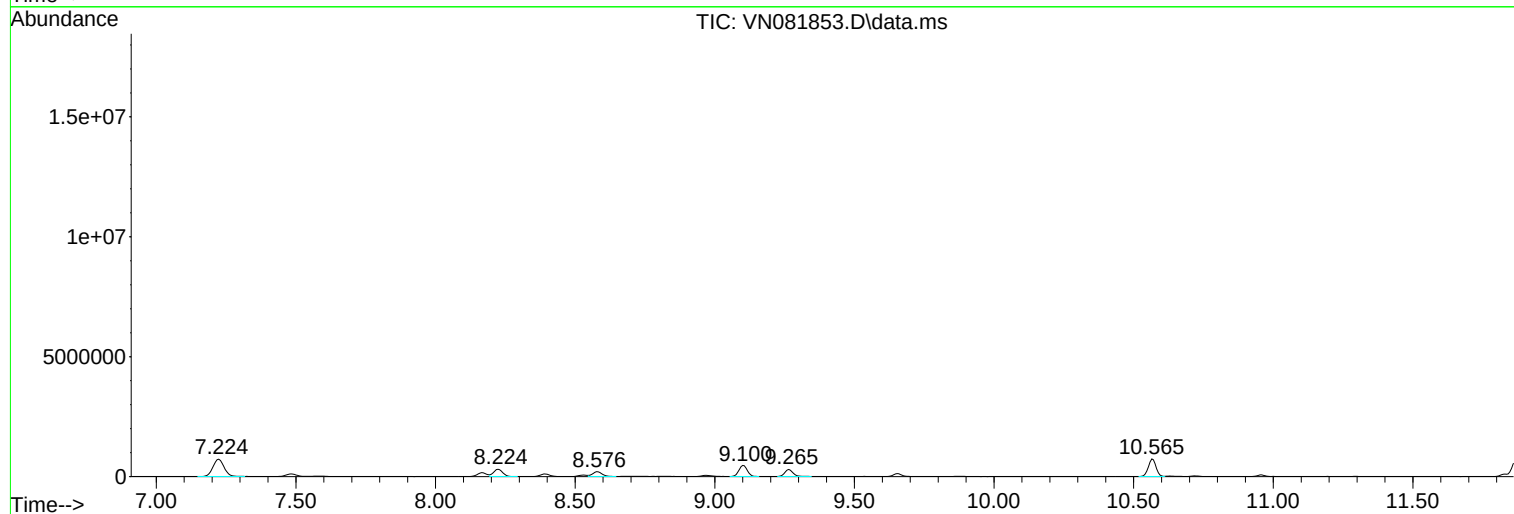
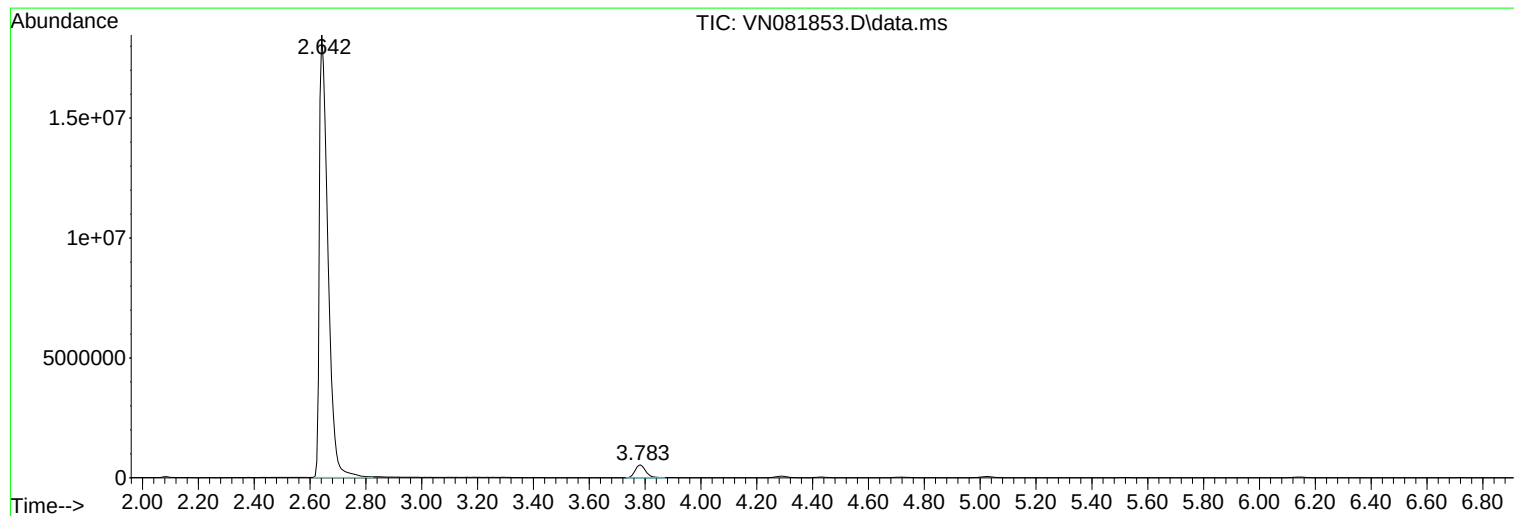
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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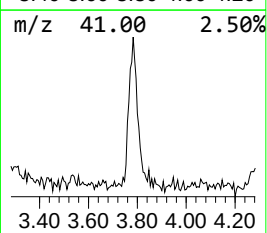
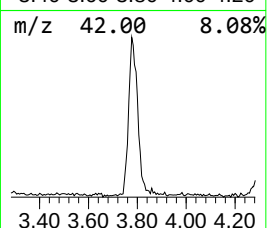
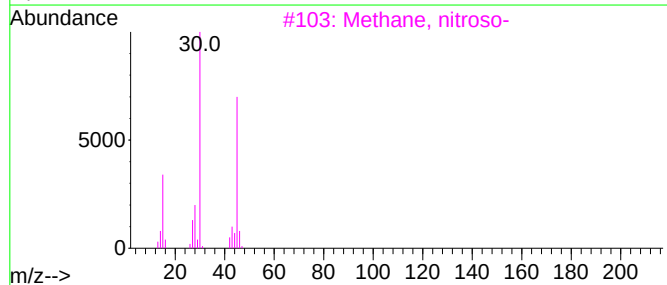
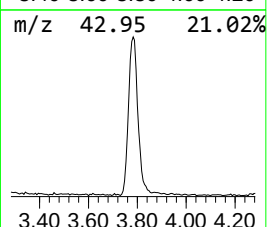
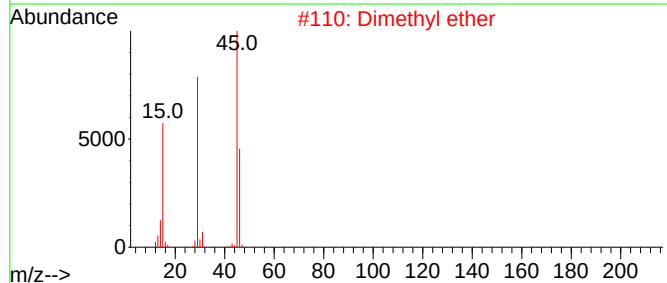
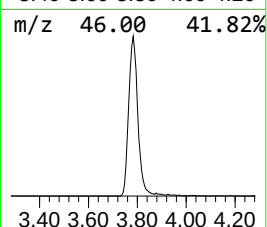
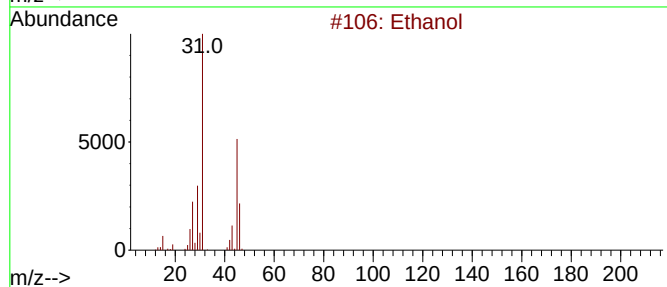
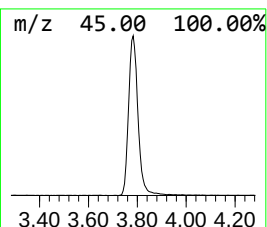
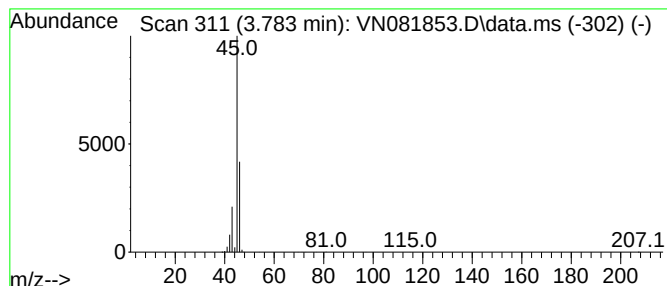
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	104.31 ug/l	1400590	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
