LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112123\
Data File : VN080232.D
Acq On : 21 Nov 2023 15:16
Operator : JC\MD
Sample : 05482-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

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\82N111623W.M
Title : SW846 8260

Signal : TIC: VN080232.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	17	21	29	rVB3	9308	15630	1.60%	0.170%
2	2.295	51	58	66	rBV3	5391	12691	1.30%	0.138%
3	2.665	114	121	129	rBV	116126	210205	21.54%	2.292%
4	4.289	387	397	411	rBV2	77065	215955	22.13%	2.355%
5	4.424	411	420	437	rVV	87018	259009	26.54%	2.825%
6	4.706	458	468	469	rBV	9974	17488	1.79%	0.191%
7	5.018	514	521	523	rBV3	5829	9876	1.01%	0.108%
8	5.512	596	605	615	rBV3	6719	21097	2.16%	0.230%
9	6.147	702	713	722	rBV4	13527	42695	4.38%	0.466%
10	6.724	803	811	824	rVB4	11975	35355	3.62%	0.386%
11	7.224	884	896	908	rBV2	346503	952491	97.61%	10.388%
12	7.483	930	940	950	rBV2	29789	75950	7.78%	0.828%
13	7.783	985	991	999	rVB2	8323	19513	2.00%	0.213%
14	8.171	1047	1057	1061	rBV	158301	368715	37.78%	4.021%
15	8.230	1061	1067	1075	rVB	232061	512490	52.52%	5.589%
16	8.530	1111	1118	1119	rBV3	10142	15822	1.62%	0.173%
17	8.583	1119	1127	1139	rVB2	154074	350503	35.92%	3.823%
18	8.977	1185	1194	1201	rBV6	3841	10574	1.08%	0.115%
19	9.100	1206	1215	1226	rVV	327697	675531	69.23%	7.367%
20	9.265	1236	1243	1251	rBV	23783	49400	5.06%	0.539%
21	9.406	1260	1267	1271	rVB2	6072	11487	1.18%	0.125%
22	9.535	1283	1289	1296	rVB2	7130	13353	1.37%	0.146%
23	9.659	1302	1310	1322	rBV2	47864	102796	10.53%	1.121%
24	10.453	1436	1445	1453	rVB2	13953	28060	2.88%	0.306%
25	10.571	1456	1465	1472	rBV	528000	975827	100.00%	10.642%
26	10.629	1472	1475	1481	rVB2	13560	22904	2.35%	0.250%
27	10.941	1521	1528	1537	rBV6	3745	10878	1.11%	0.119%
28	11.206	1565	1573	1584	rBV2	49966	148324	15.20%	1.618%
29	11.300	1584	1589	1601	rVB2	20369	38246	3.92%	0.417%
30	11.865	1674	1685	1694	rBV	512402	946406	96.99%	10.321%
31	11.982	1697	1705	1710	rBV6	5741	12526	1.28%	0.137%
32	12.076	1716	1721	1728	rVB5	6313	12614	1.29%	0.138%
33	12.212	1739	1744	1754	rVB	32051	51230	5.25%	0.559%
34	12.382	1767	1773	1777	rBV	39001	71300	7.31%	0.778%
35	12.459	1782	1786	1794	rVB2	23425	40123	4.11%	0.438%
36	12.565	1798	1804	1808	rBV4	6901	11199	1.15%	0.122%

LSC Area Percent Report

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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

