LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081135.D
Acq On : 22 Feb 2024 15:11
Operator : JC\MD
Sample : P1546-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1332

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\82N021624W.M
Title : SW846 8260

Signal : TIC: VN081135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	15	22	28	rBV	193627	281535	1.16%	0.339%
2	2.659	112	120	141	rBV	13711191	24181138	100.00%	29.111%
3	3.783	301	311	324	rBV	686993	1815590	7.51%	2.186%
4	4.283	385	396	414	rBV	5814568	16520984	68.32%	19.889%
5	4.706	459	468	485	rVB	84179	269401	1.11%	0.324%
6	6.718	787	810	826	rBV4	319103	1246667	5.16%	1.501%
7	7.224	884	896	912	rBV	710762	1979123	8.18%	2.383%
8	7.482	931	940	950	rBV2	118496	293659	1.21%	0.354%
9	8.171	1047	1057	1061	rBV	246363	599349	2.48%	0.722%
10	8.224	1061	1066	1079	rVB2	505363	1136588	4.70%	1.368%
11	8.577	1121	1126	1132	rVV2	260840	588372	2.43%	0.708%
12	8.647	1132	1138	1166	rVB	94329	477516	1.97%	0.575%
13	9.106	1206	1216	1231	rVB	765488	1613518	6.67%	1.942%
14	9.265	1235	1243	1254	rBV	355736	747390	3.09%	0.900%
15	10.571	1456	1465	1473	rBV	904956	1749099	7.23%	2.106%
16	11.829	1671	1679	1681	rBV3	200095	354256	1.47%	0.426%
17	11.865	1681	1685	1696	rVB	1033931	1852495	7.66%	2.230%
18	12.423	1774	1780	1790	rVB	899849	1393533	5.76%	1.678%
19	12.853	1844	1853	1859	rBV2	686061	1367534	5.66%	1.646%
20	13.241	1913	1919	1922	rBV	431110	738431	3.05%	0.889%
21	13.270	1922	1924	1930	rVV	418211	610360	2.52%	0.735%
22	13.341	1930	1936	1943	rVB	4301062	6440661	26.64%	7.754%
23	13.688	1981	1995	2004	rBV3	738821	1429044	5.91%	1.720%
24	13.794	2006	2013	2020	rBV	1030939	1701102	7.03%	2.048%
25	13.876	2020	2027	2036	rBV	8173920	12605078	52.13%	15.175%
26	13.959	2036	2041	2046	rVB3	170041	276405	1.14%	0.333%
27	15.400	2281	2286	2292	rVB	307895	506115	2.09%	0.609%
28	15.464	2292	2297	2305	rBV2	153806	290138	1.20%	0.349%

