LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081470.D
Acq On : 19 Mar 2024 14:58
Operator : JC\MD
Sample : P1772-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1349

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: VN081470.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	17	22	32	rVB2	36651	59970	1.76%	0.318%
2	2.807	139	145	152	rVB2	29993	67606	1.99%	0.359%
3	4.424	412	420	429	rBV	19317	54907	1.61%	0.291%
4	7.224	885	896	908	rBV4	77961	220274	6.48%	1.169%
5	8.165	1046	1056	1061	rBV2	341093	829747	24.40%	4.403%
6	8.224	1061	1066	1078	rVB2	645051	1388193	40.82%	7.367%
7	8.577	1118	1126	1141	rVB	355572	819836	24.11%	4.351%
8	9.101	1205	1215	1229	rBV	891878	1813197	53.32%	9.622%
9	9.265	1236	1243	1254	rBV	45674	97801	2.88%	0.519%
10	10.565	1455	1464	1474	rBV	1334296	2439994	71.75%	12.949%
11	11.865	1672	1685	1695	rBV	1157946	2100445	61.76%	11.147%
12	12.212	1738	1744	1750	rBV3	30356	55430	1.63%	0.294%
13	12.424	1774	1780	1784	rBV2	82883	127044	3.74%	0.674%
14	12.847	1843	1852	1864	rBV	899484	1630158	47.93%	8.651%
15	13.259	1913	1922	1930	rBV	2190069	3400878	100.00%	18.048%
16	13.336	1930	1935	1943	rVB	484916	748286	22.00%	3.971%
