LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075832.D
Acq On : 15 Dec 2022 20:59
Operator : JC\MD
Sample : N6066-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-597

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\82N121422W.M
Title : SW846 8260

Signal : TIC: VN075832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.495	70	75	82	rBV2	21527	37107	1.42%	0.191%
2	2.677	99	106	117	rBV	142479	252545	9.66%	1.299%
3	2.830	125	132	140	rVB5	17392	42197	1.61%	0.217%
4	3.806	286	298	315	rBV	457260	1219252	46.63%	6.270%
5	4.306	375	383	396	rVB	16302	43378	1.66%	0.223%
6	4.448	396	407	419	rBV	51639	156174	5.97%	0.803%
7	4.730	443	455	468	rBV3	9058	30761	1.18%	0.158%
8	5.536	579	592	605	rBV2	33462	118502	4.53%	0.609%
9	6.153	686	697	710	rVB3	23052	72574	2.78%	0.373%
10	6.736	782	796	808	rBV3	26986	86111	3.29%	0.443%
11	7.236	866	881	893	rBV	524891	1443445	55.20%	7.423%
12	7.494	914	925	934	rBV	160308	421287	16.11%	2.166%
13	8.171	1030	1040	1045	rBV	236345	576016	22.03%	2.962%
14	8.230	1045	1050	1064	rVB	469838	1047097	40.04%	5.385%
15	8.536	1093	1102	1104	rBV2	42202	82103	3.14%	0.422%
16	8.588	1104	1111	1130	rVB2	253606	714025	27.31%	3.672%
17	8.824	1143	1151	1159	rVB2	13143	26534	1.01%	0.136%
18	8.983	1171	1178	1185	rBV5	12991	30857	1.18%	0.159%
19	9.106	1190	1199	1209	rBV	620778	1252012	47.88%	6.438%
20	9.271	1219	1227	1238	rBV	226406	454551	17.38%	2.338%
21	9.659	1286	1293	1302	rVB2	66877	141907	5.43%	0.730%
22	10.571	1439	1448	1454	rBV	972692	1801194	68.88%	9.263%
23	10.630	1454	1458	1469	rVB	108993	206910	7.91%	1.064%
24	10.959	1506	1514	1525	rBV2	88844	170743	6.53%	0.878%
25	11.300	1565	1572	1576	rBV2	22337	38558	1.47%	0.198%
26	11.353	1576	1581	1587	rVB3	14432	26605	1.02%	0.137%
27	11.865	1655	1668	1680	rBV	810014	1552853	59.39%	7.986%
28	11.976	1680	1687	1697	rVV5	25527	77300	2.96%	0.398%
29	12.071	1697	1703	1712	rVB	71539	143209	5.48%	0.736%
30	12.212	1722	1727	1737	rVB	38540	71436	2.73%	0.367%
31	12.412	1747	1761	1767	rBV5	133346	340625	13.03%	1.752%
32	12.459	1767	1769	1779	rVB	27704	43572	1.67%	0.224%
33	12.853	1827	1836	1844	rBV	660594	1172494	44.84%	6.030%
34	12.935	1847	1850	1857	rVB6	12284	27730	1.06%	0.143%
35	13.123	1872	1882	1887	rBV3	32877	83073	3.18%	0.427%
36	13.247	1897	1903	1905	rBV	32242	51222	1.96%	0.263%

LSC Area Percent Report

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ORA-597

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

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Title : SW846 8260

37	13.341	1914	1919	1931	rVB	159305	253369	9.69%	1.303%
38	13.488	1939	1944	1947	rVV3	46177	82502	3.16%	0.424%
39	13.535	1947	1952	1959	rVB7	60888	126610	4.84%	0.651%
40	13.694	1973	1979	1987	rVB2	52894	96855	3.70%	0.498%
41	13.794	1989	1996	2004	rBV	841366	1429418	54.67%	7.351%
42	13.876	2004	2010	2019	rBV	1662344	2614807	100.00%	13.447%
43	13.959	2019	2024	2034	rVB7	59887	111319	4.26%	0.572%
44	14.176	2052	2061	2067	rVB8	24950	56820	2.17%	0.292%
45	14.253	2068	2074	2078	rBV4	40596	77904	2.98%	0.401%
46	14.465	2107	2110	2117	rVB5	18589	33737	1.29%	0.173%
47	14.541	2117	2123	2131	rBV3	17478	40773	1.56%	0.210%
48	14.618	2131	2136	2145	rVV7	15956	40603	1.55%	0.209%
49	14.794	2161	2166	2176	rVB9	18168	53088	2.03%	0.273%
50	15.347	2252	2260	2266	rVB7	14627	39308	1.50%	0.202%
51	15.465	2275	2280	2287	rBV3	41302	87594	3.35%	0.450%
52	15.588	2296	2301	2305	rBV3	20735	39818	1.52%	0.205%
53	15.647	2305	2311	2322	rVB	81598	205283	7.85%	1.056%