Sum of corrected areas: 83065081

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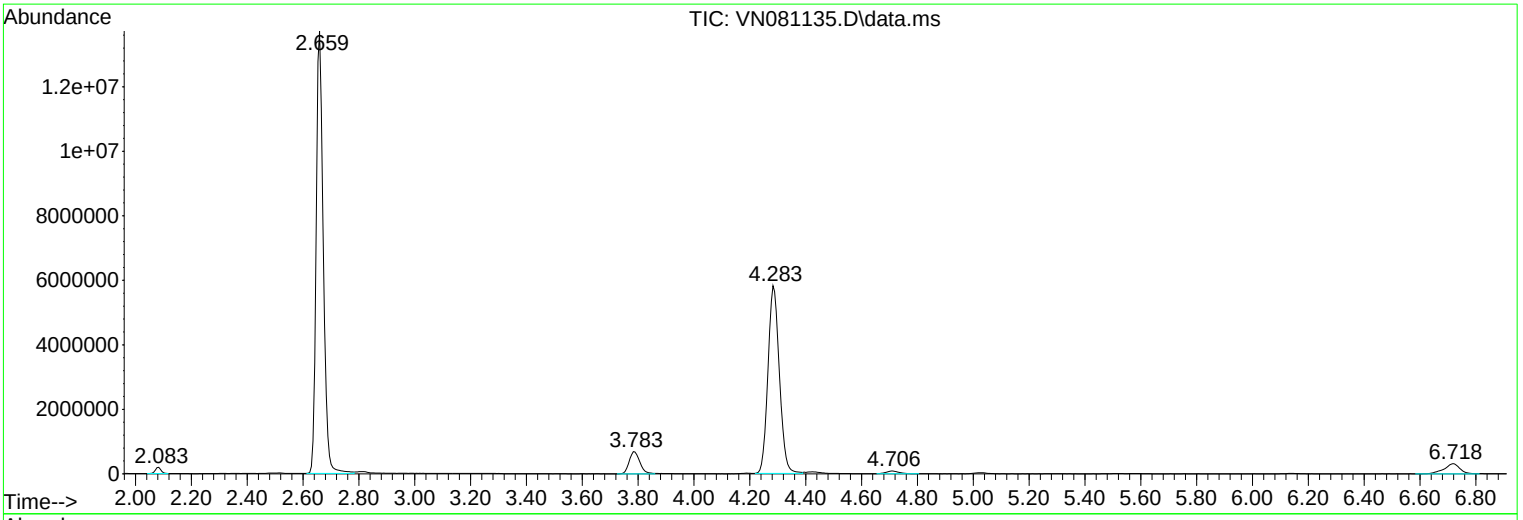
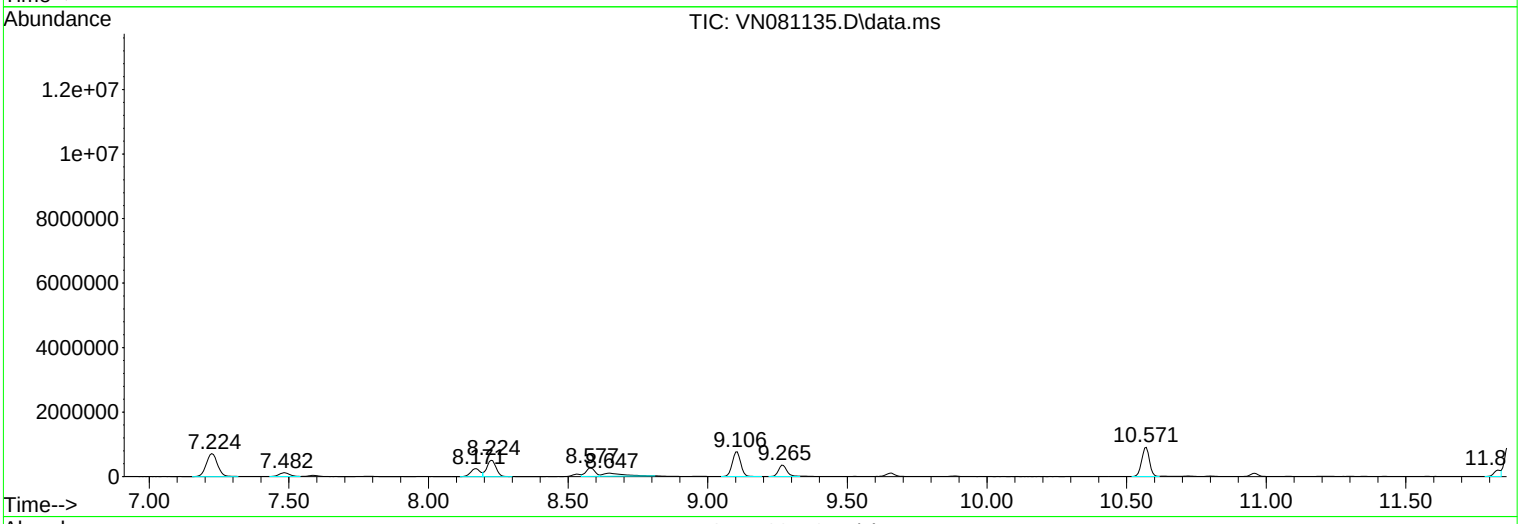
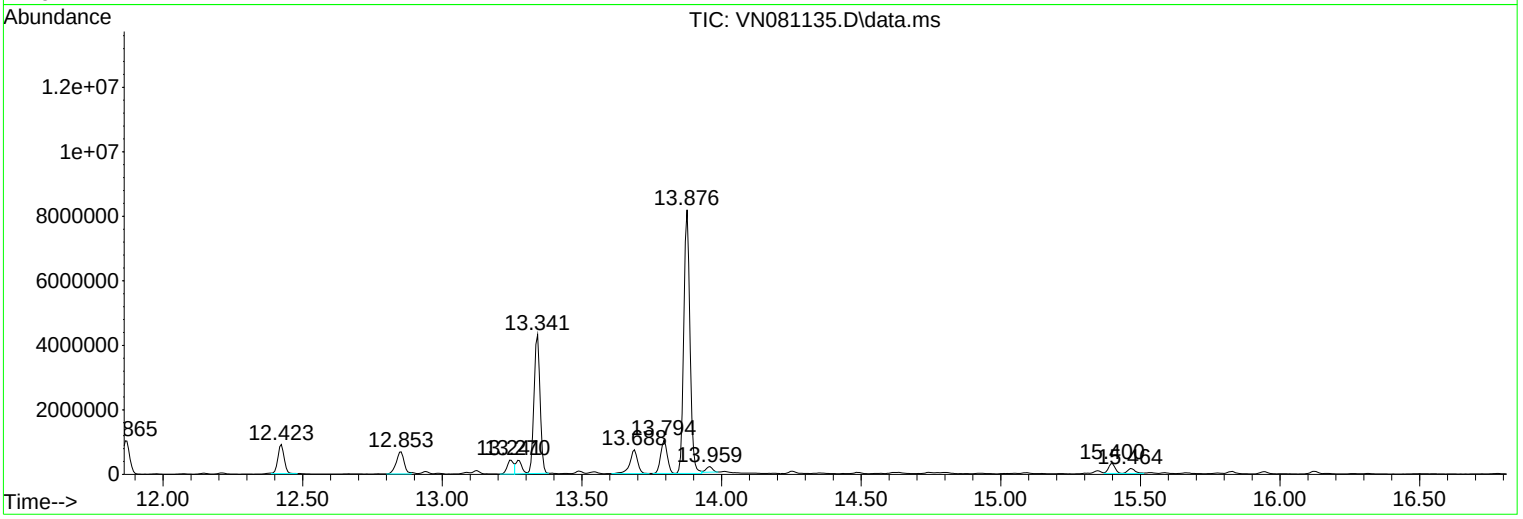
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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