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Title : SW846 8260

37	12.853	1845	1853	1864	rVB	437876	782992	80.24%	8.539%
38	13.088	1886	1893	1896	rBV6	13576	25278	2.59%	0.276%
39	13.118	1896	1898	1903	rVB3	7222	10567	1.08%	0.115%
40	13.259	1911	1922	1931	rBV	91835	172045	17.63%	1.876%
41	13.335	1931	1935	1945	rVB	65834	106539	10.92%	1.162%
42	13.506	1957	1964	1976	rVB7	31387	70662	7.24%	0.771%
43	13.612	1976	1982	1987	rBV6	11149	25071	2.57%	0.273%
44	13.688	1987	1995	2006	rVB3	95318	182452	18.70%	1.990%
45	13.794	2006	2013	2020	rBV	559536	939081	96.23%	10.242%
46	13.870	2020	2026	2036	rVV	219622	377626	38.70%	4.118%
47	13.959	2036	2041	2046	rVB5	9201	15998	1.64%	0.174%
48	14.247	2086	2090	2096	rVB4	10938	14723	1.51%	0.161%
49	14.559	2136	2143	2148	rVB7	14192	24312	2.49%	0.265%
50	14.629	2148	2155	2162	rVB4	6291	13390	1.37%	0.146%
51	15.400	2280	2286	2290	rBV3	17286	30095	3.08%	0.328%
52	15.464	2290	2297	2302	rVV4	6130	10193	1.04%	0.111%

Sum of corrected areas: 9169287

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ClientSampleId :
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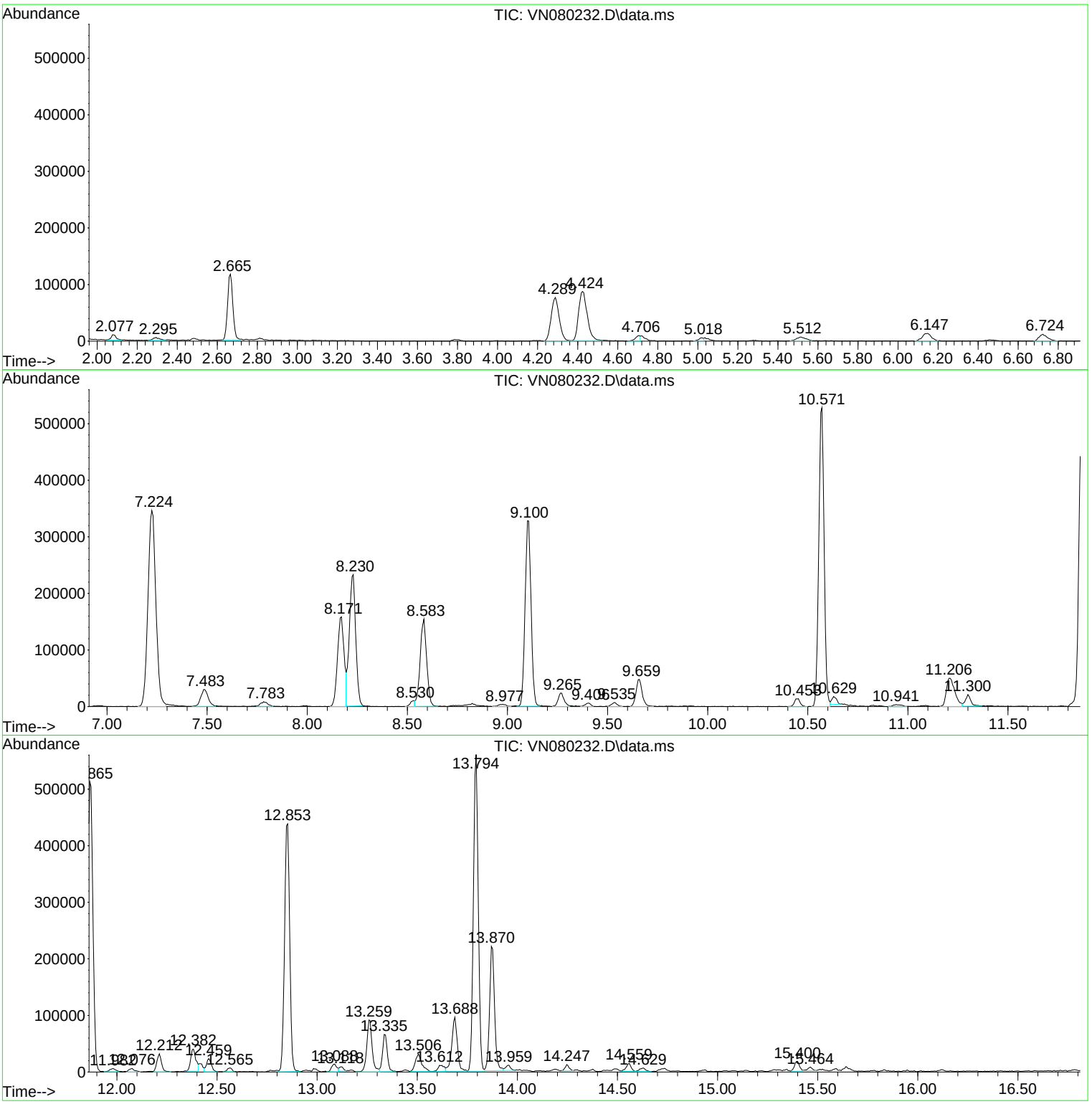
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112123\
Data File : VN080232.D
Acq On : 21 Nov 2023 15:16
Operator : JC\MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