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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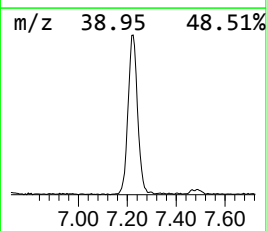
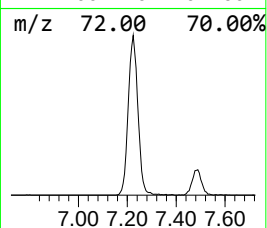
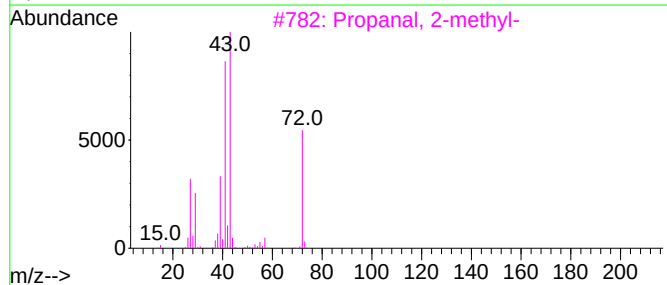
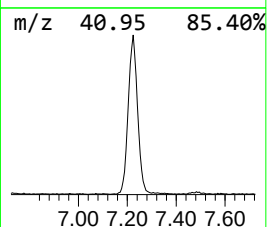
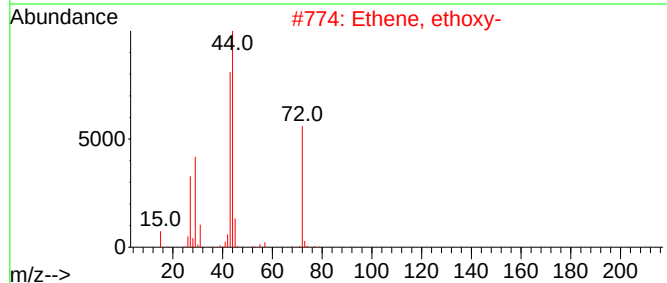
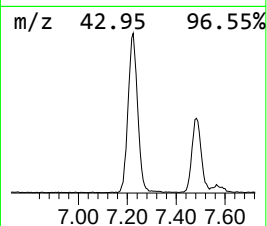
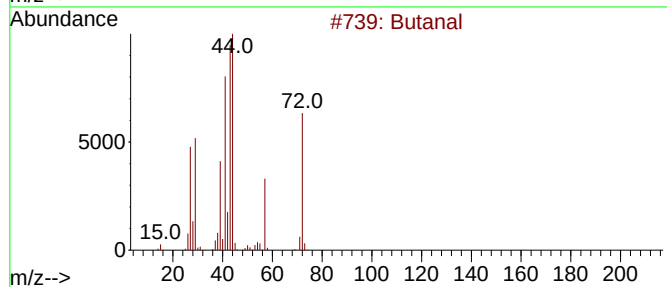
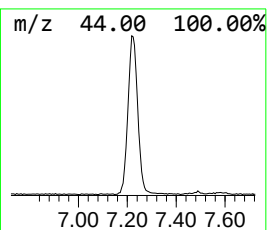
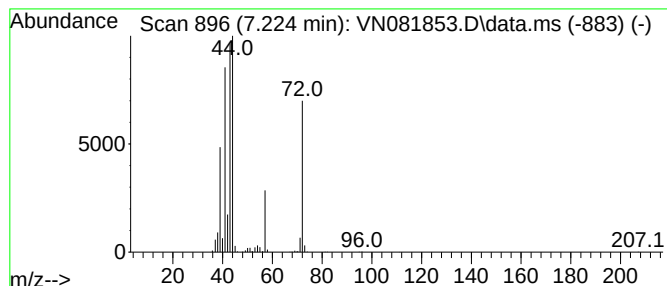
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	150.34 ug/l	2018590	Pentafluorobenzene	8.229

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	49
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	25
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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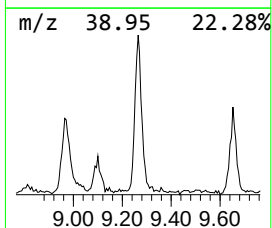
