LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080850.D
Acq On : 31 Jan 2024 19:07
Operator : JC\MD
Sample : P1284-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1249

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\82N012924W.M
Title : SW846 8260

Signal : TIC: VN080850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	18	21	28	rVB	35614	53059	3.03%	0.742%
2	4.430	413	421	431	rBV	12719	34166	1.95%	0.478%
3	7.218	886	895	907	rBV3	32812	88432	5.05%	1.237%
4	8.165	1047	1056	1061	rBV2	80717	190685	10.90%	2.668%
5	8.224	1061	1066	1076	rVB2	135725	288799	16.51%	4.040%
6	8.577	1119	1126	1137	rVB3	101965	242274	13.85%	3.390%
7	9.100	1207	1215	1226	rBV	280963	576225	32.93%	8.062%
8	9.265	1236	1243	1254	rBV2	50152	113962	6.51%	1.594%
9	10.571	1457	1465	1472	rBV	344190	648842	37.08%	9.078%
10	10.953	1524	1530	1540	rBV4	15438	31016	1.77%	0.434%
11	11.865	1679	1685	1696	rVB	410968	748028	42.75%	10.465%
12	12.424	1774	1780	1789	rVB2	62625	106541	6.09%	1.491%
13	12.847	1844	1852	1864	rBV	262573	499365	28.54%	6.986%
14	12.941	1864	1868	1874	rVB3	22699	34505	1.97%	0.483%
15	13.082	1887	1892	1896	rBV5	12380	22142	1.27%	0.310%
16	13.247	1913	1920	1922	rBV4	30181	51995	2.97%	0.727%
17	13.271	1922	1924	1929	rVV3	27706	41479	2.37%	0.580%
18	13.341	1929	1936	1945	rVB	1163646	1749640	100.00%	24.478%
19	13.688	1988	1995	2005	rVB	135406	225004	12.86%	3.148%
20	13.794	2005	2013	2020	rBV	376584	634572	36.27%	8.878%
21	13.876	2020	2027	2037	rBV	278561	461770	26.39%	6.460%
22	13.959	2037	2041	2046	rVB4	15276	26571	1.52%	0.372%
23	14.253	2083	2091	2099	rBV3	17086	30612	1.75%	0.428%
24	14.618	2145	2153	2158	rBV5	11327	20559	1.18%	0.288%
25	15.353	2271	2278	2281	rBV4	28951	55484	3.17%	0.776%
26	15.394	2281	2285	2292	rVB2	53888	94883	5.42%	1.327%
27	15.829	2352	2359	2364	rBV4	14470	24880	1.42%	0.348%
28	15.941	2371	2378	2385	rBV4	15441	28758	1.64%	0.402%
29	16.123	2402	2409	2414	rBV3	13343	23474	1.34%	0.328%