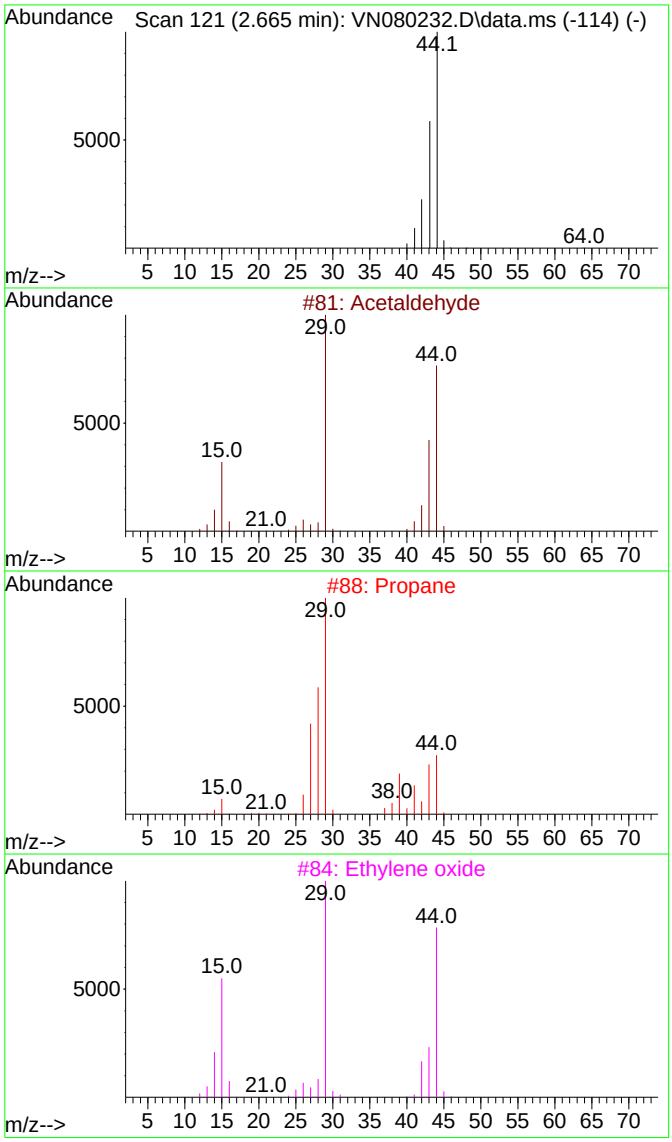
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