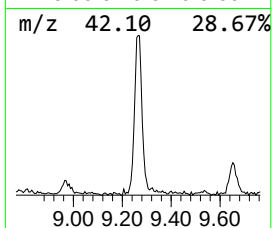
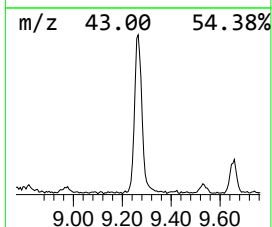
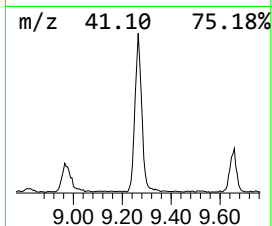
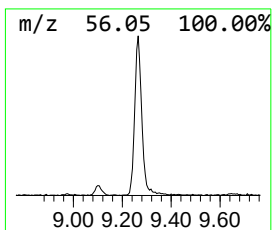
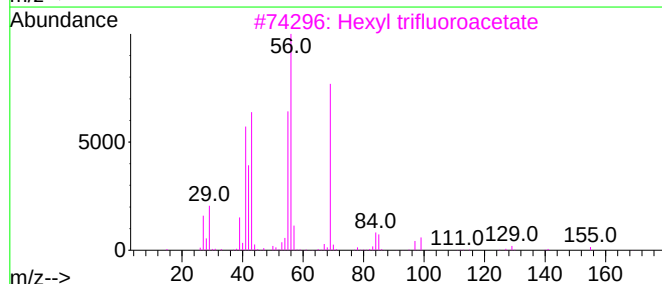
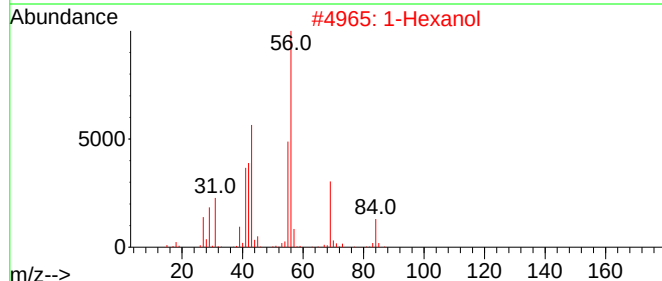
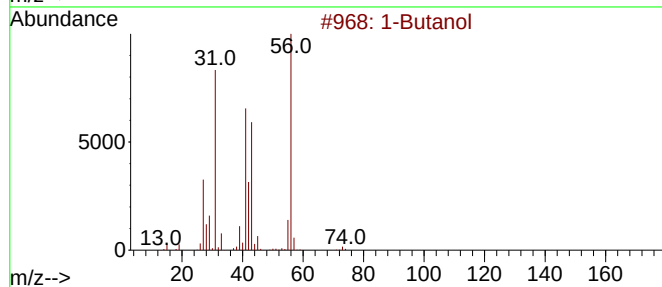
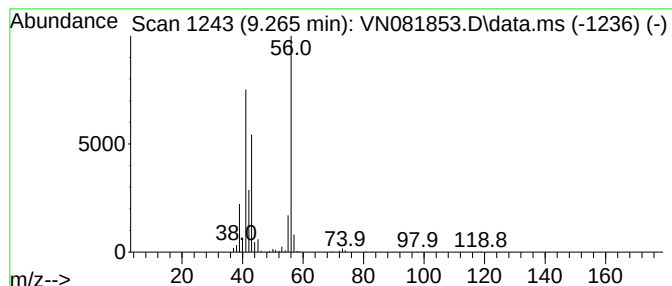
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Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	31.72 ug/l	604407	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			1-Hexanol	102	C6H14O	000111-27-3	39
3			Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	39
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