Sum of corrected areas: 7147722

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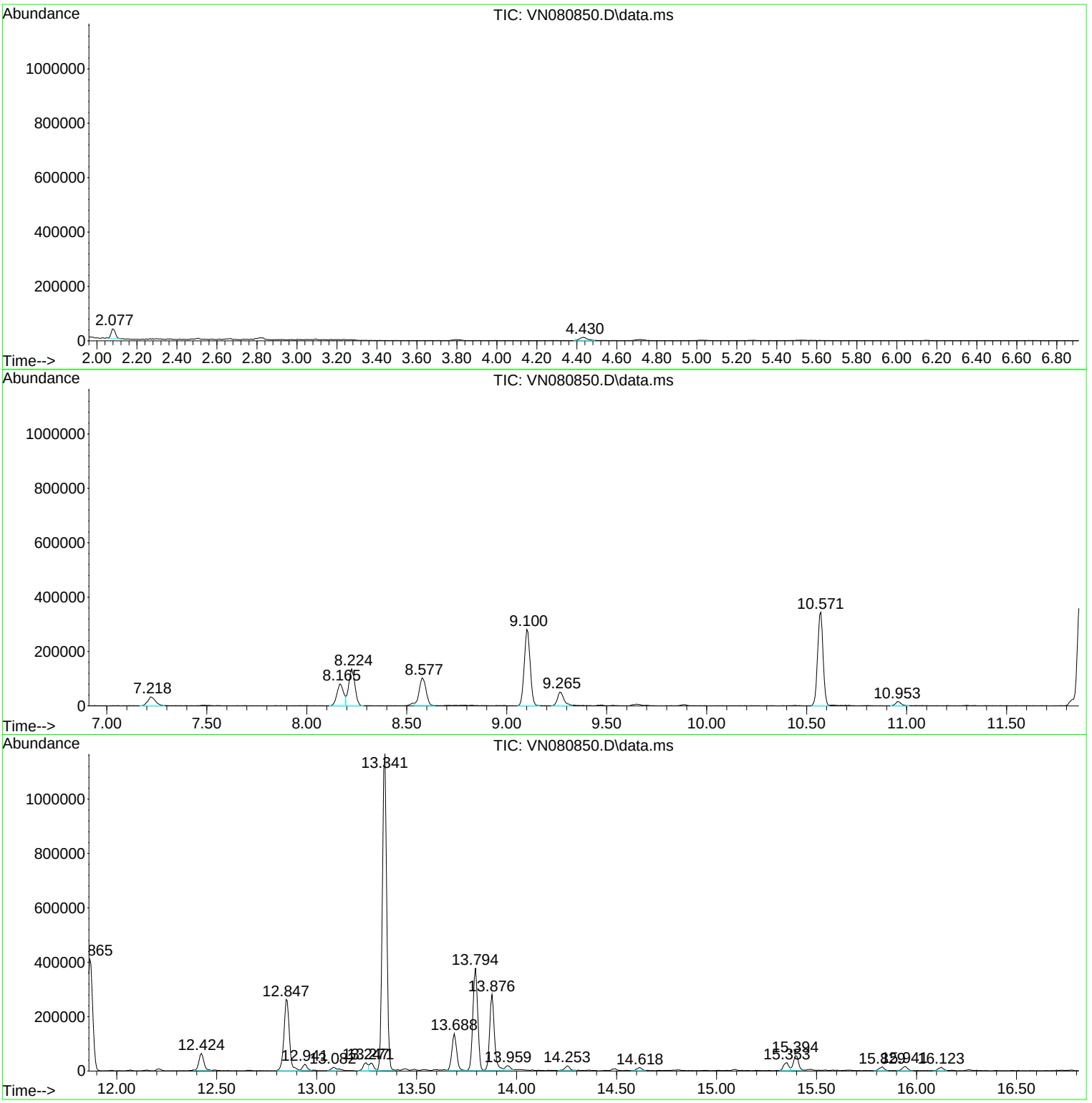
ClientSampleId :
1249

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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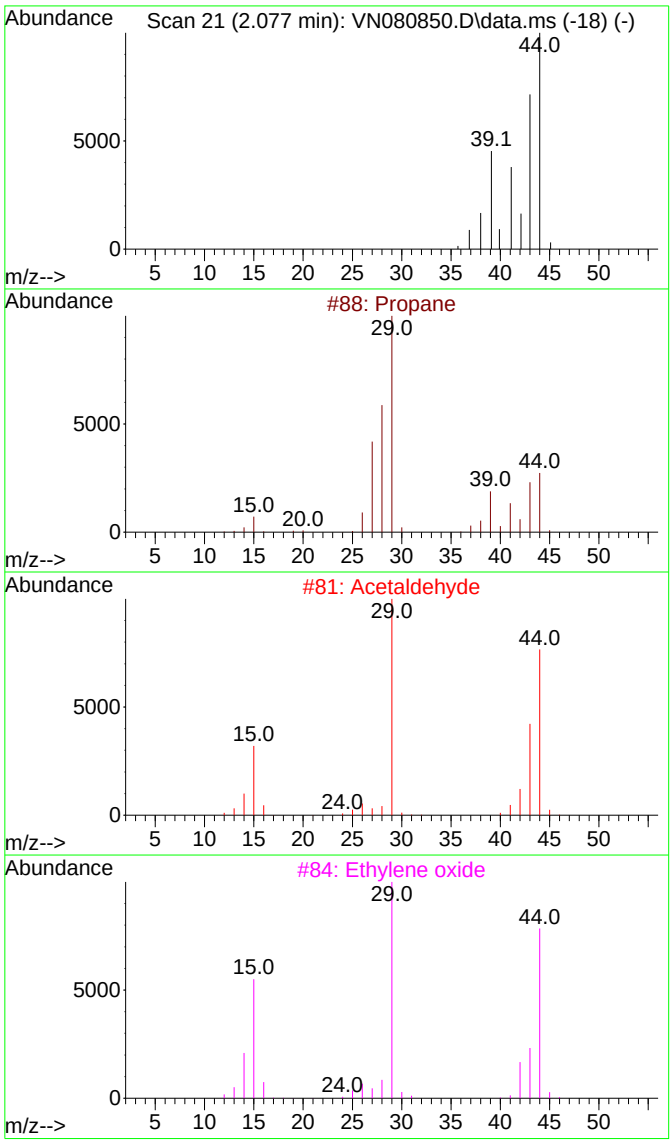
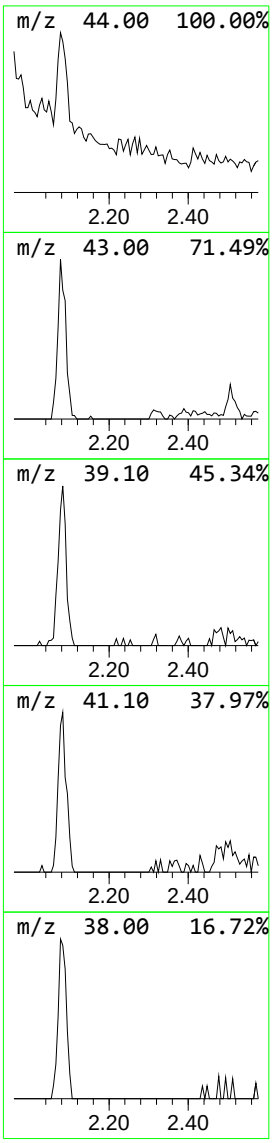
Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.077	9.19 ug/l	53059	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Ethyne, fluoro-	44	C2HF	002713-09-9	3
5	Acetonitrile-d3	44	C2D3N	002206-26-0	3