17	13.506	1956	1964	1975	rVB2	86596	172882	5.08%	0.917%
18	13.612	1975	1982	1987	rBV4	51614	95979	2.82%	0.509%
19	13.794	2006	2013	2020	rVV	1071377	1816444	53.41%	9.640%
20	13.877	2020	2027	2035	rVV	393228	694253	20.41%	3.684%
21	13.953	2035	2040	2049	rVB8	25339	53217	1.56%	0.282%
22	14.241	2083	2089	2095	rBV7	15732	34094	1.00%	0.181%
23	15.400	2279	2286	2293	rBV2	68688	123084	3.62%	0.653%

Sum of corrected areas: 18843719

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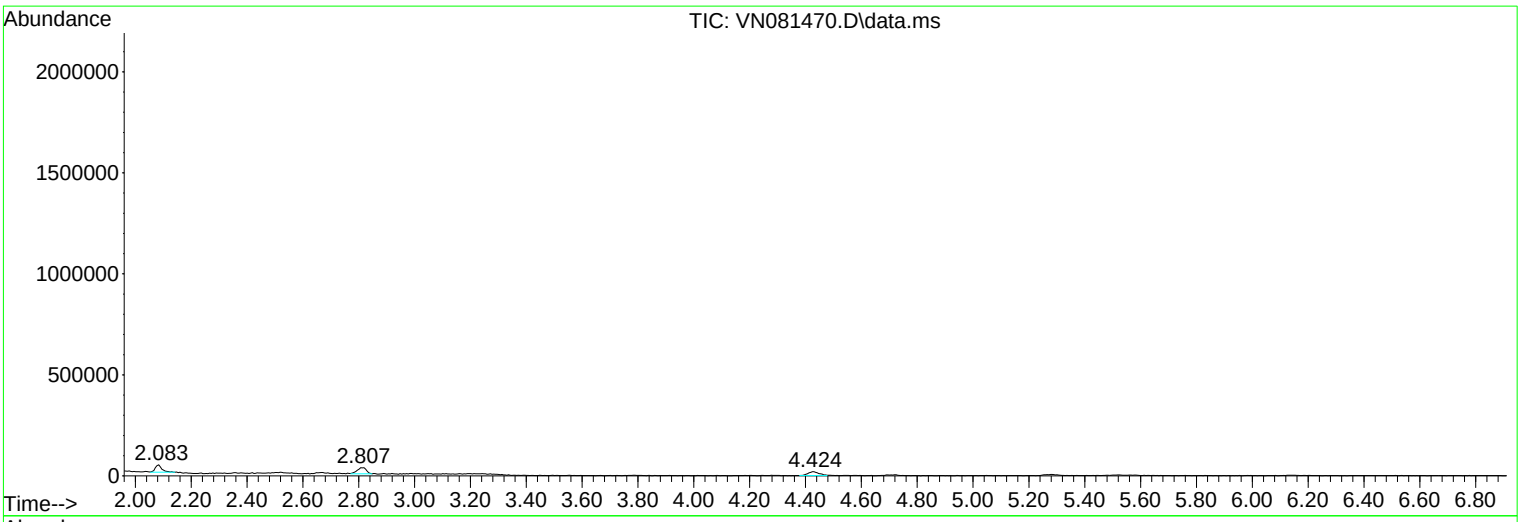
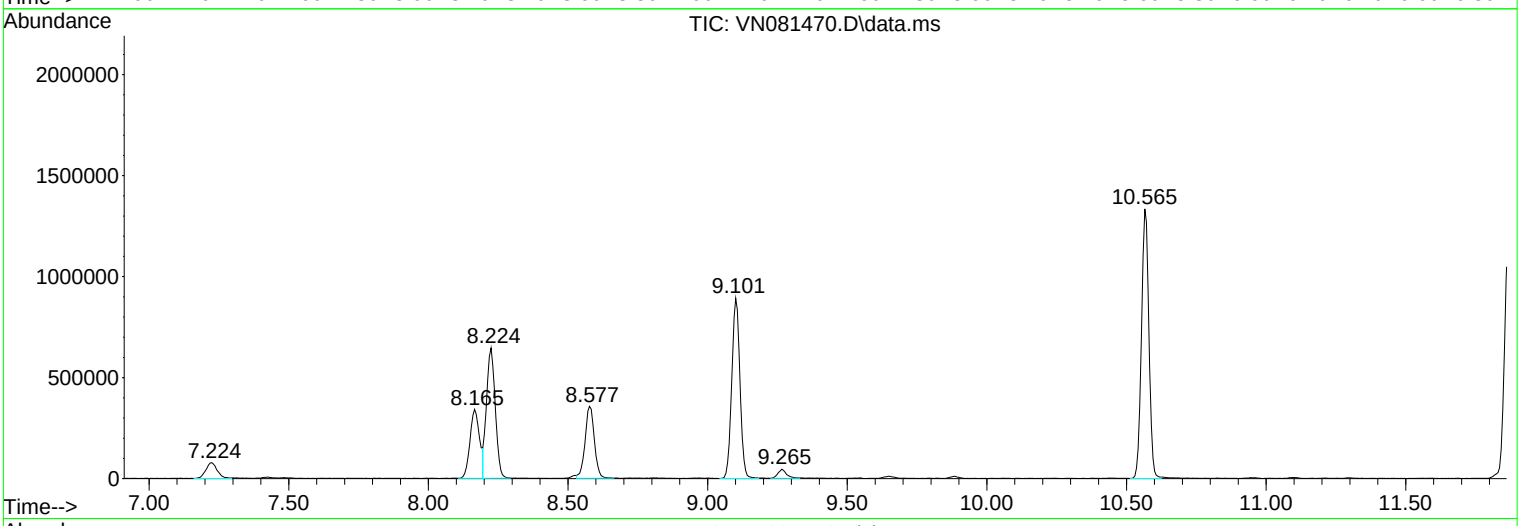
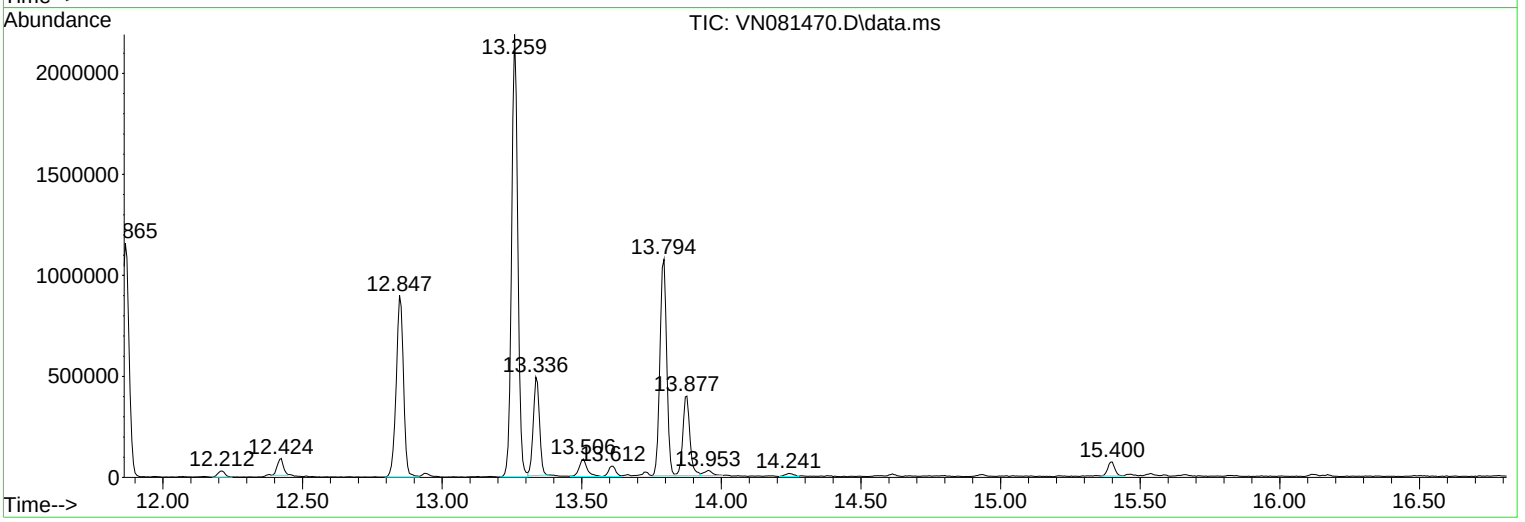