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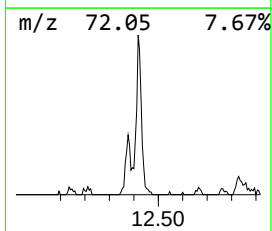
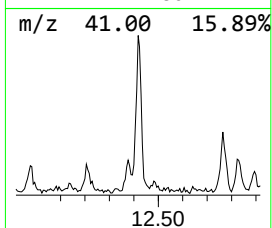
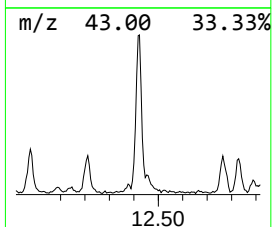
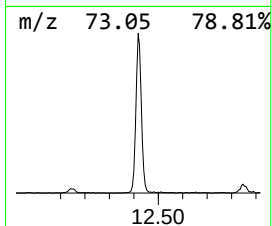
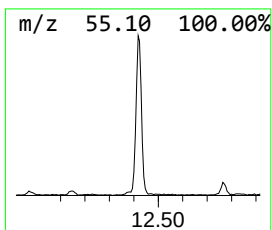
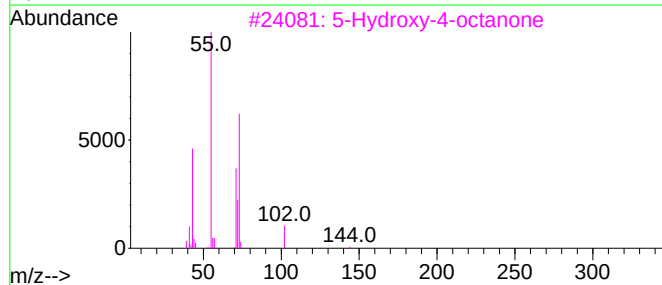
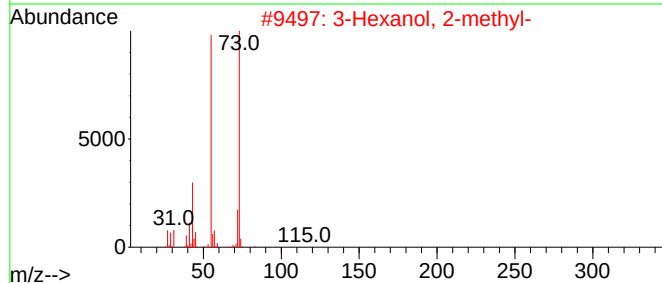
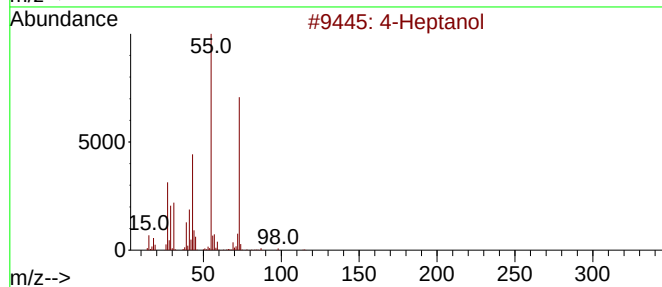
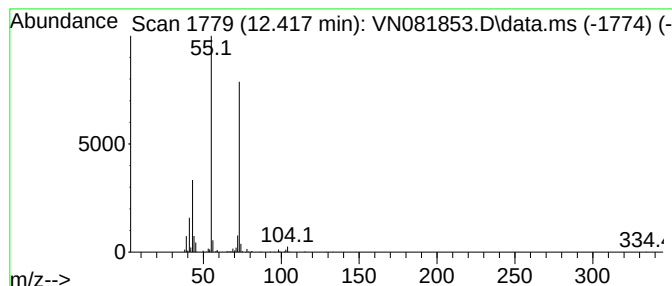
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Peak Number 5 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.417	26.78 ug/l	599284	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	78
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	53
3			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	39