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Quant Title : SW846 8260

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

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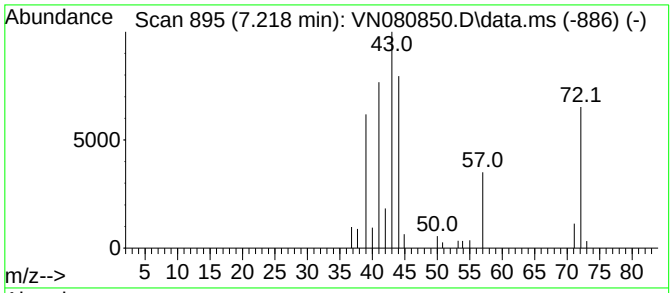
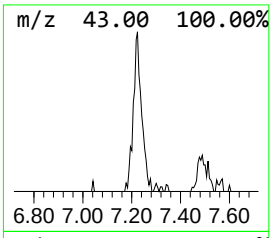
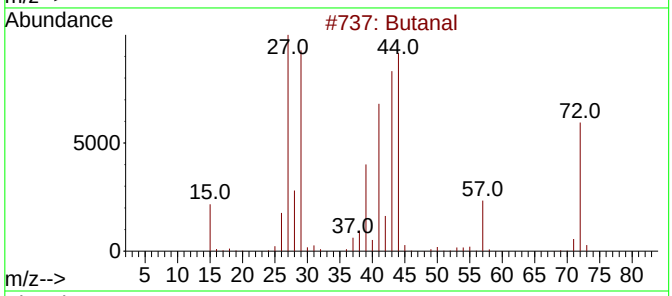
Peak Number 2 Butanal Concentration Rank 4

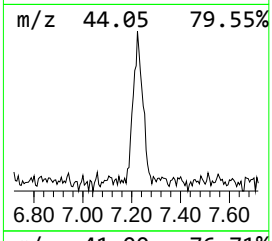
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.218	15.31 ug/l	88432	Pentafluorobenzene	8.224

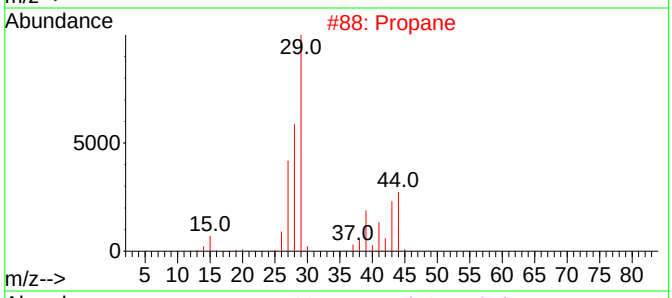
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	80
2	Propane	44	C3H8	000074-98-6	45
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27
4	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23
5	Methacrolein	70	C4H6O	000078-85-3	16

