LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081468.D
Acq On : 19 Mar 2024 14:10
Operator : JC\MD
Sample : P1772-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1351

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081468.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	16	22	29	rBV	28647	45804	1.19%	0.206%
2	4.424	410	420	435	rBV2	15766	50492	1.31%	0.227%
3	7.224	885	896	906	rBV3	67208	193496	5.02%	0.868%
4	8.165	1046	1056	1061	rBV3	332195	827390	21.45%	3.713%
5	8.224	1061	1066	1080	rVB	636936	1393475	36.12%	6.254%
6	8.577	1111	1126	1140	rBV	361847	839393	21.76%	3.767%
7	9.100	1206	1215	1226	rBV	874690	1802383	46.72%	8.089%
8	9.265	1236	1243	1257	rBV3	60112	149772	3.88%	0.672%
9	10.565	1455	1464	1479	rBV	1313280	2456969	63.69%	11.027%
10	11.865	1672	1685	1696	rBV	1167090	2098457	54.40%	9.418%
11	12.424	1775	1780	1785	rVB	83085	128271	3.33%	0.576%
12	12.847	1842	1852	1863	rBV	899135	1601160	41.51%	7.186%
13	12.941	1863	1868	1875	rVB2	34018	54321	1.41%	0.244%
14	13.082	1886	1892	1896	rBV4	28758	53634	1.39%	0.241%
15	13.259	1913	1922	1929	rBV	2441464	3857746	100.00%	17.314%
16	13.335	1929	1935	1949	rVB	2015612	3032637	78.61%	13.611%
17	13.506	1957	1964	1974	rVB7	33582	79772	2.07%	0.358%
18	13.606	1974	1981	1987	rBV6	45605	79207	2.05%	0.355%
19	13.688	1987	1995	2001	rBV2	262801	492185	12.76%	2.209%
20	13.794	2006	2013	2020	rVV	1100909	1859995	48.21%	8.348%