Sum of corrected areas: 19445767

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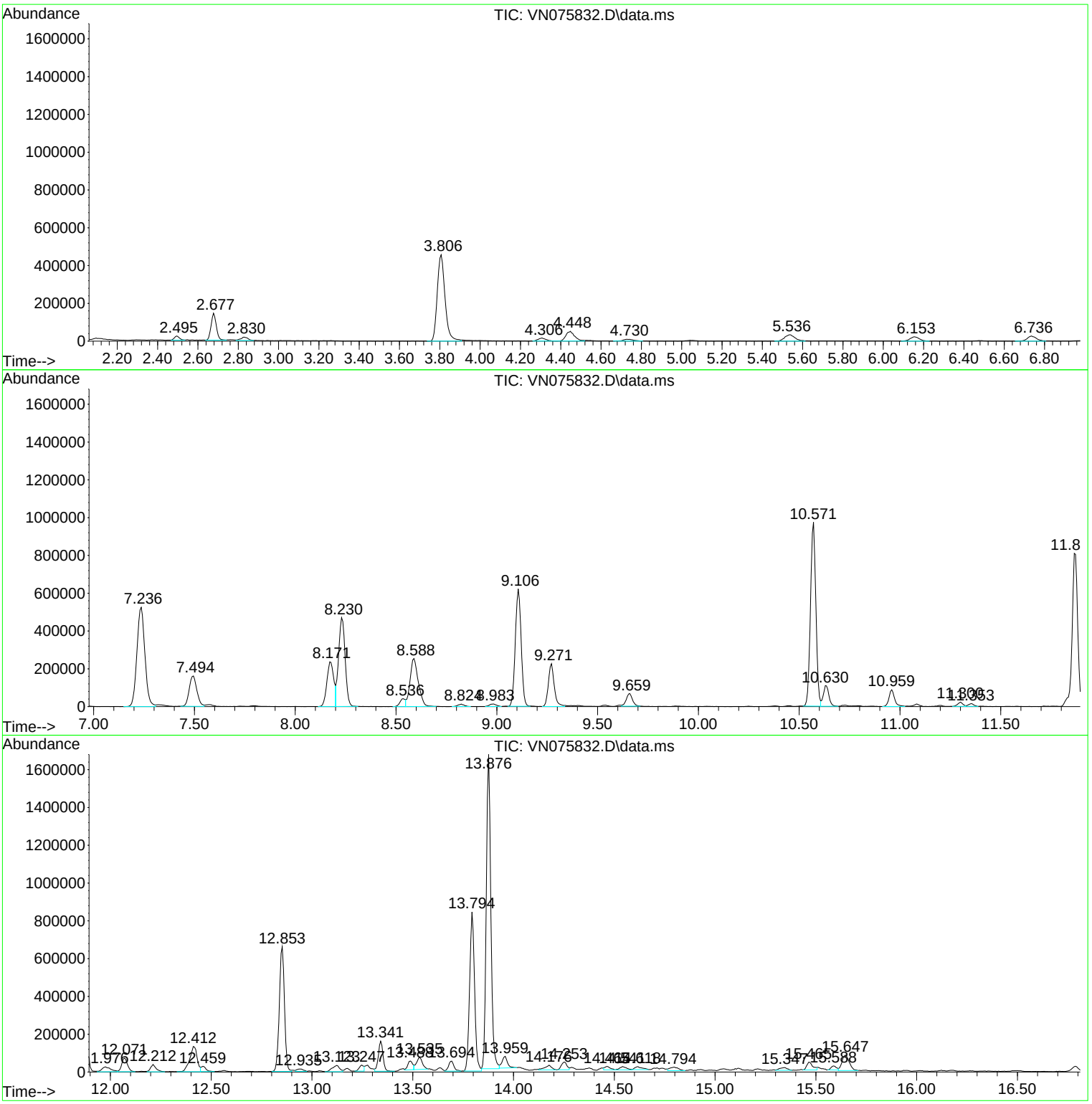
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