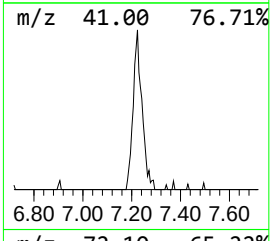


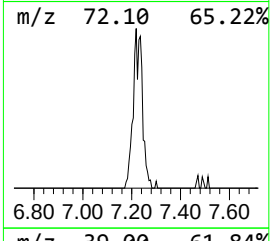


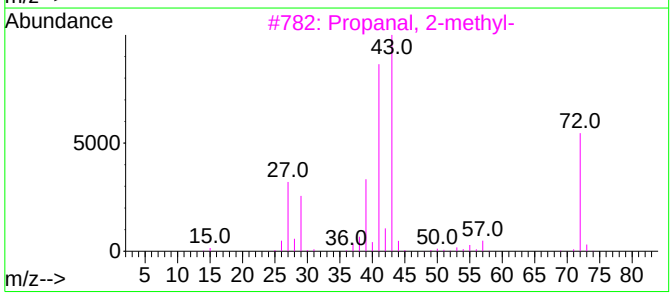


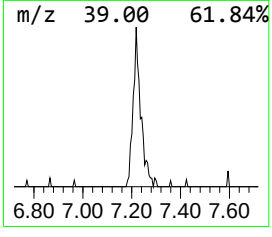












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1249

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

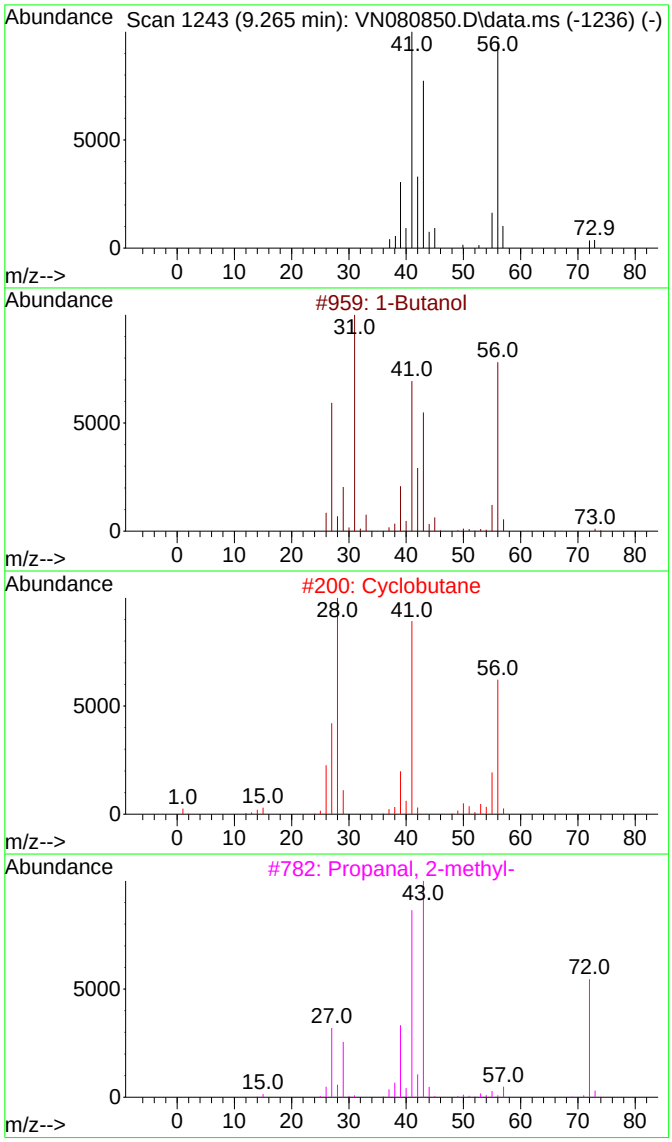
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

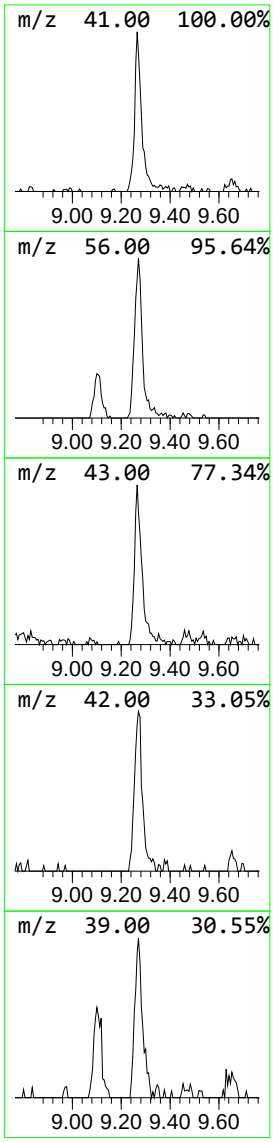
****

Peak Number 3 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	9.89 ug/l	113962	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	78
2	Cyclobutane	56	C4H8	000287-23-0	38
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	14
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