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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







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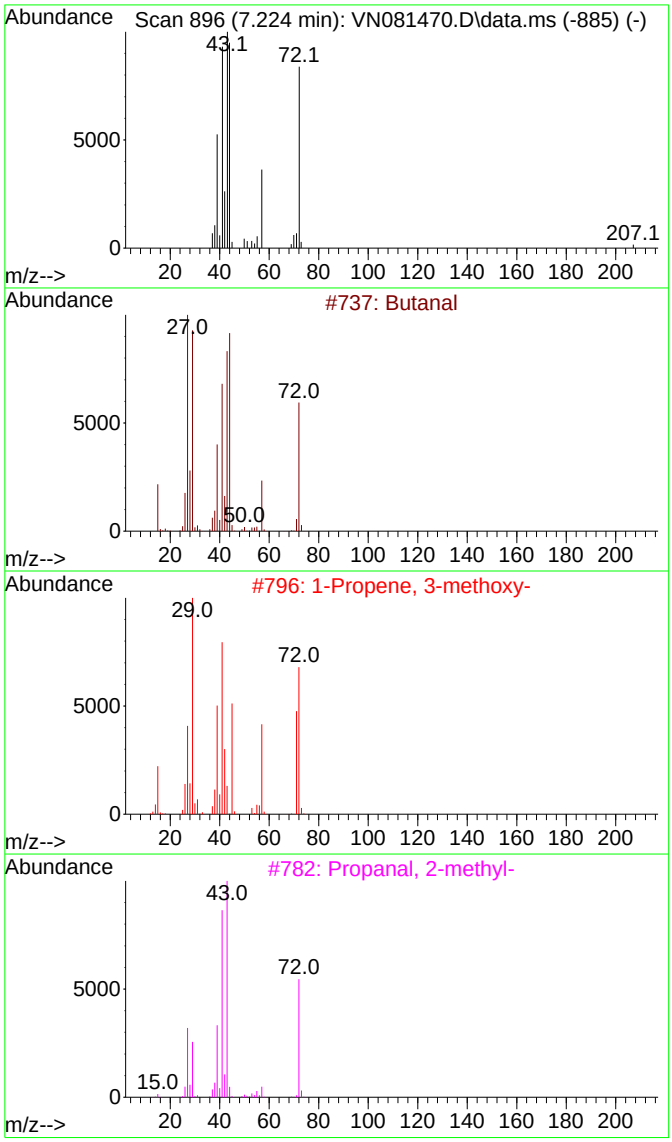
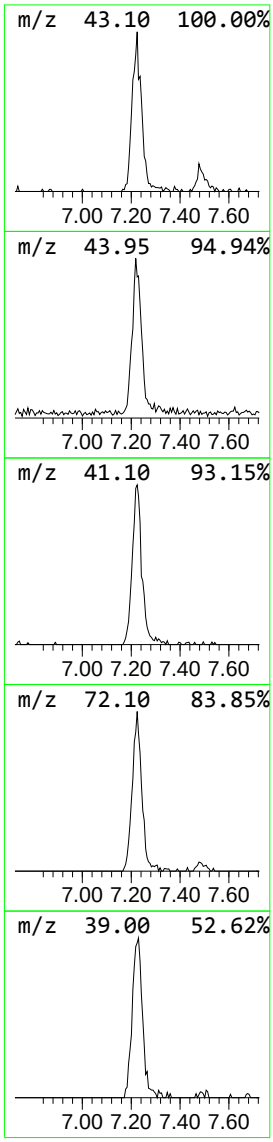
****

Peak Number 1 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	7.93 ug/l	220274	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	49
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	37
5	Furazan-3,4-diol	102	C2H2N2O3	143876-06-6	33





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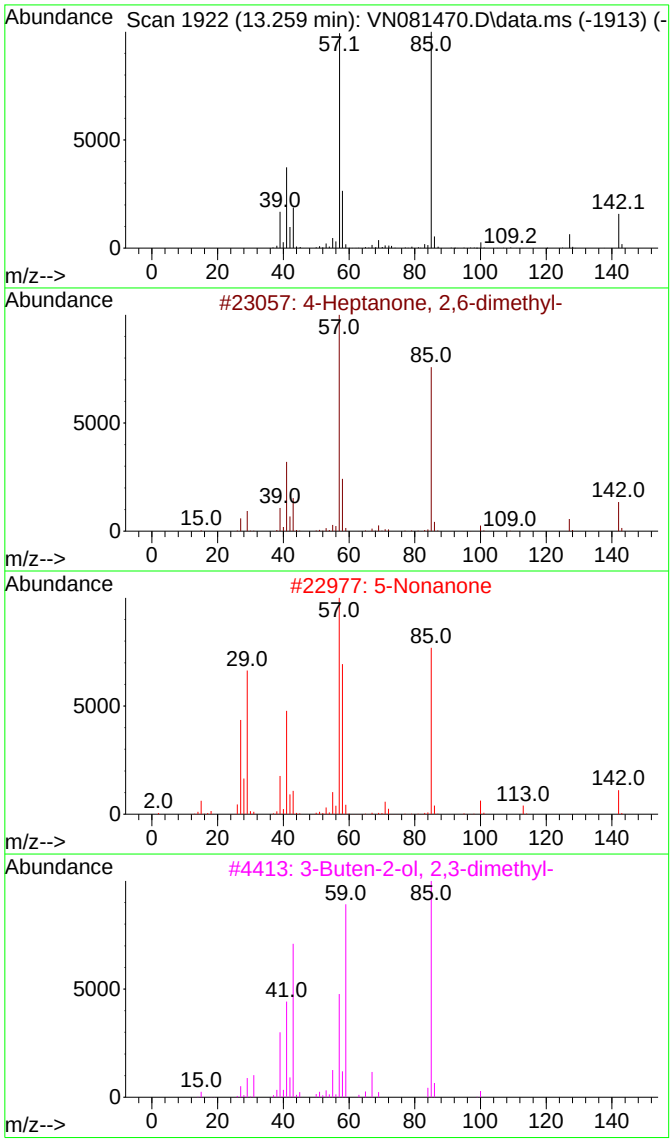