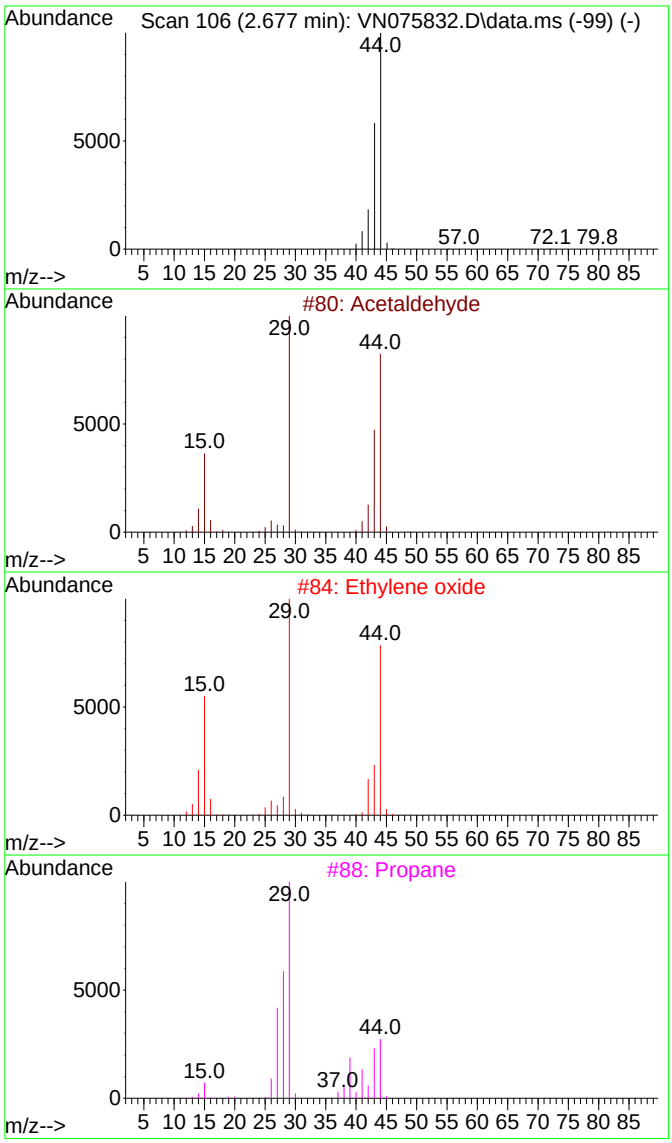
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

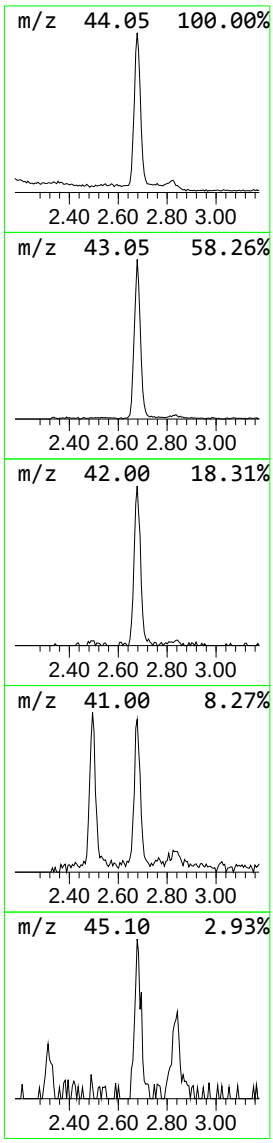
****

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.677	12.06 ug/l	252545	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Ethylene oxide	44	C2H4O	000075-21-8	9
3	Propane	44	C3H8	000074-98-6	5
4	Cyclobutanol	72	C4H8O	002919-23-5	4
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





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ClientSampleId :
ORA-597

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

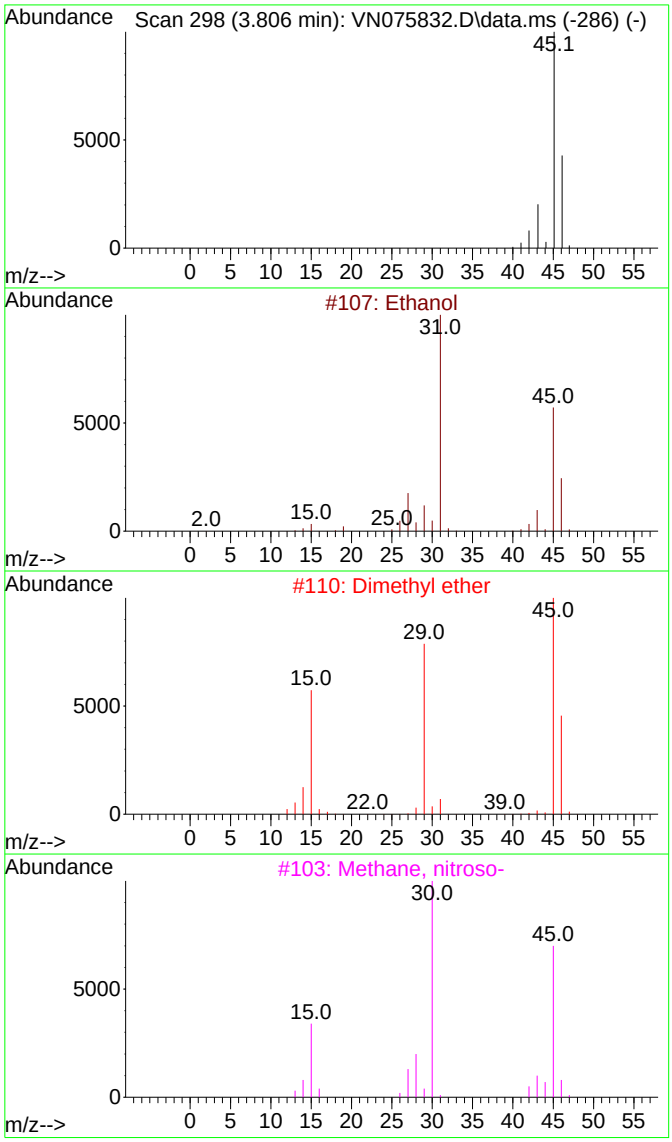
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