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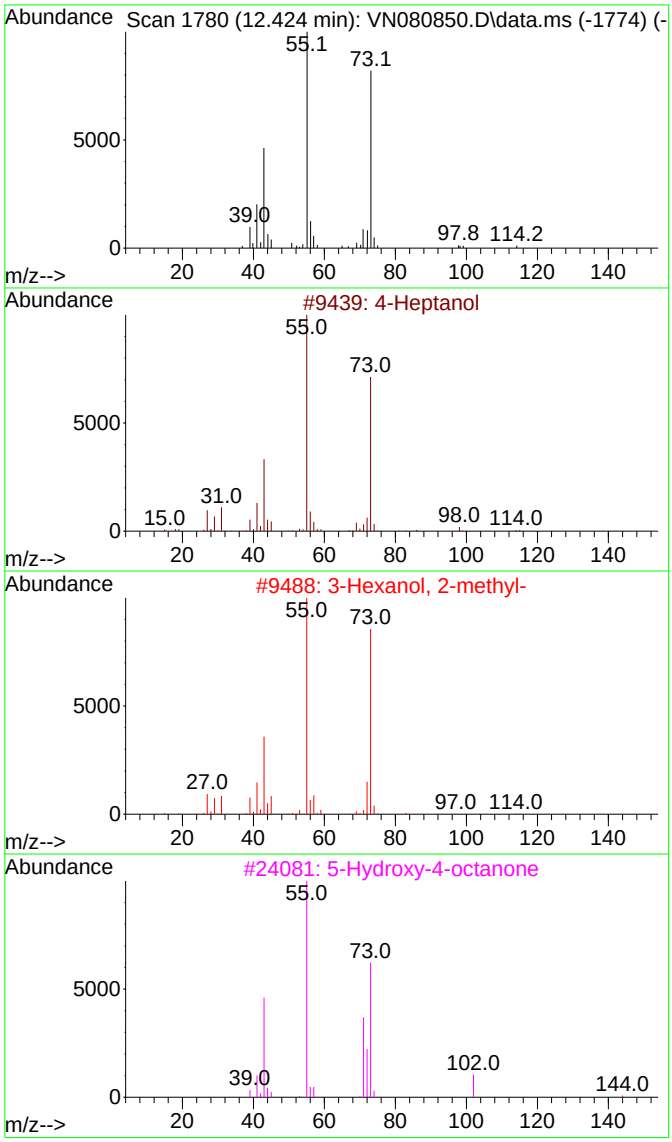
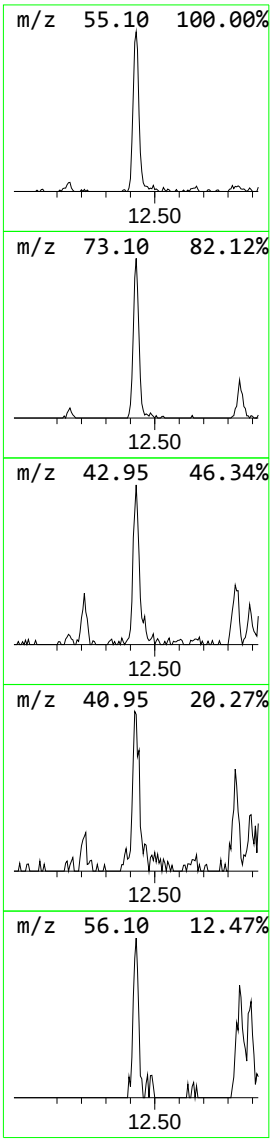
****

Peak Number 4 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.424	7.12 ug/l	106541	Chlorobenzene-d5	11.871

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	45
3	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	42
4	DL-4,5-Octanediol	146	C8H18O2	1000099-07-1	42
5	4,5-Octanediol	146	C8H18O2	022607-10-9	38