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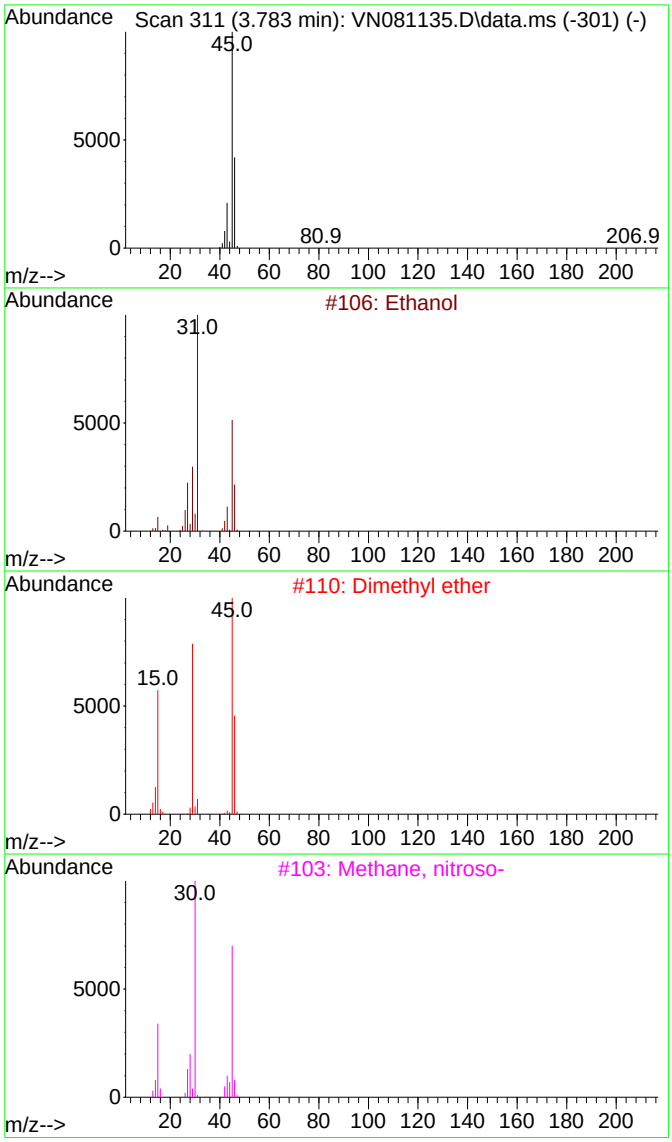
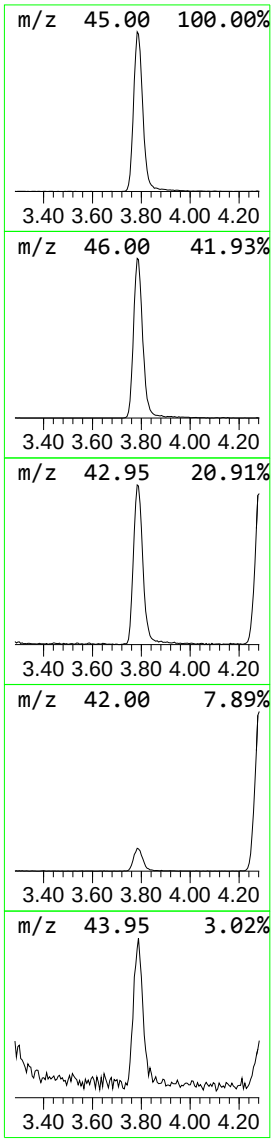
****
Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	79.87 ug/l	1815590	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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Data File : VN081135.D
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Instrument :
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ClientSampleId :
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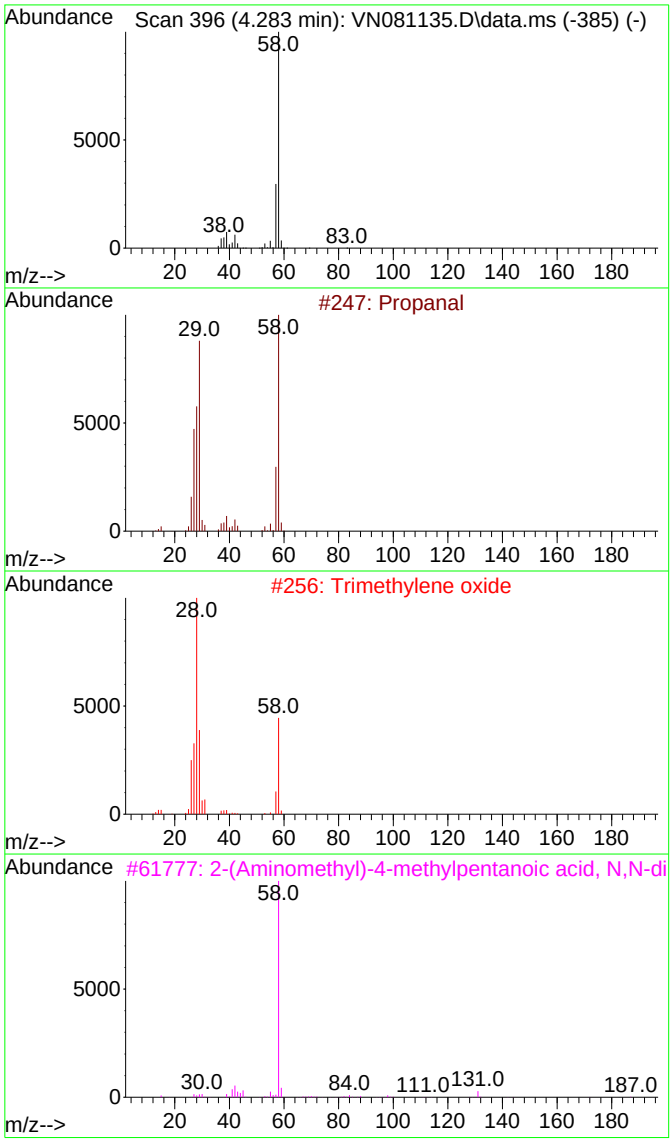
Quant Title : SW846 8260