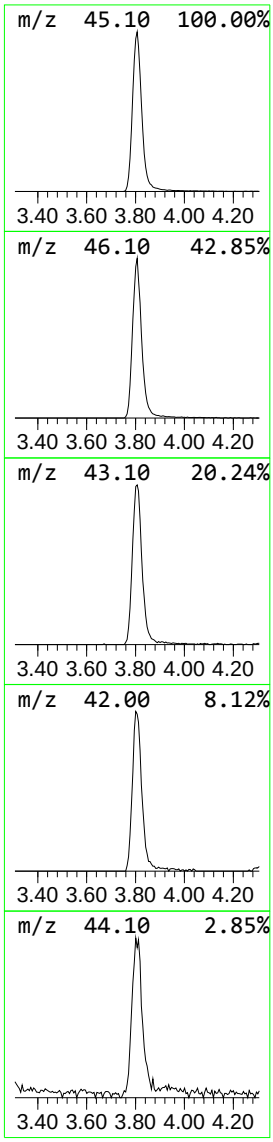
****

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.806	58.22 ug/l	1219250	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-597

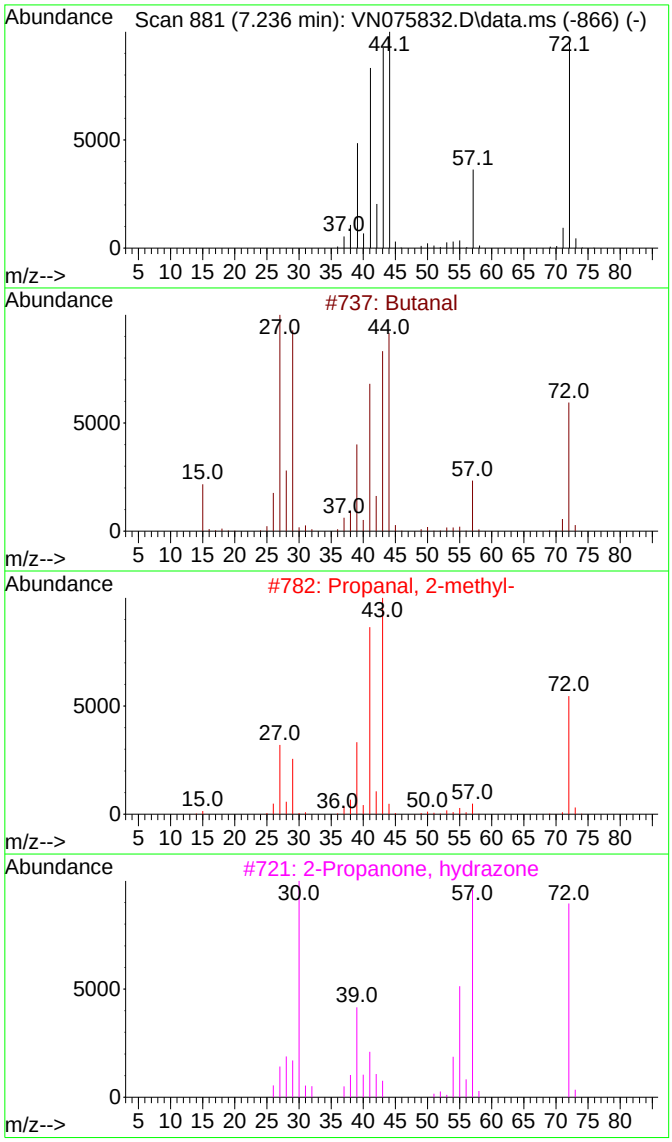
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

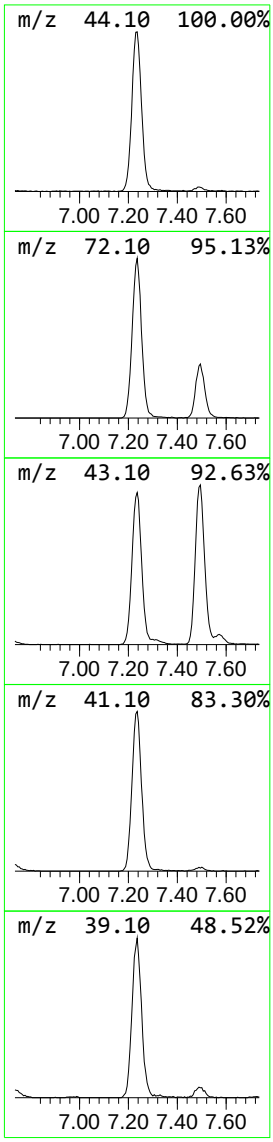
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.236	68.93 ug/l	1443450	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Instrument :
MSVOA_N
ClientSampleId :
ORA-597