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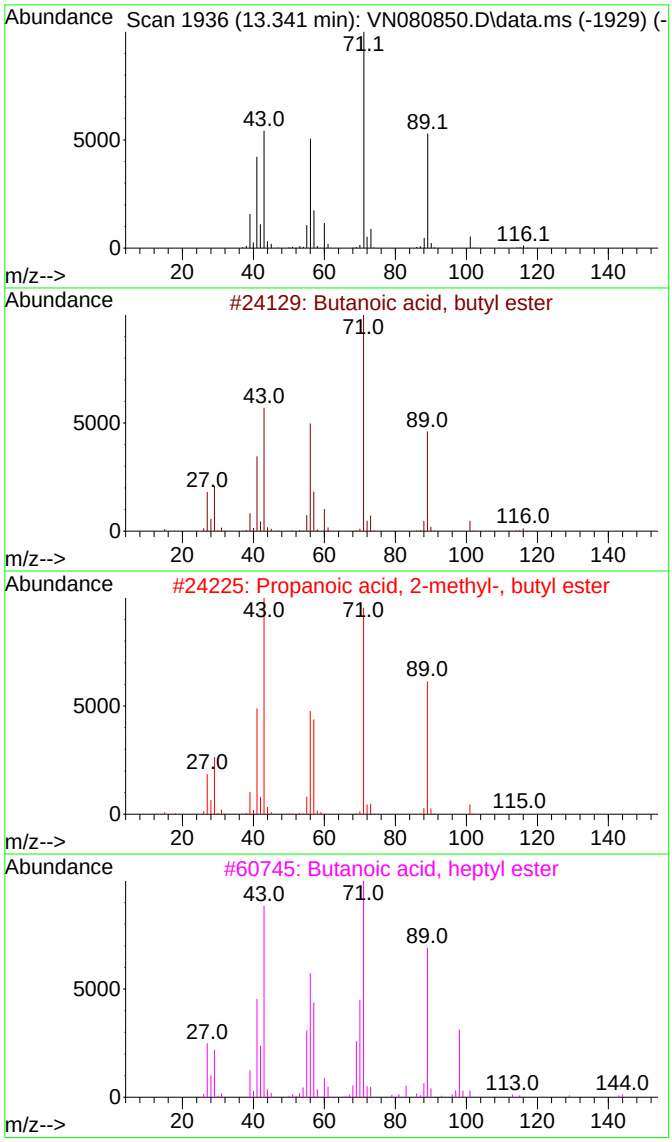
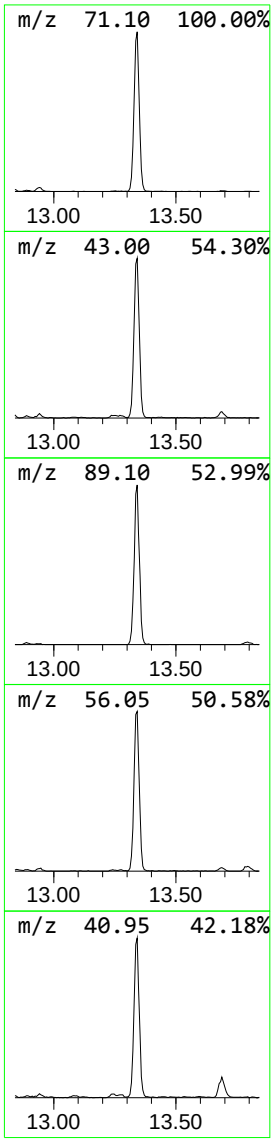
****
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	137.86 ug/l	1749640	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	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	78
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72





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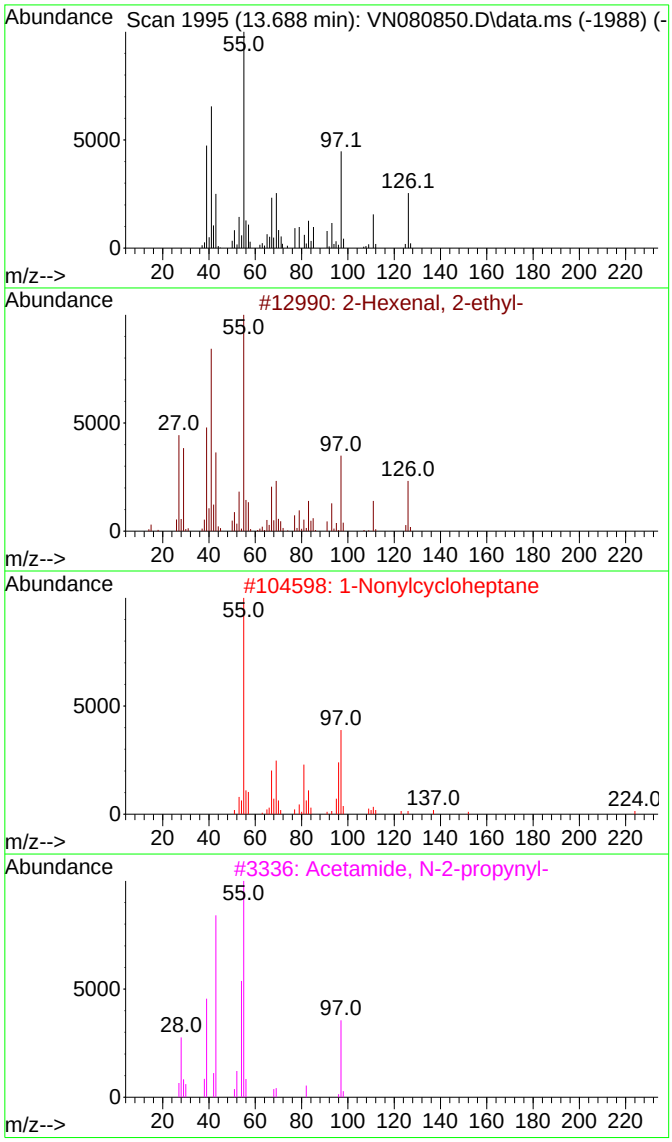
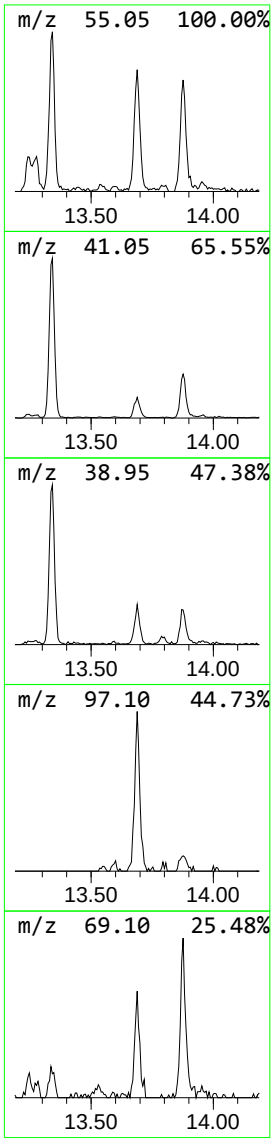
****
Peak Number 6 2-Hexenal, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	17.73 ug/l	225004	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	90
2	1-Nonylcycloheptane	224	C16H32	1000371-47-7	50
3	Acetamide, N-2-propynyl-	97	C5H7NO	065881-41-6	46
4	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	38
5	Cyclopropane, 1-bromo-2,2-diethyl-	176	C7H13Br	343926-55-6	35