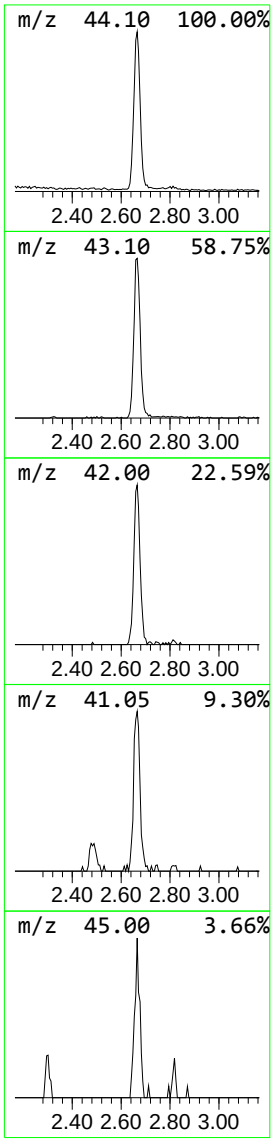
****

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.665	20.51 ug/l	210205	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	1-Propanol, 2-amino-, (.+/-.)-	75	C3H9NO	006168-72-5	4





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Data File : VN080232.D
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

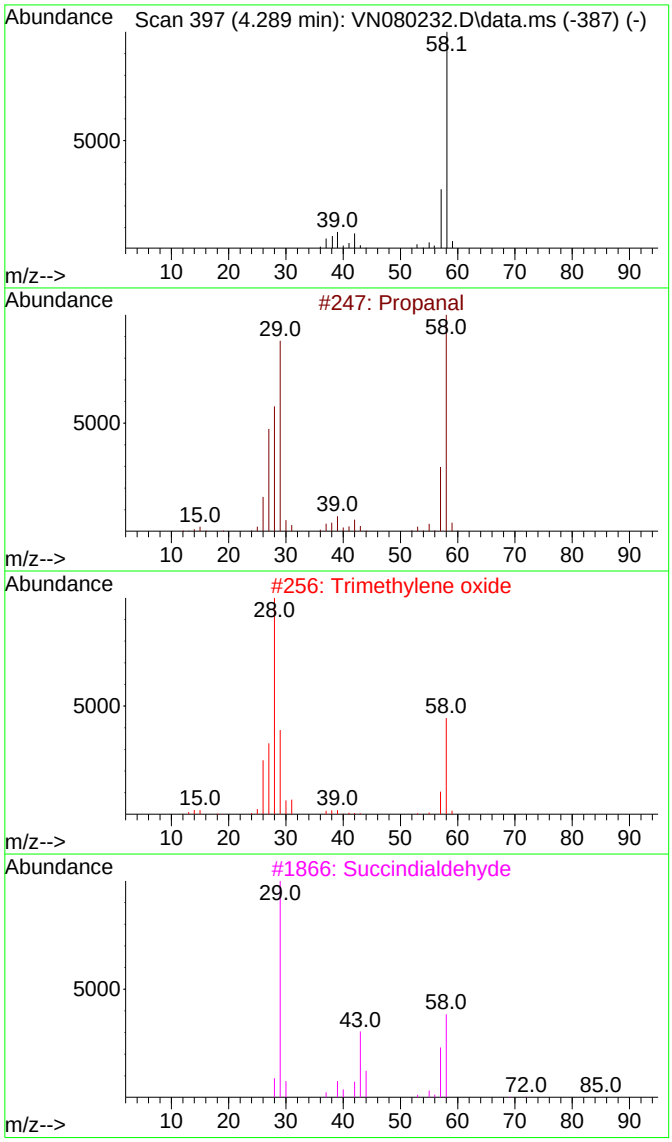
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

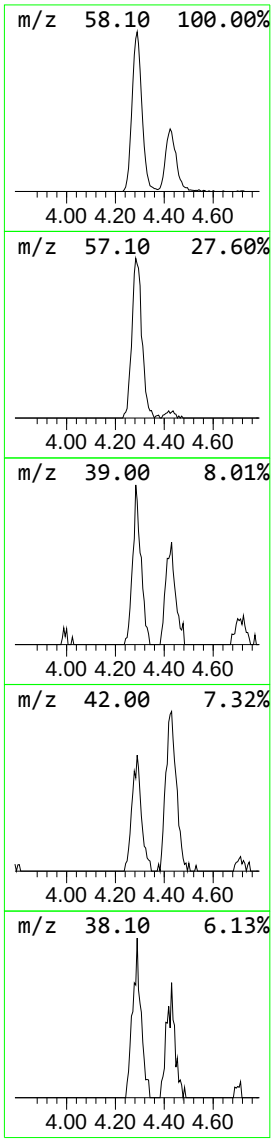
****

Peak Number 2 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.289	21.07 ug/l	215955	Pentafluorobenzene	8.230