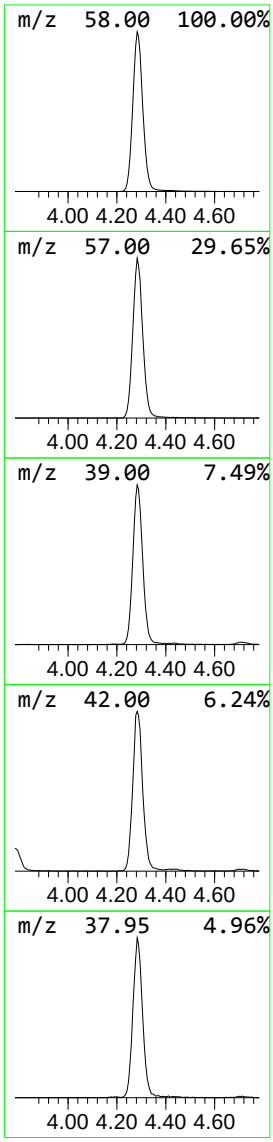
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	726.78 ug/l	16521000	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	56
3	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7





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Instrument :
MSVOA_N
ClientSampleId :
1332

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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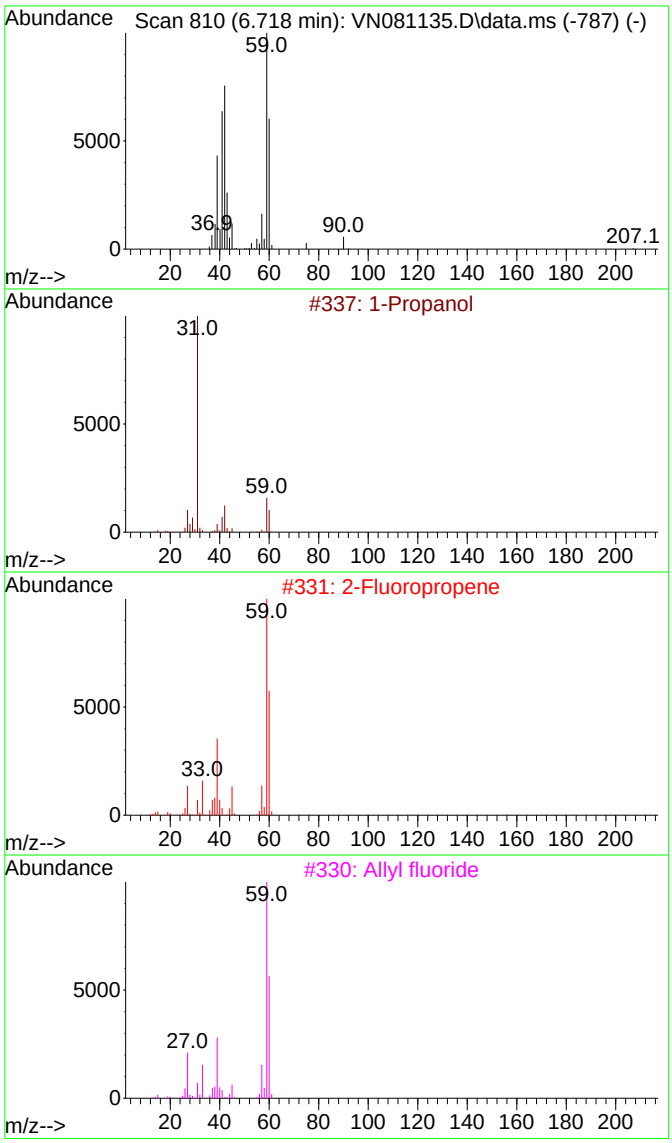
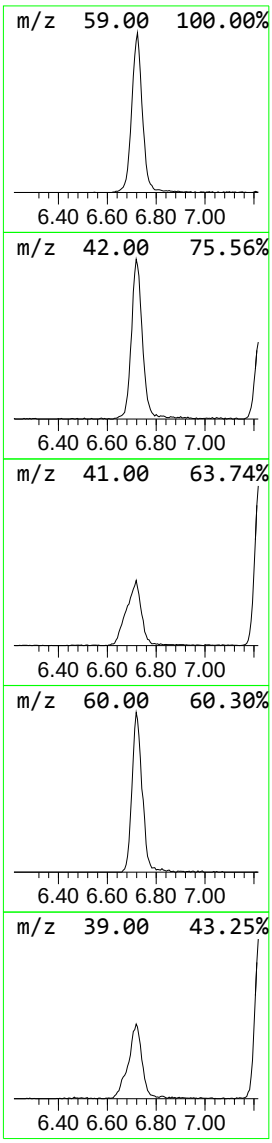
****
Peak Number 4 1-Propanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.718	54.84 ug/l	1246670	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	58
3	Allyl fluoride	60	C3H5F	000818-92-8	43
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Propene	42	C3H6	000115-07-1	25