4			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	25
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	23



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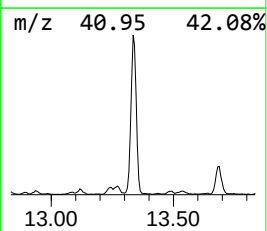
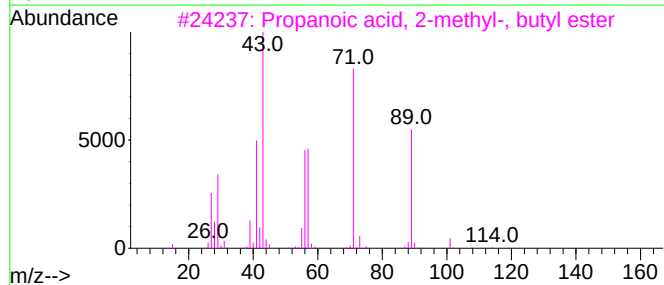
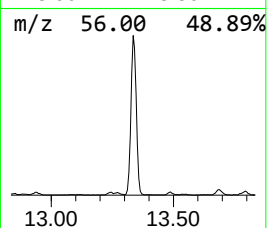
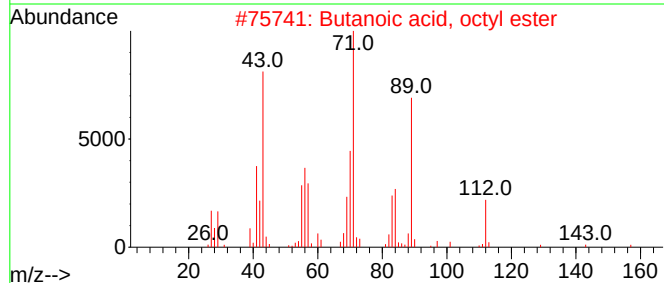
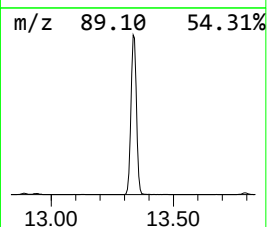
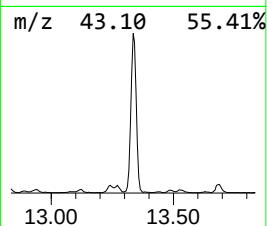
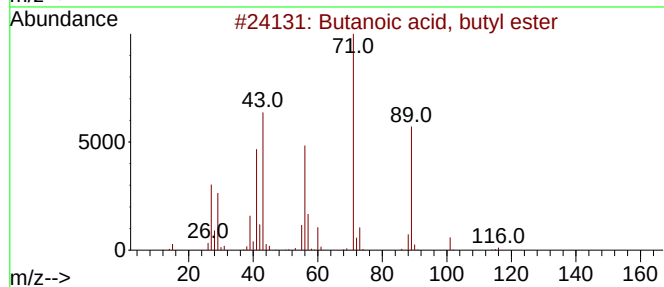
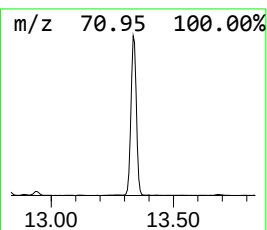
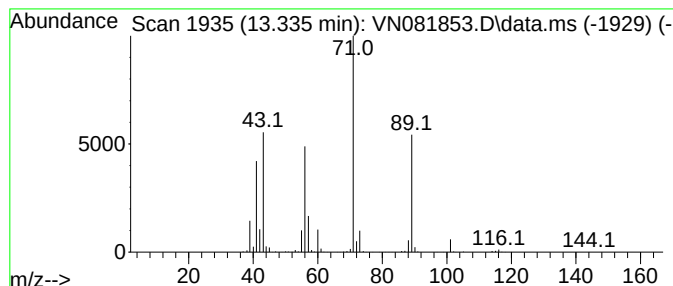
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	179.53 ug/l	3156100	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			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64