21	13.876	2020	2027	2035	rVV	463785	793834	20.58%	3.563%
22	13.953	2035	2040	2046	rVB6	36100	69052	1.79%	0.310%
23	14.253	2082	2091	2096	rBV5	26807	50197	1.30%	0.225%
24	14.612	2145	2152	2157	rBV6	22926	39951	1.04%	0.179%
25	15.347	2270	2277	2281	rBV4	57988	105985	2.75%	0.476%
26	15.394	2281	2285	2291	rVB2	76326	125800	3.26%	0.565%

Sum of corrected areas: 22281378

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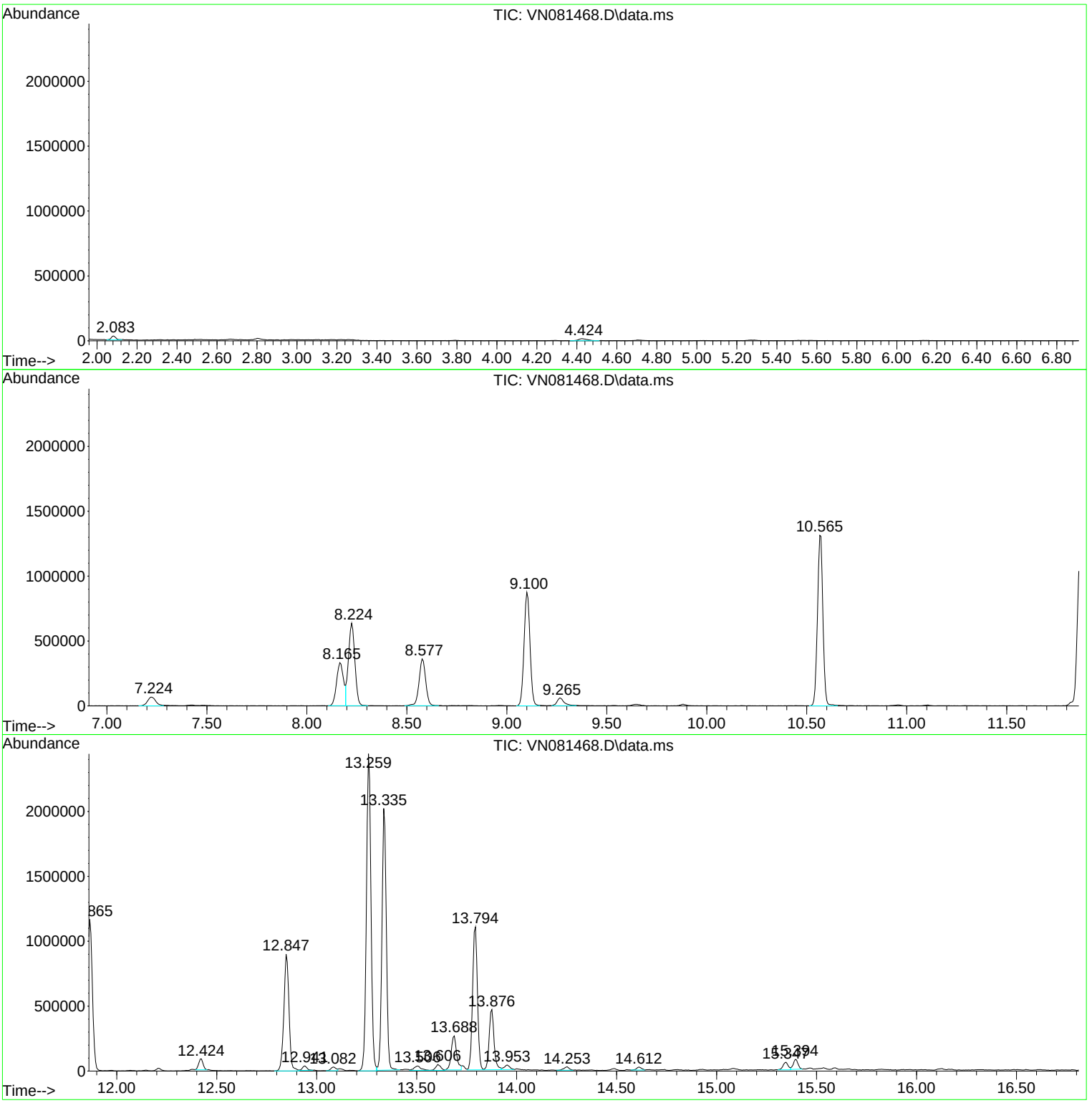
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



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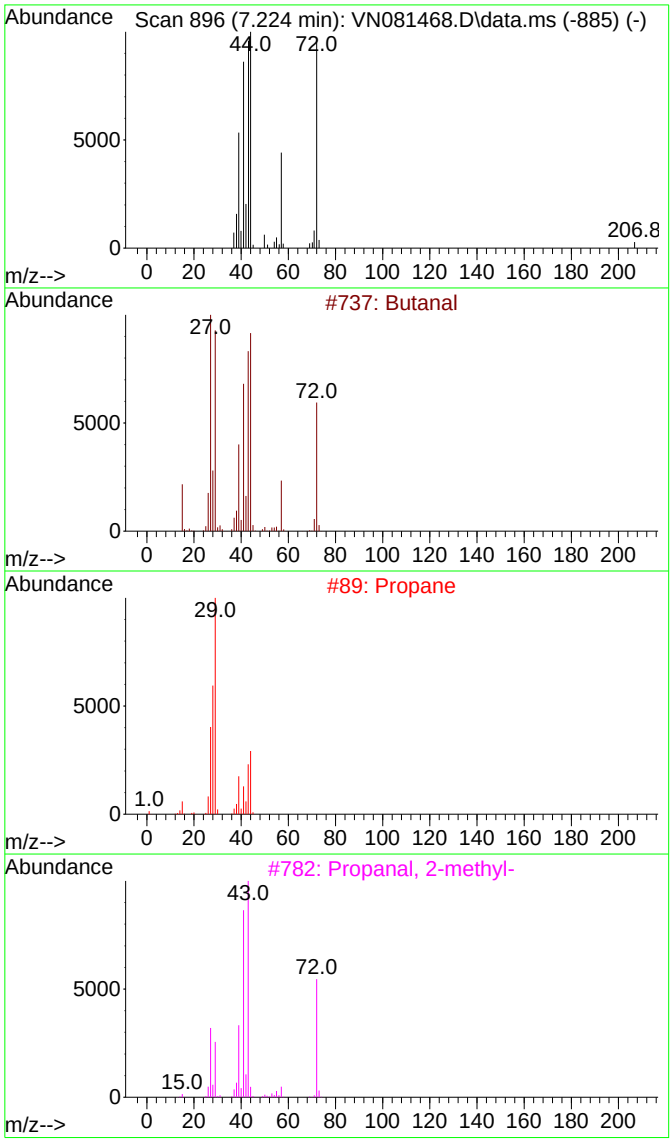
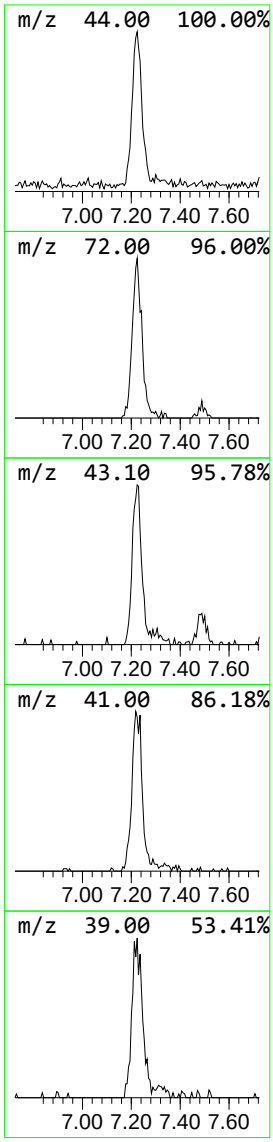