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Misc : 5.0mL/MSVOA_N/WATER
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Instrument :
MSVOA_N
ClientSampleId :
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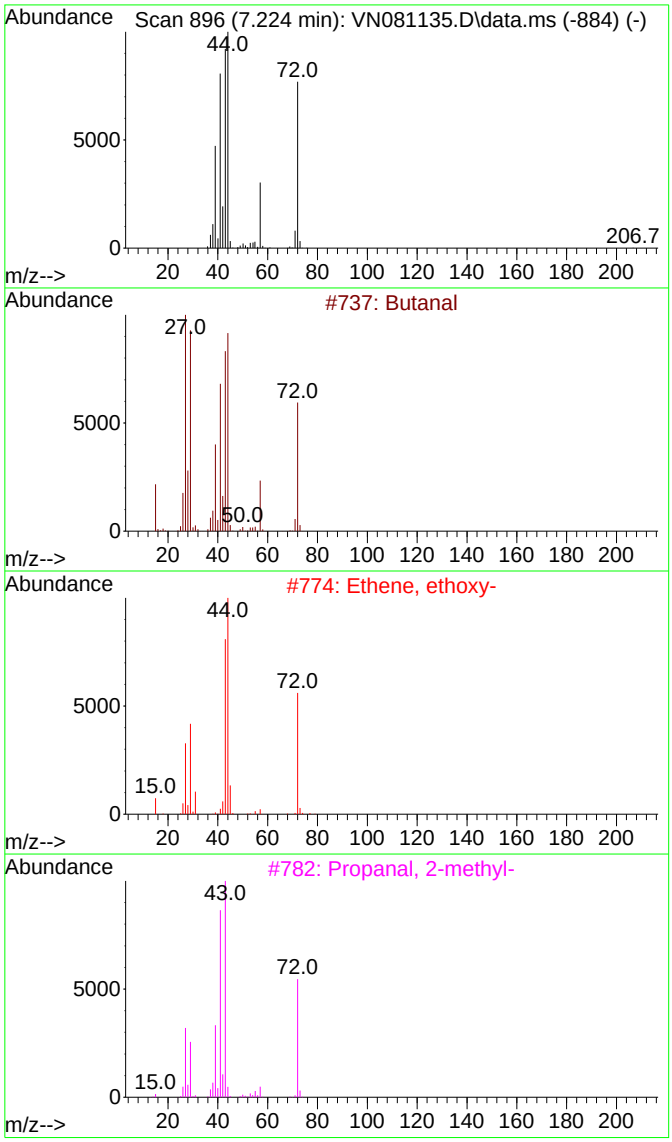
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

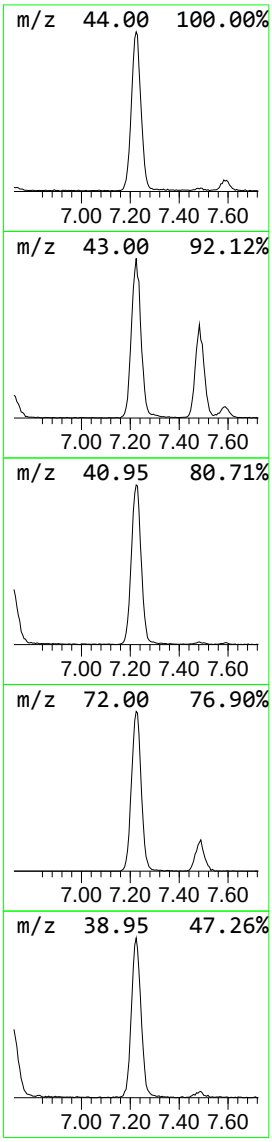
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	87.06 ug/l	1979120	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Operator : JC\MD
Sample : P1546-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1332

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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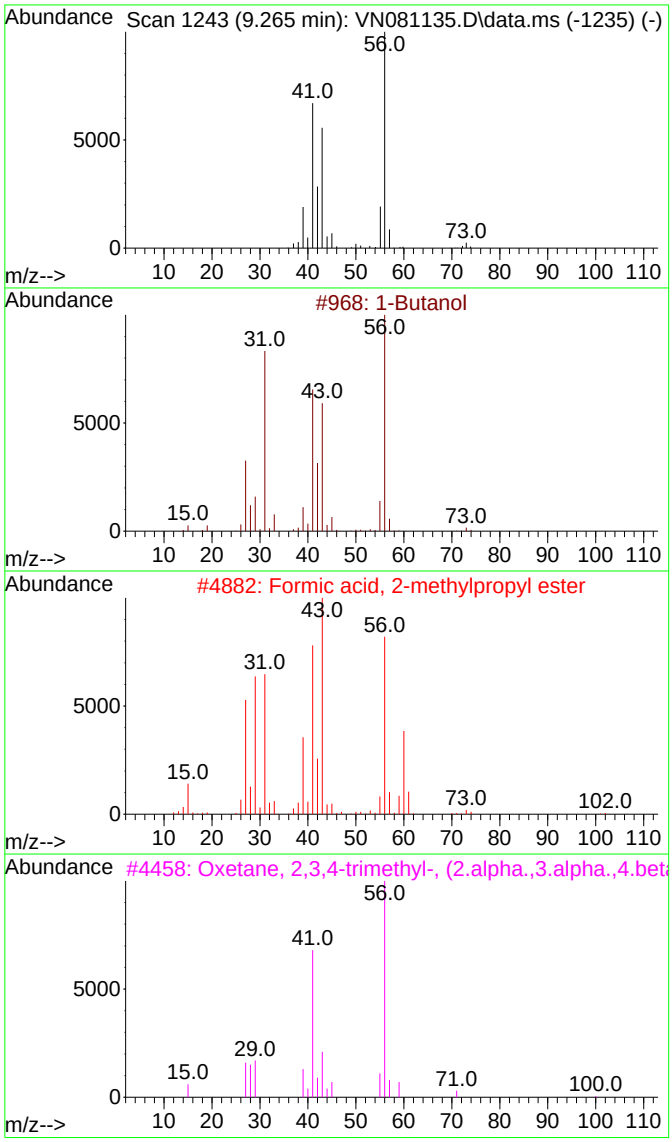
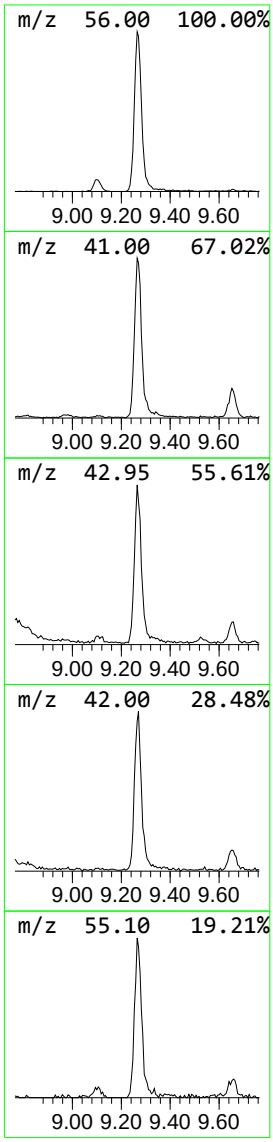
****
Peak Number 6 1-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	23.16 ug/l	747390	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	39
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	38
4	.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	9
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9