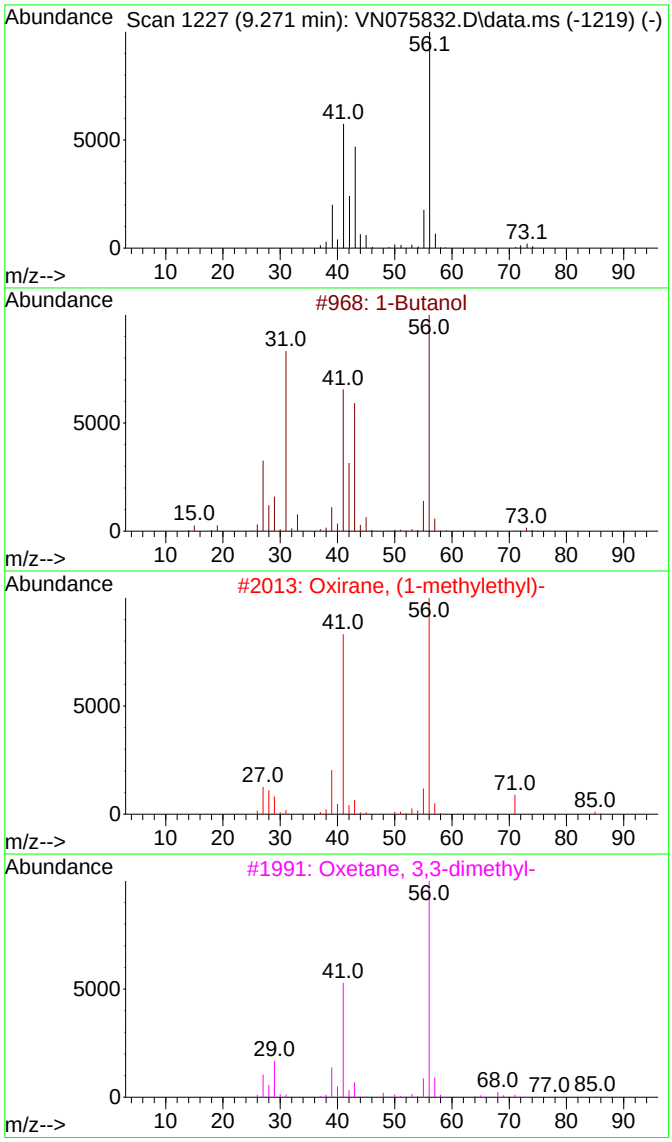
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