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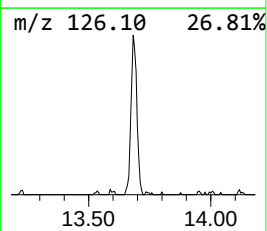
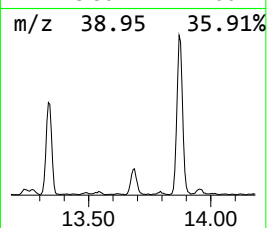
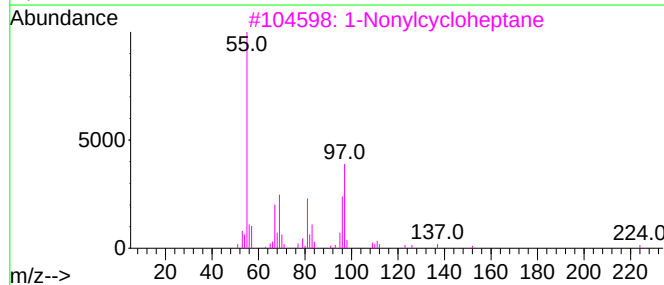
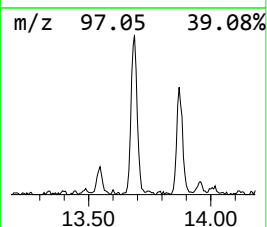
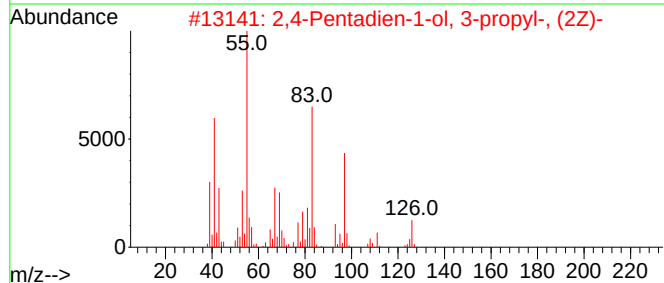
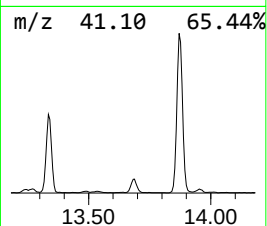
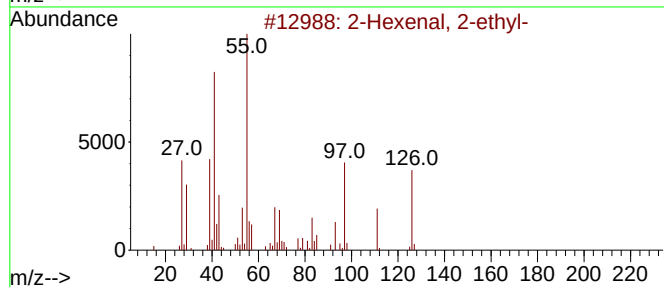
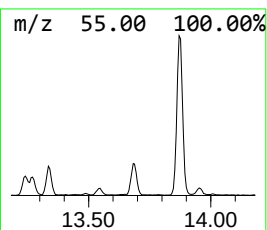
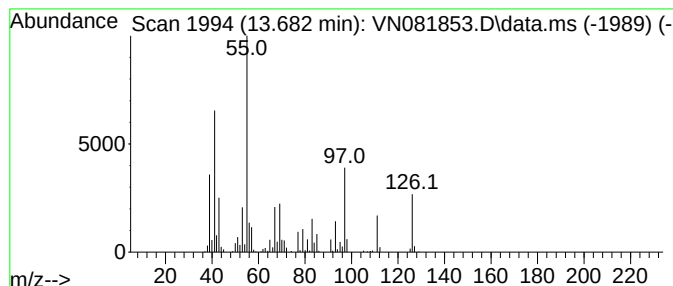
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Quant Title : SW846 8260

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

Peak Number 7 2-Hexenal, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.682	29.79 ug/l	523718	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	95
2			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	47