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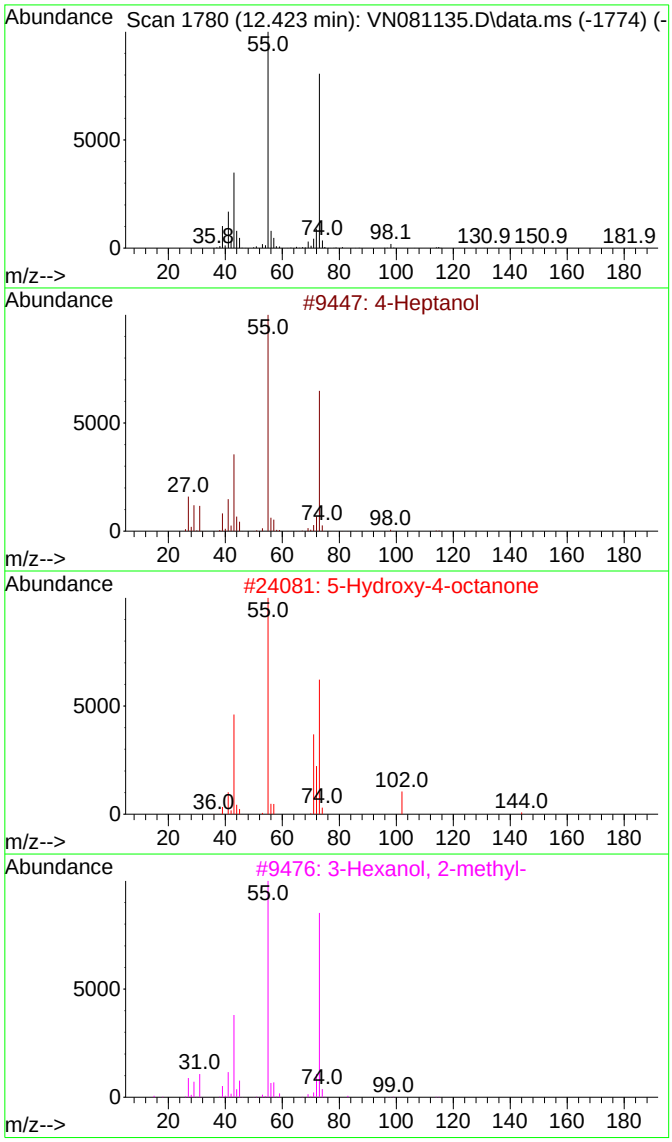
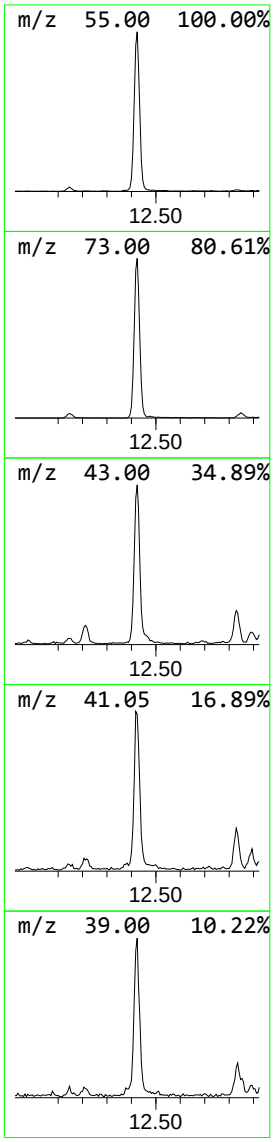
****

Peak Number 7 4-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.423	37.61 ug/l	1393530	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	83
2	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	50
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	45
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	27
5	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	17