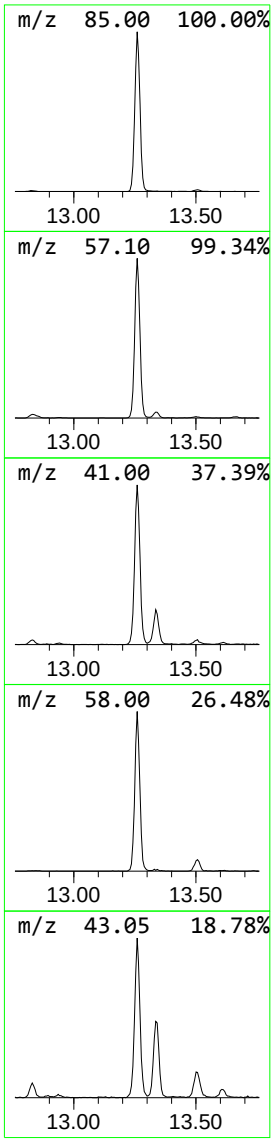
****
Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	93.61 ug/l	3400880	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	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47





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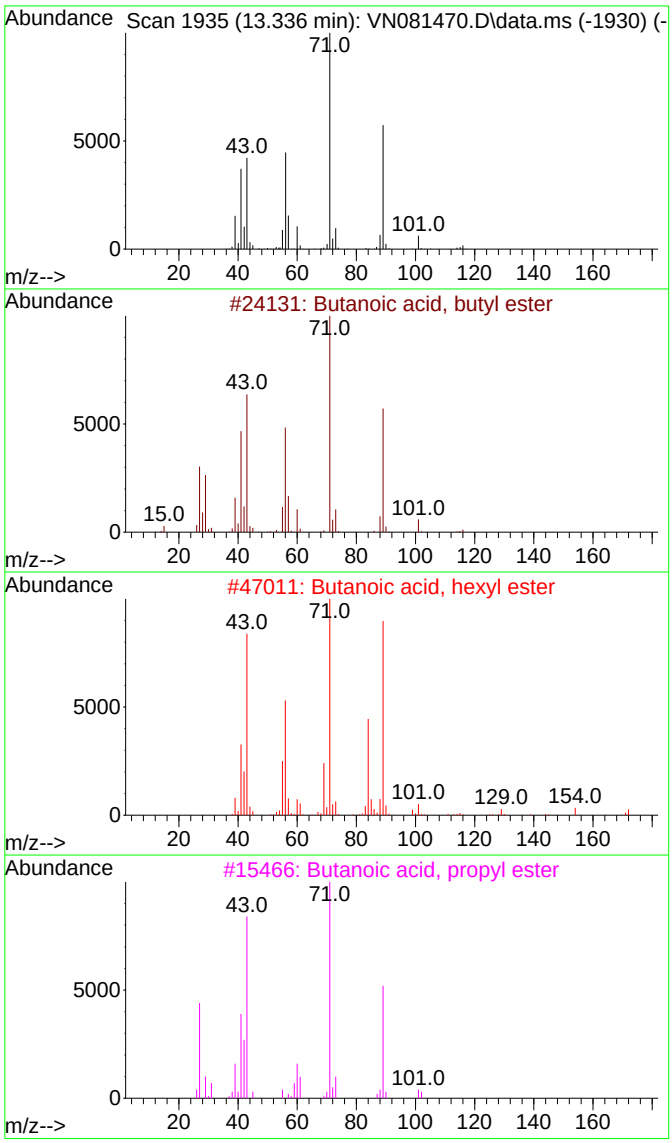
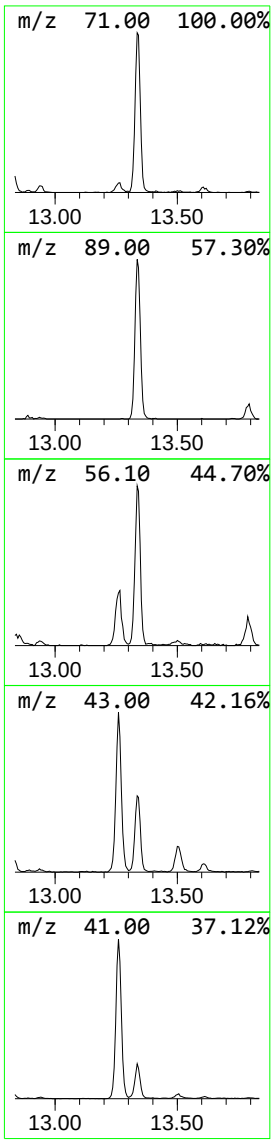
****
Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.336	20.60 ug/l	748286	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, propyl ester	130	C7H14O2	000105-66-8	59
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59