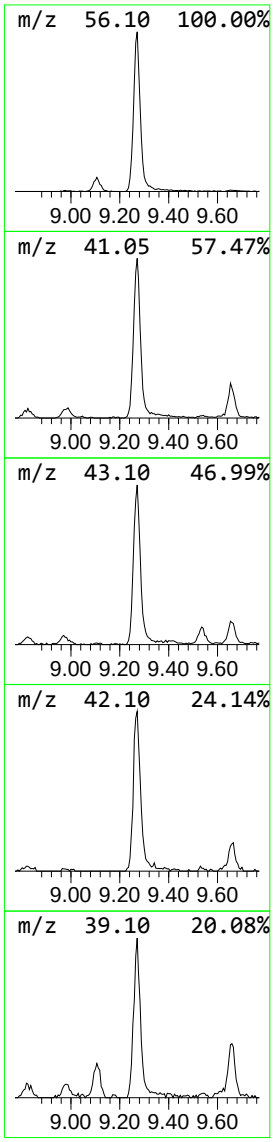
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	18.15 ug/l	454551	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	33
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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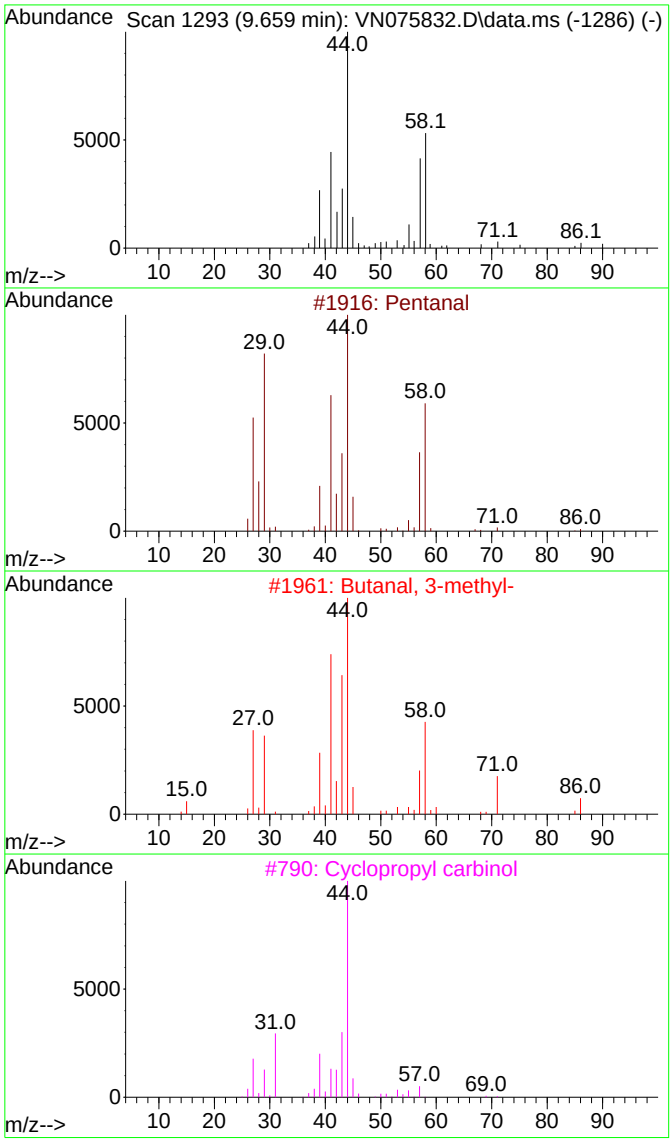
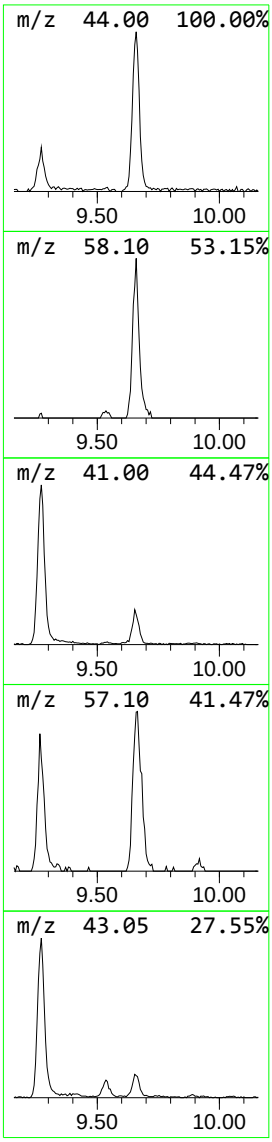
****
Peak Number 5 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.659	5.67 ug/l	141907	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	78
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	78
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	40
4	2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5	Alanylglycine, TMS	218	C8H18N2O3Si	1000475-96-7	23





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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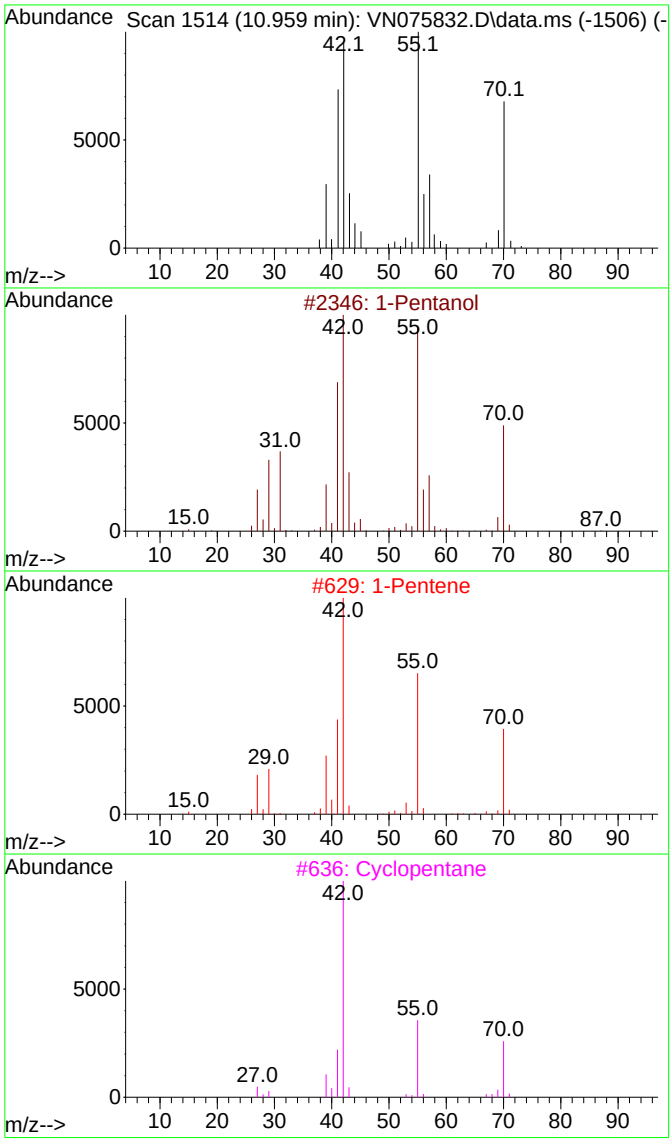
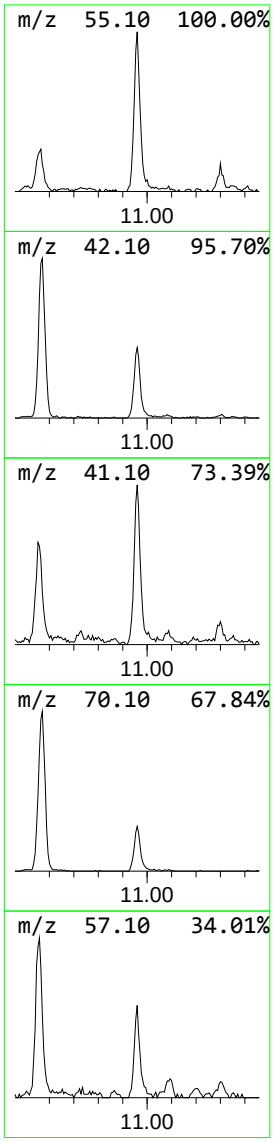
Peak Number 6 1-Pentanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.959	5.50 ug/l	170743	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	86
2	1-Pentene	70	C5H10	000109-67-1	64
3	Cyclopentane	70	C5H10	000287-92-3	52
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
5	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	45