3			1-Nonylcycloheptane	224	C16H32	1000371-47-7	35
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	32
5			Acetamide, N-2-propynyl-	97	C5H7NO	065881-41-6	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081853.D
Acq On : 25 Apr 2024 16:17
Operator : JC\MD
Sample : P2257-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41A

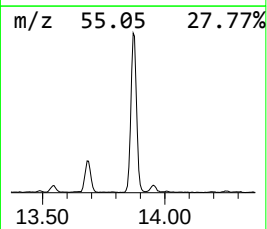
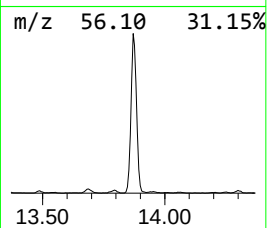
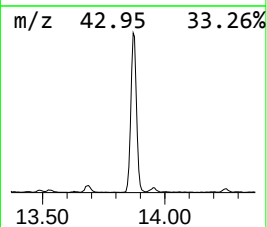
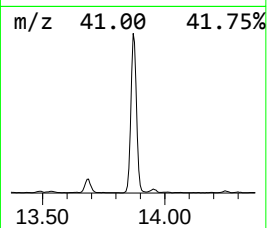
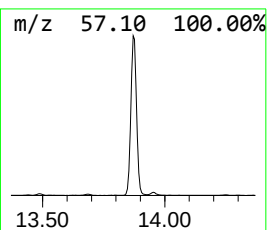
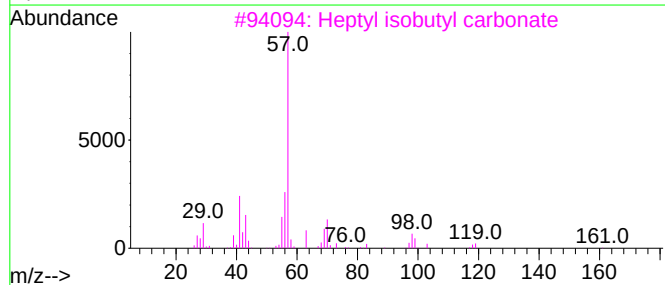
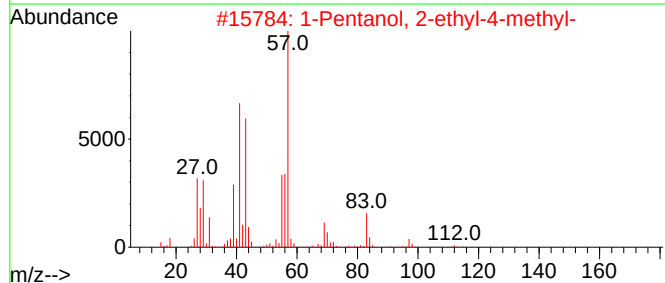
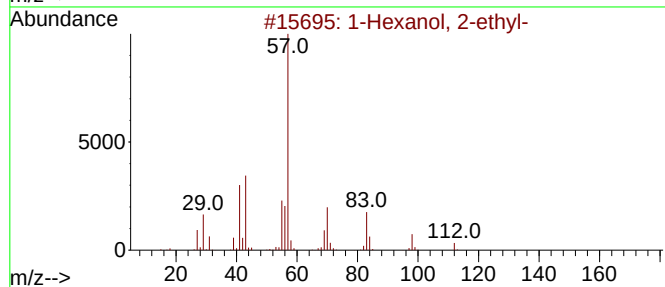
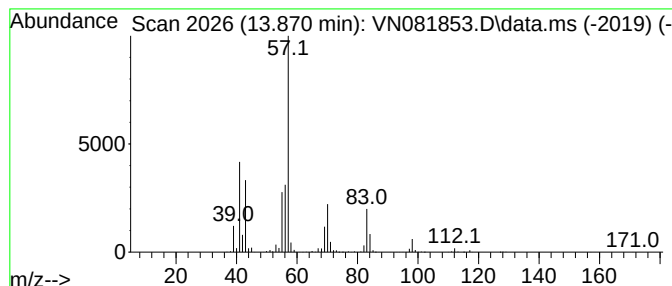
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	343.23 ug/l	6034030	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	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081853.D
Acq On : 25 Apr 2024 16:17
Operator : JC\MD
Sample : P2257-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41A

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
Ethanol	3.783	104.3	ug/l	1400590	1	8.229	671339	50.0
Butanal	7.224	150.3	ug/l	2018590	1	8.229	671339	50.0
1-Butanol	9.265	31.7	ug/l	604407	2	9.100	952810	50.0
4-Heptanol	12.417	26.8	ug/l	599284	3	11.865	1118880	50.0
Butanoic acid, ...	13.335	179.5	ug/l	3156100	4	13.794	878997	50.0
2-Hexenal, 2-et...	13.682	29.8	ug/l	523718	4	13.794	878997	50.0
1-Hexanol, 2-et...	13.870	343.2	ug/l	6034030	4	13.794	878997	50.0