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	Succindialdehyde	86	C4H6O2	000638-37-9	9
4	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9





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Data File : VN080232.D
Acq On : 21 Nov 2023 15:16
Operator : JC\MD
Sample : 05482-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

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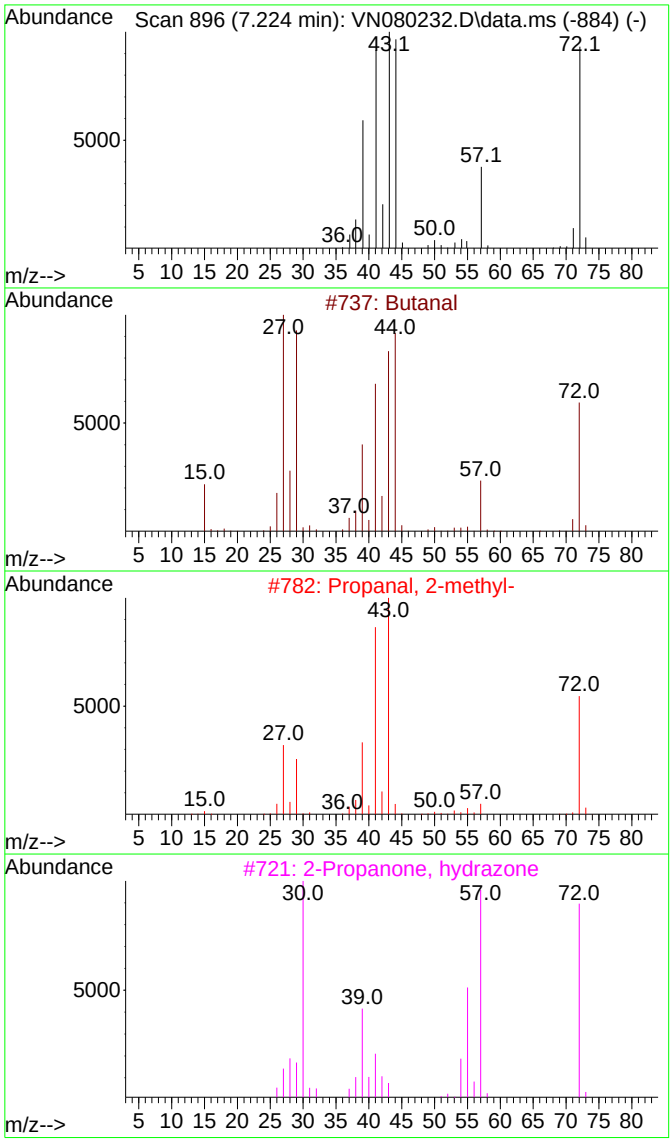
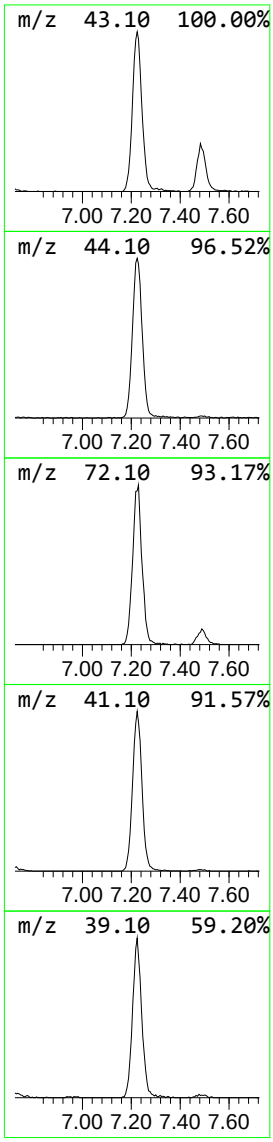
Peak Number 3 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	92.93 ug/l	952491	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	35
4	Propane	44	C3H8	000074-98-6	35
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