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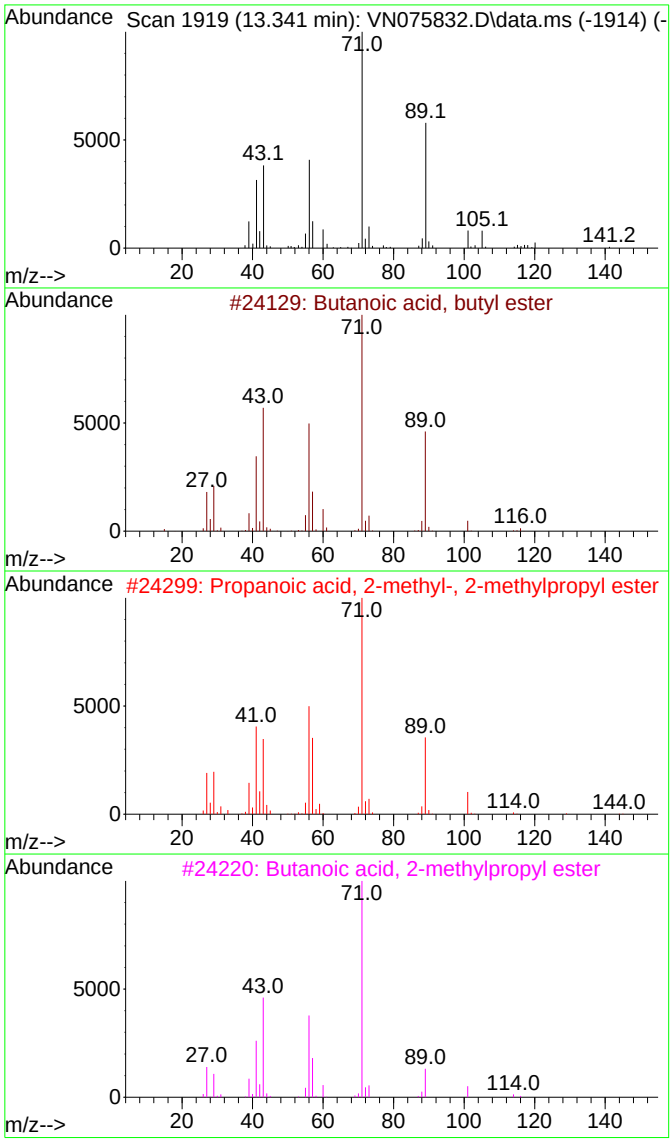
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

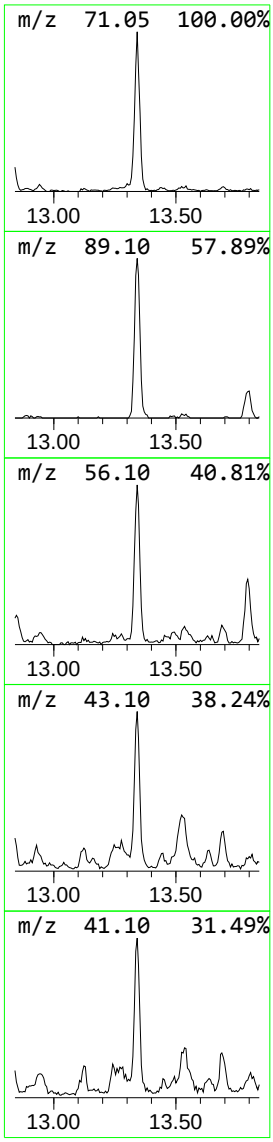
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	8.86 ug/l	253369	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	72
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	45
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	42
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	42