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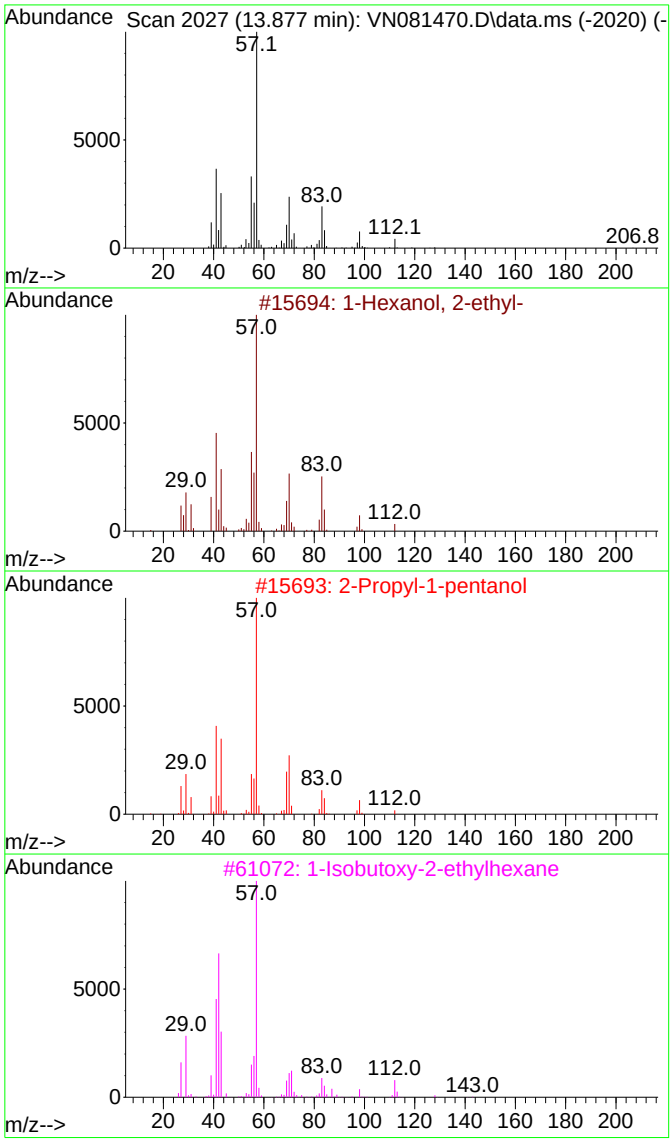
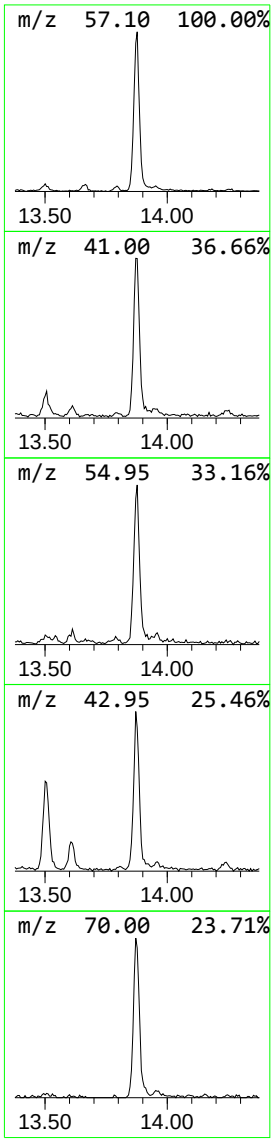
****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.877	19.11 ug/l	694253	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	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	7.224	7.9	ug/l	220274	1	8.224	1388190	50.0
4-Heptanone, 2,...	13.259	93.6	ug/l	3400880	4	13.794	1816440	50.0
Butanoic acid, ...	13.336	20.6	ug/l	748286	4	13.794	1816440	50.0
1-Hexanol, 2-et...	13.877	19.1	ug/l	694253	4	13.794	1816440	50.0