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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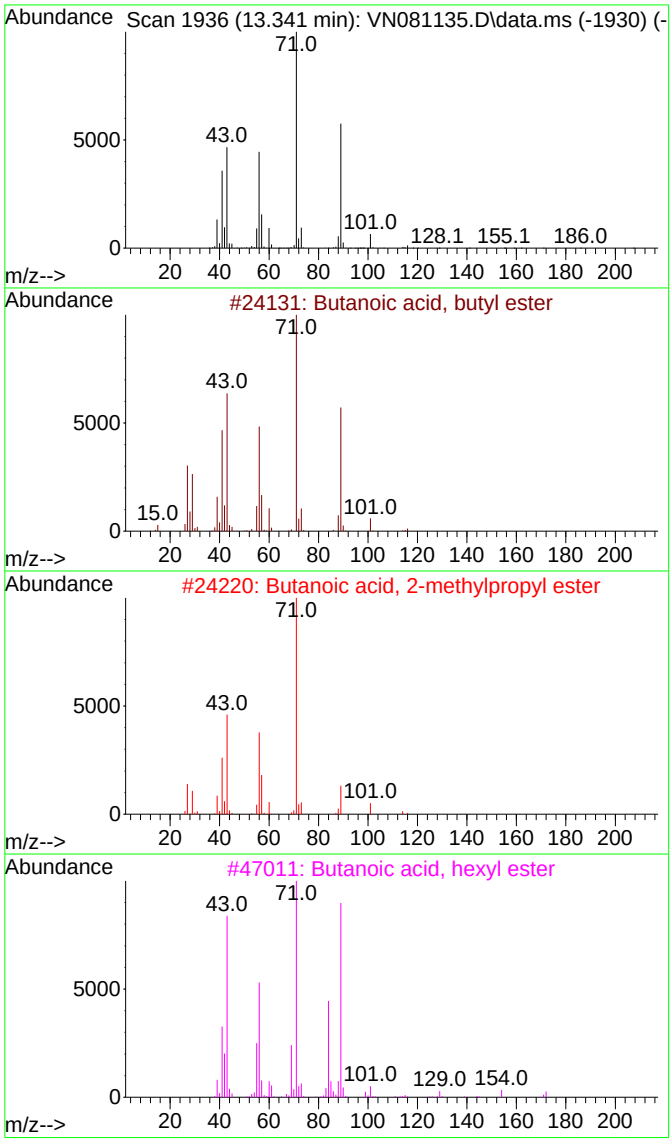
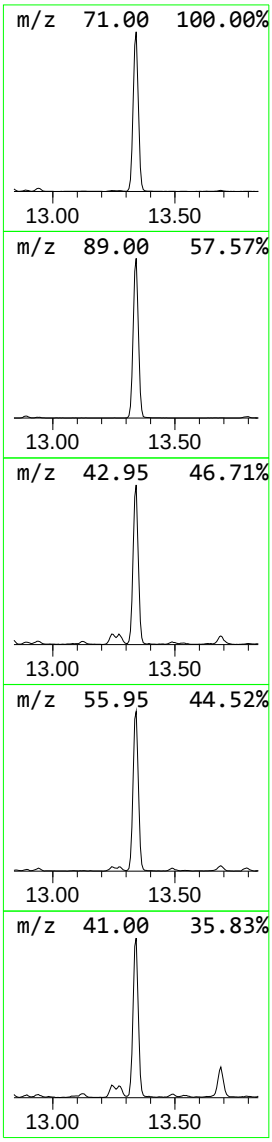
****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	189.31 ug/l	6440660	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59





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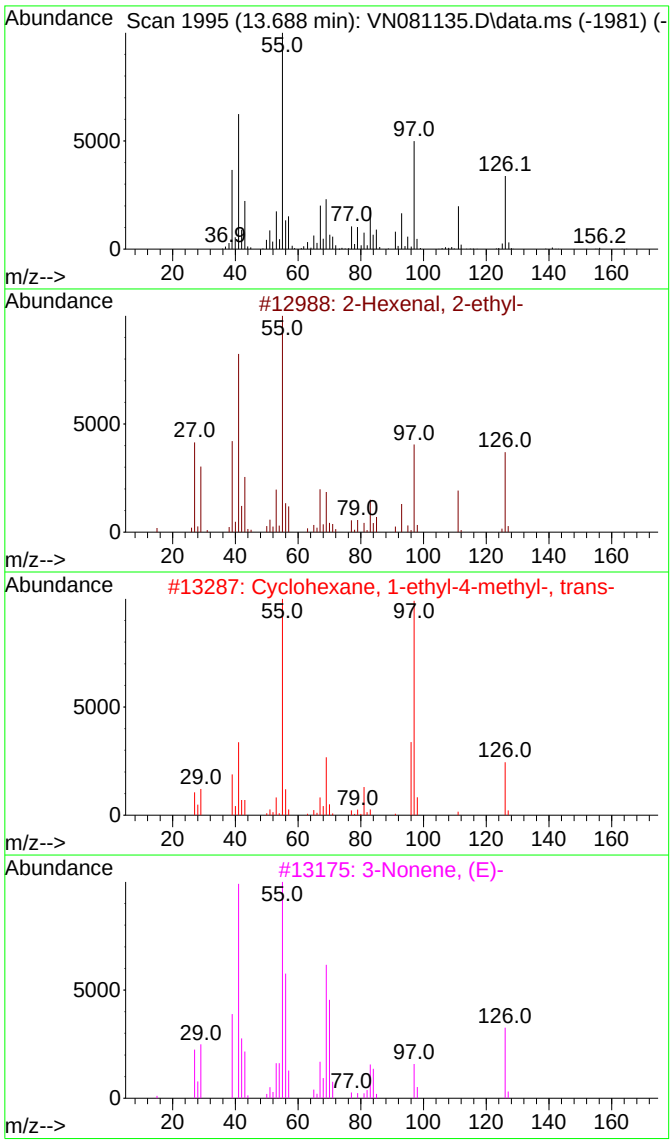
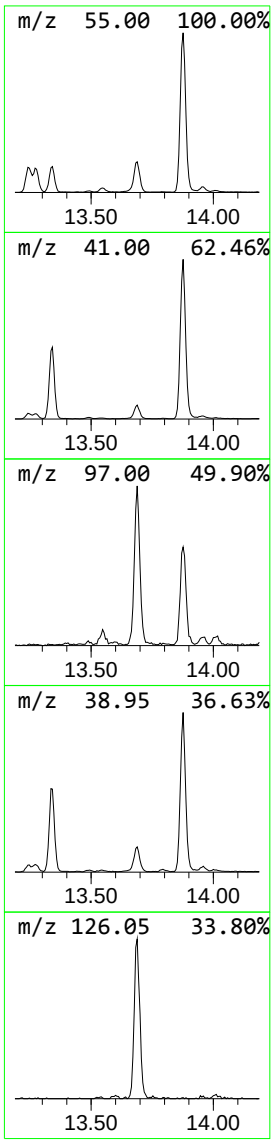
****
Peak Number 9 2-Hexenal, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	42.00 ug/l	1429040	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	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	46
3	3-Nonene, (E)-	126	C9H18	020063-92-7	43
4	3,5-Octadien-2-ol	126	C8H14O	069668-82-2	43
5	cis-2-Nonene	126	C9H18	006434-77-1	35