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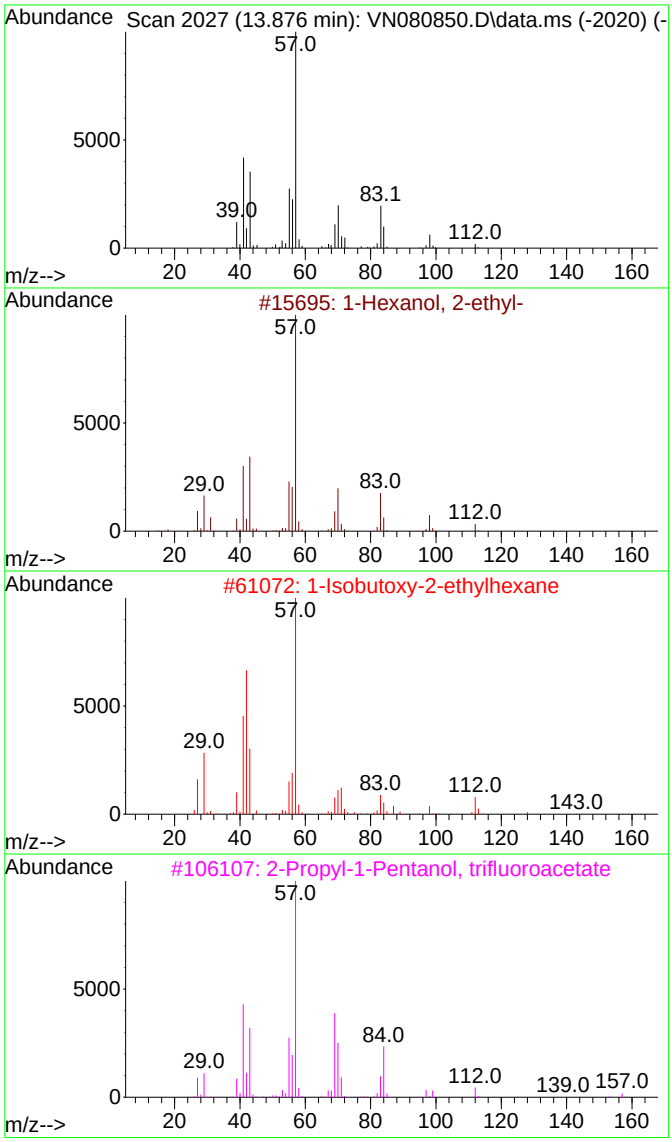
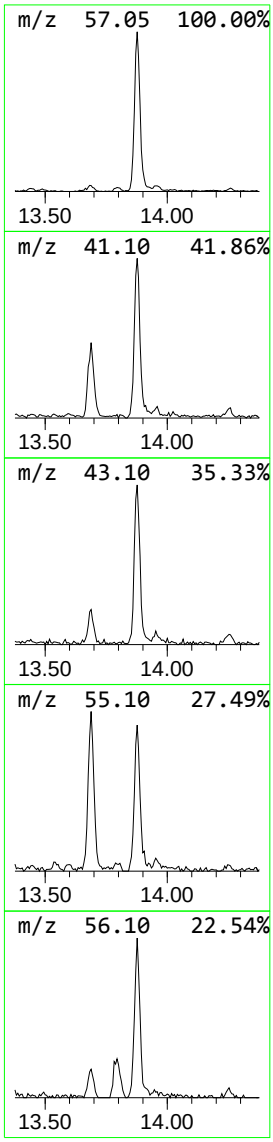
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	36.38 ug/l	461770	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-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	47
4	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	45
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43