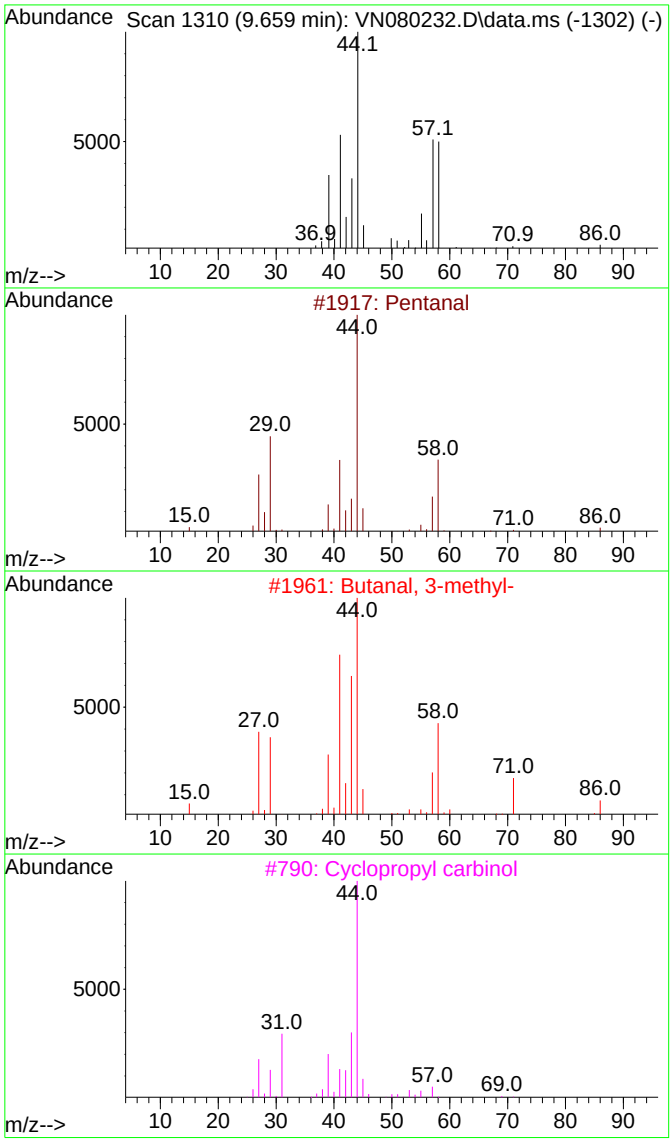
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

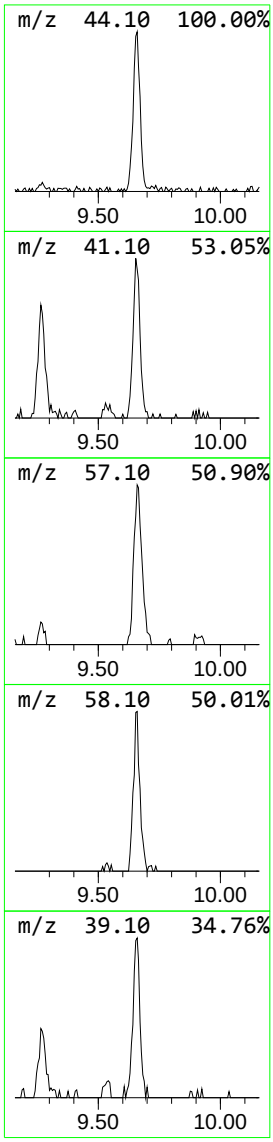
****

Peak Number 4 Pentanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.659	7.61 ug/l	102796	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	83
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	56
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	50
4	Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	12
5	Allyl ethyl ether	86	C5H10O	000557-31-3	10