Peak Number 1 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	6.94 ug/l	193496	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	1-Butanamine, N-(1-methylethyl)-	115	C7H17N	039099-23-5	39
5	1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	38





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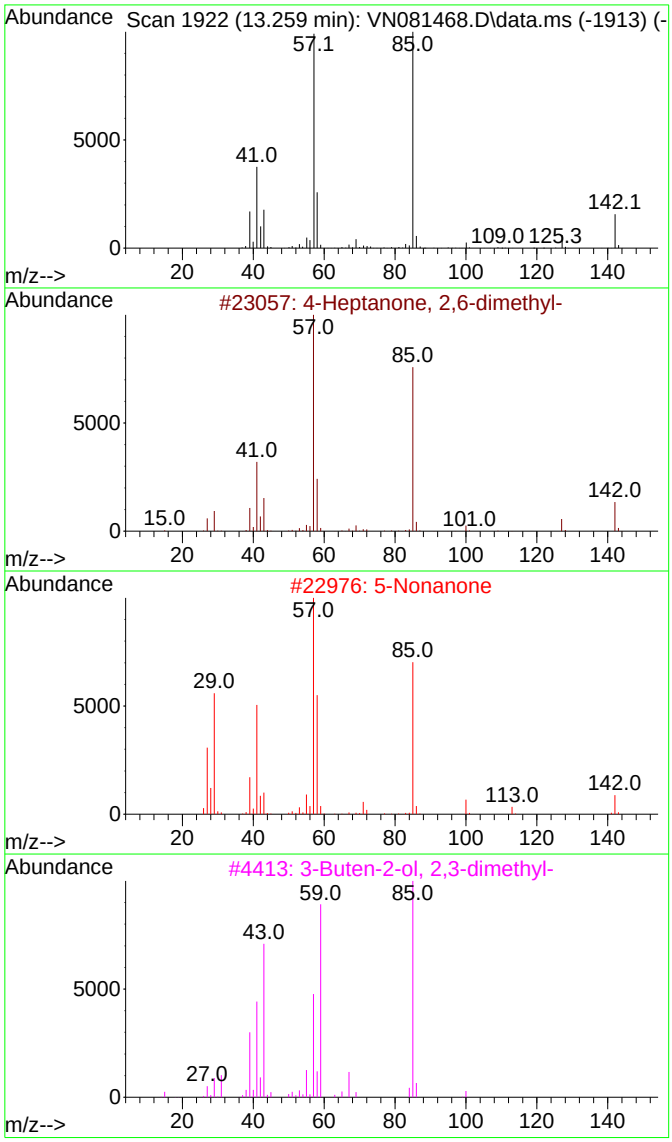
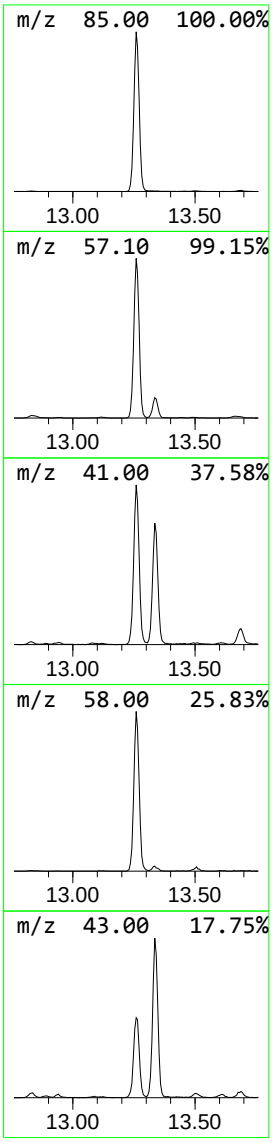
****
Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	103.70 ug/l	3857750	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	50
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47





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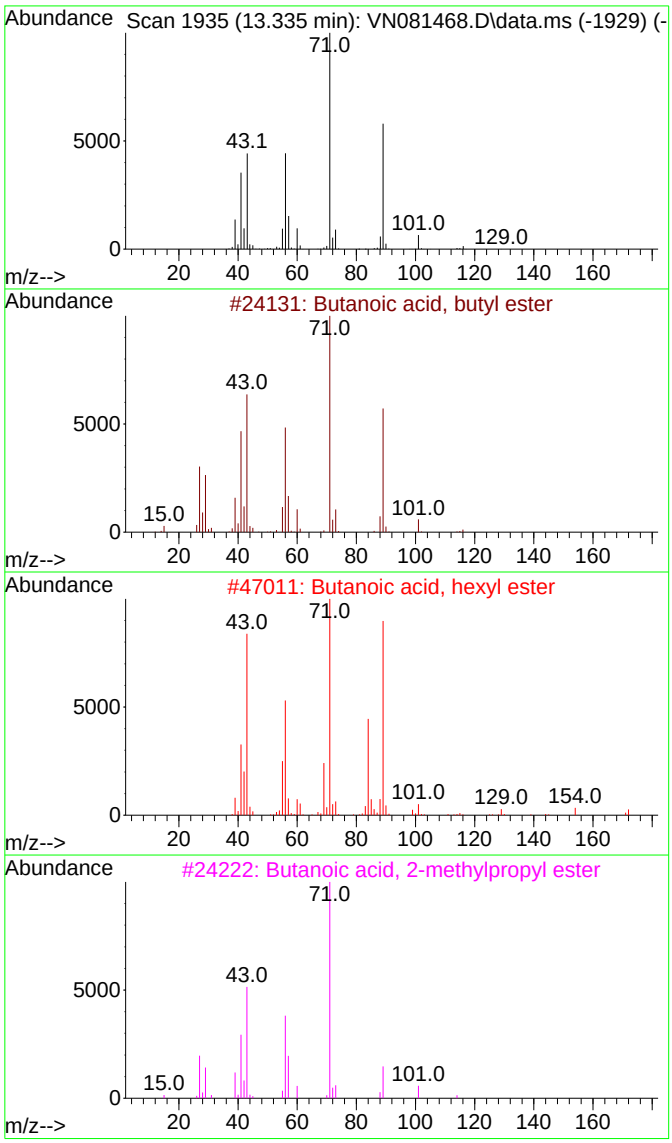
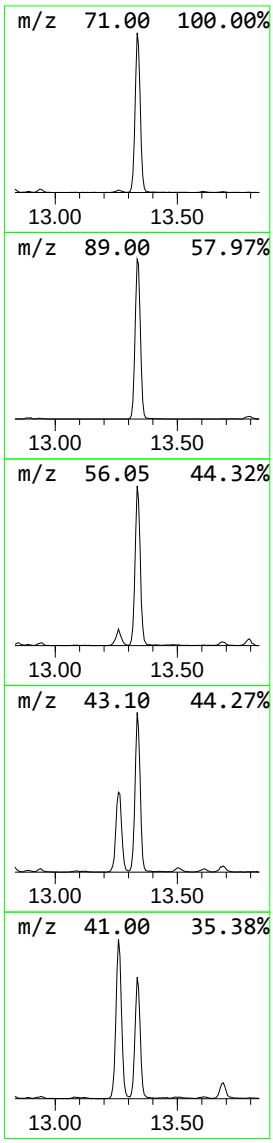