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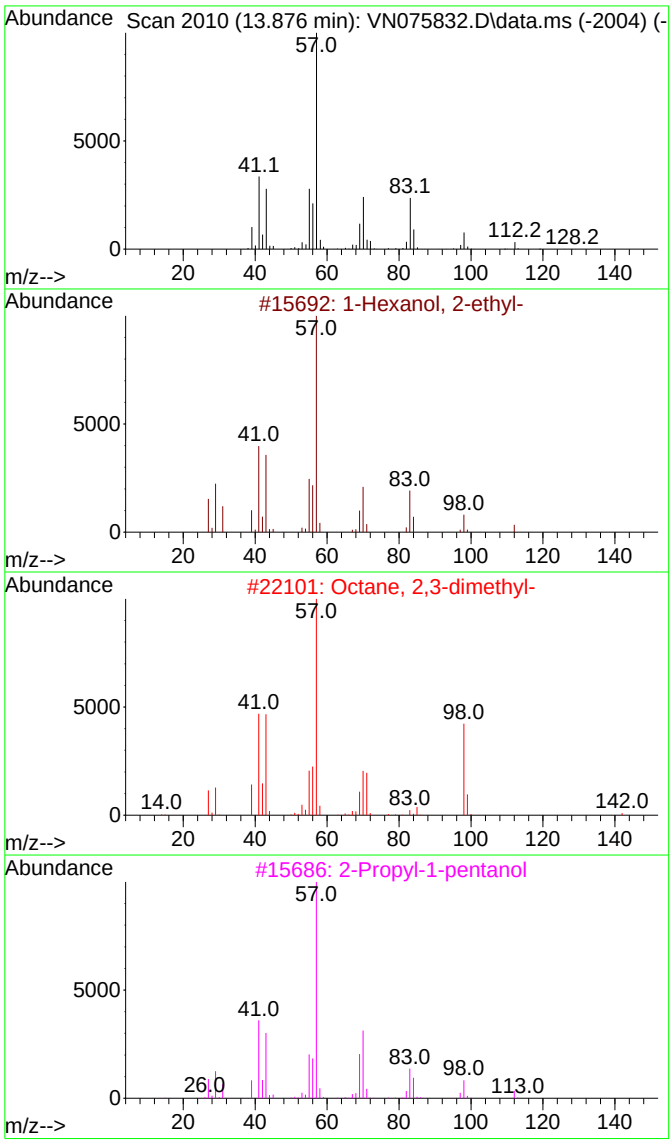
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

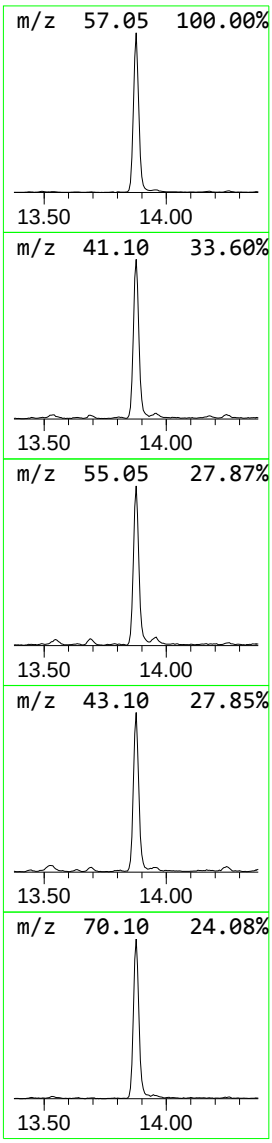
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	91.46 ug/l	2614810	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	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075832.D
Acq On : 15 Dec 2022 20:59
Operator : JC\MD
Sample : N6066-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-597

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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
Acetaldehyde	2.677	12.1	ug/l	252545	1	8.230	1047100	50.0
Ethanol	3.806	58.2	ug/l	1219250	1	8.230	1047100	50.0
Butanal	7.236	68.9	ug/l	1443450	1	8.230	1047100	50.0
1-Butanol	9.271	18.1	ug/l	454551	2	9.106	1252010	50.0
Pentanal	9.659	5.7	ug/l	141907	2	9.106	1252010	50.0
1-Pentanol	10.959	5.5	ug/l	170743	3	11.865	1552850	50.0
Butanoic acid, ...	13.341	8.9	ug/l	253369	4	13.794	1429420	50.0
1-Hexanol, 2-et...	13.876	91.5	ug/l	2614810	4	13.794	1429420	50.0