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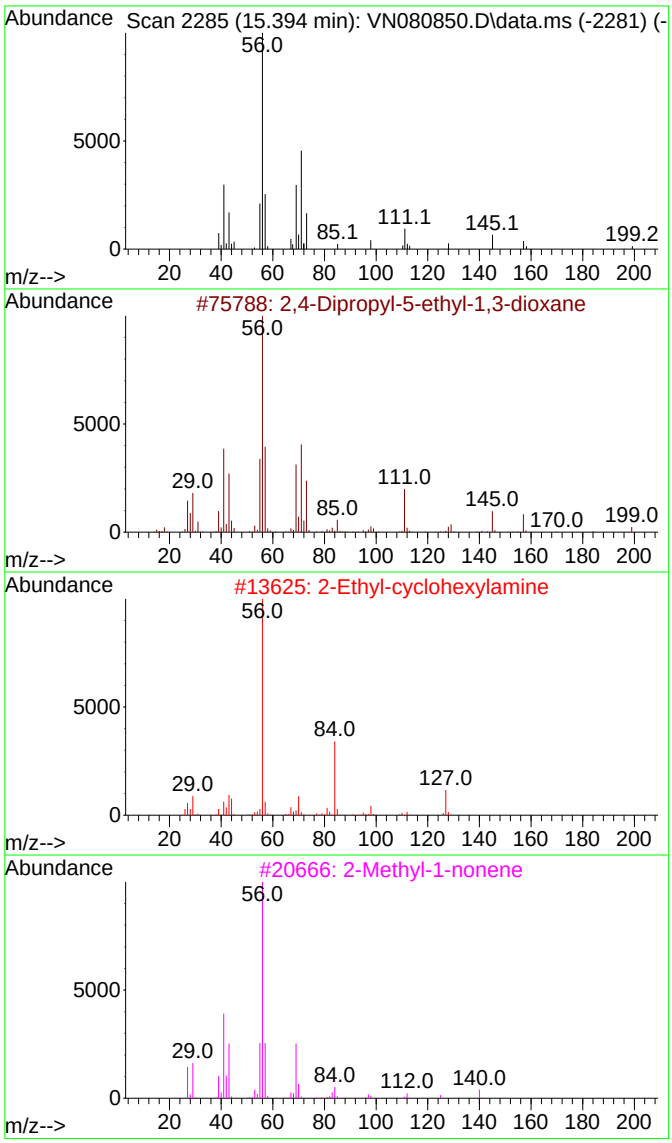
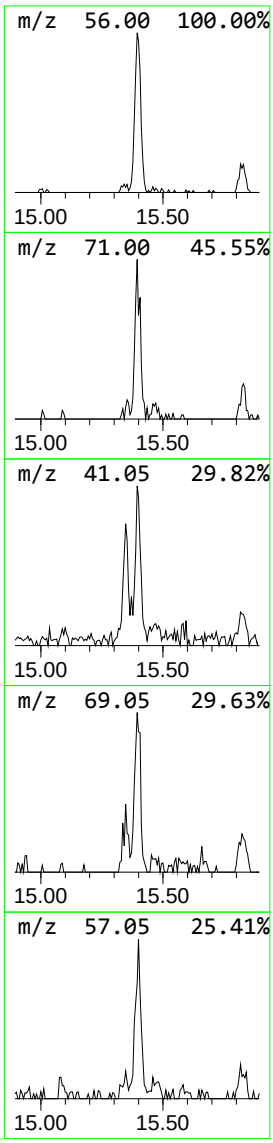
Peak Number 8 unknown15.394 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	7.48 ug/l	94883	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	39
2	2-Ethyl-cyclohexylamine	127	C8H17N	024216-90-8	32
3	2-Methyl-1-nonene	140	C10H20	002980-71-4	25
4	2-Propanone, 2-propenylhydrazone	112	C6H12N2	019031-79-9	25
5	2,3-Dimethylcyclohexylamine	127	C8H17N	042195-92-6	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080850.D
Acq On : 31 Jan 2024 19:07
Operator : JC\MD
Sample : P1284-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1249

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.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
Propane	2.077	9.2	ug/l	53059	1	8.224	288799	50.0
Butanal	7.218	15.3	ug/l	88432	1	8.224	288799	50.0
1-Butanol	9.265	9.9	ug/l	113962	2	9.100	576225	50.0
4-Heptanol	12.424	7.1	ug/l	106541	3	11.871	748028	50.0
Butanoic acid, ...	13.341	137.9	ug/l	1749640	4	13.794	634572	50.0
2-Hexenal, 2-et...	13.688	17.7	ug/l	225004	4	13.794	634572	50.0
1-Hexanol, 2-et...	13.876	36.4	ug/l	461770	4	13.794	634572	50.0
unknown15.394	15.394	7.5	ug/l	94883	4	13.794	634572	50.0