****
Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	81.52 ug/l	3032640	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, hexyl ester	172	C10H20O2	002639-63-6	74
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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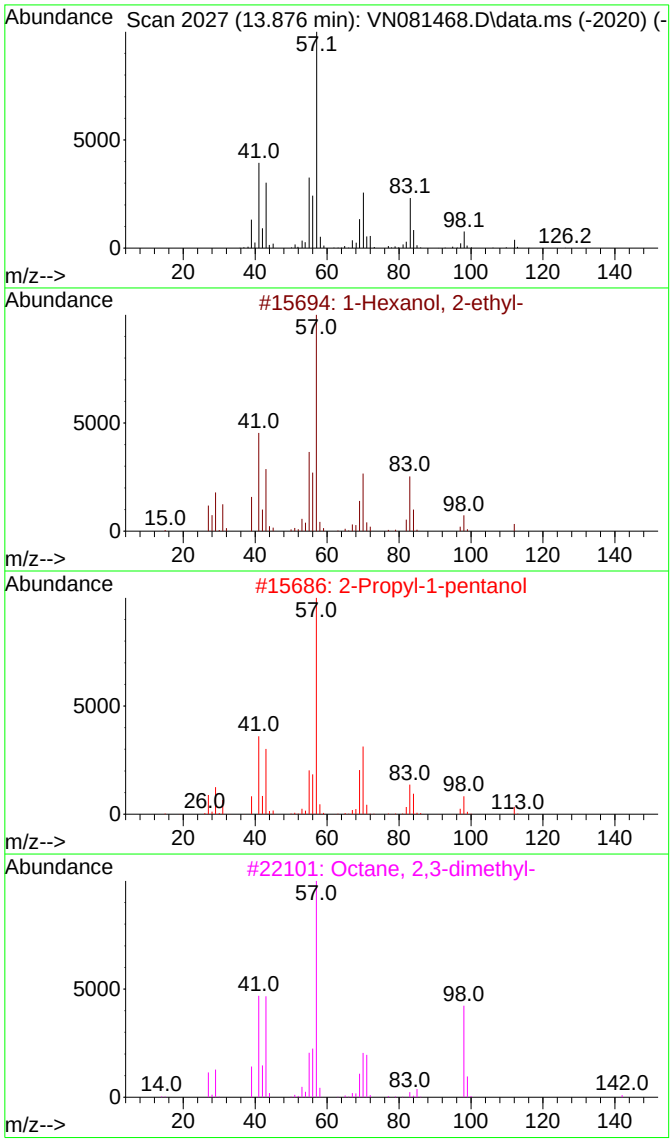
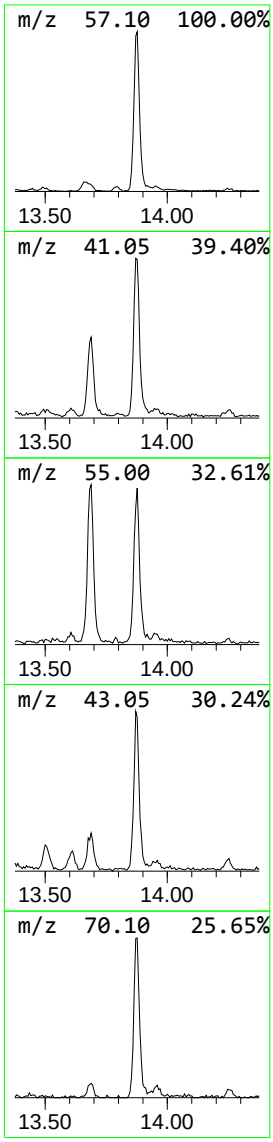
****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	21.34 ug/l	793834	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-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	7.224	6.9	ug/l	193496	1	8.224	1393480	50.0
4-Heptanone, 2,...	13.259	103.7	ug/l	3857750	4	13.794	1860000	50.0
Butanoic acid, ...	13.335	81.5	ug/l	3032640	4	13.794	1860000	50.0
1-Hexanol, 2-et...	13.876	21.3	ug/l	793834	4	13.794	1860000	50.0