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MSVOA_N
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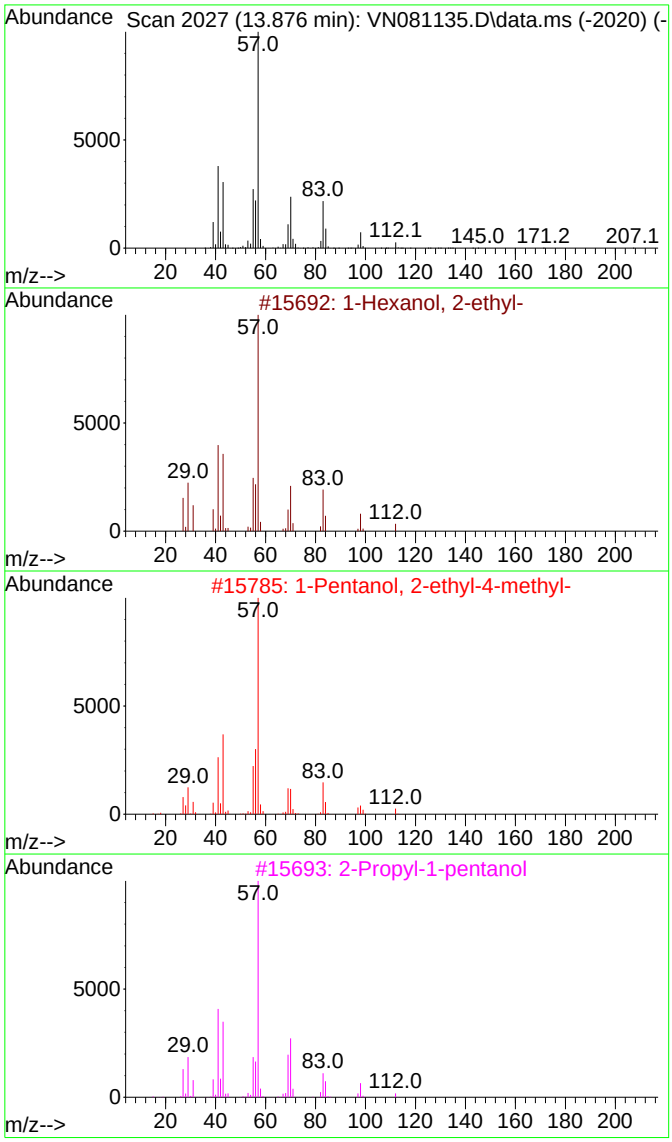
Quant Title : SW846 8260

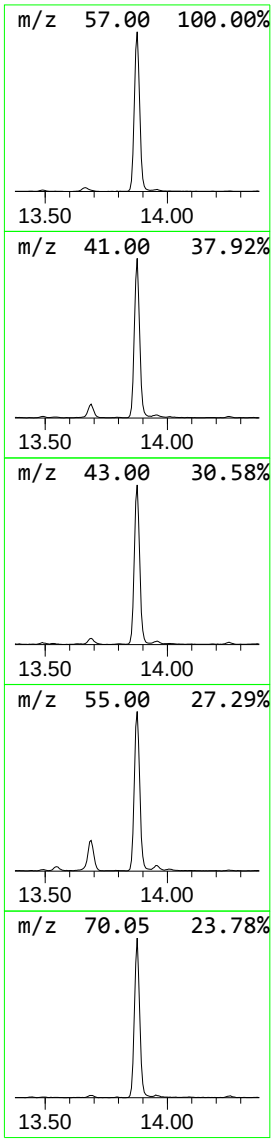
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	370.50 ug/l	12605100	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	53
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081135.D
Acq On : 22 Feb 2024 15:11
Operator : JC\MD
Sample : P1546-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1332

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.783	79.9	ug/l	1815590	1	8.224	1136590	50.0
Propanal	4.283	726.8	ug/l	16521000	1	8.224	1136590	50.0
1-Propanol	6.718	54.8	ug/l	1246670	1	8.224	1136590	50.0
Butanal	7.224	87.1	ug/l	1979120	1	8.224	1136590	50.0
1-Butanol	9.265	23.2	ug/l	747390	2	9.106	1613520	50.0
4-Heptanol	12.423	37.6	ug/l	1393530	3	11.865	1852500	50.0
Butanoic acid, ...	13.341	189.3	ug/l	6440660	4	13.794	1701100	50.0
2-Hexenal, 2-et...	13.688	42.0	ug/l	1429040	4	13.794	1701100	50.0
1-Hexanol, 2-et...	13.876	370.5	ug/l	12605100	4	13.794	1701100	50.0