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Instrument :
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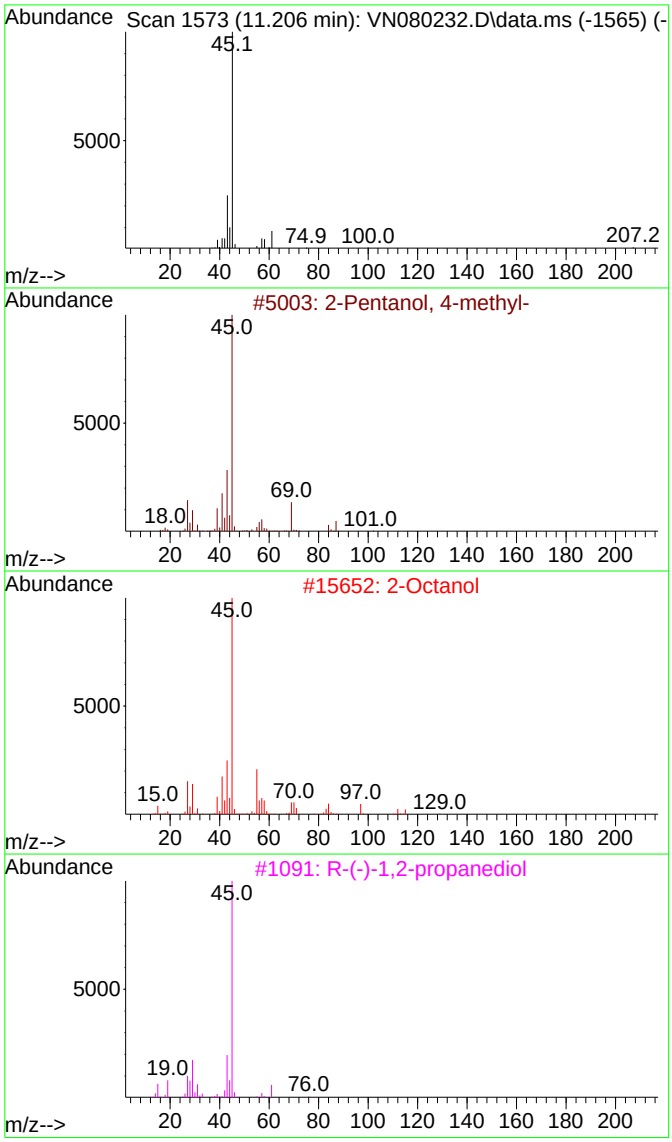
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

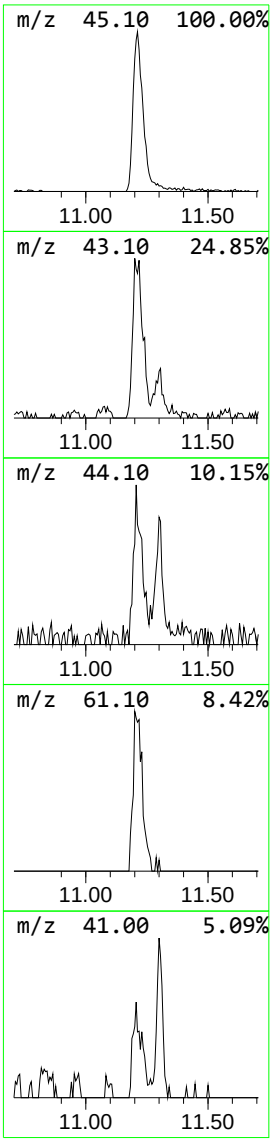
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanol, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	7.84 ug/l	148324	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	56
2	2-Octanol	130	C8H18O	000123-96-6	43
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Acetic acid, cyano-, 2-methoxyet...	143	C6H9NO3	010258-54-5	9





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Quant Title : SW846 8260

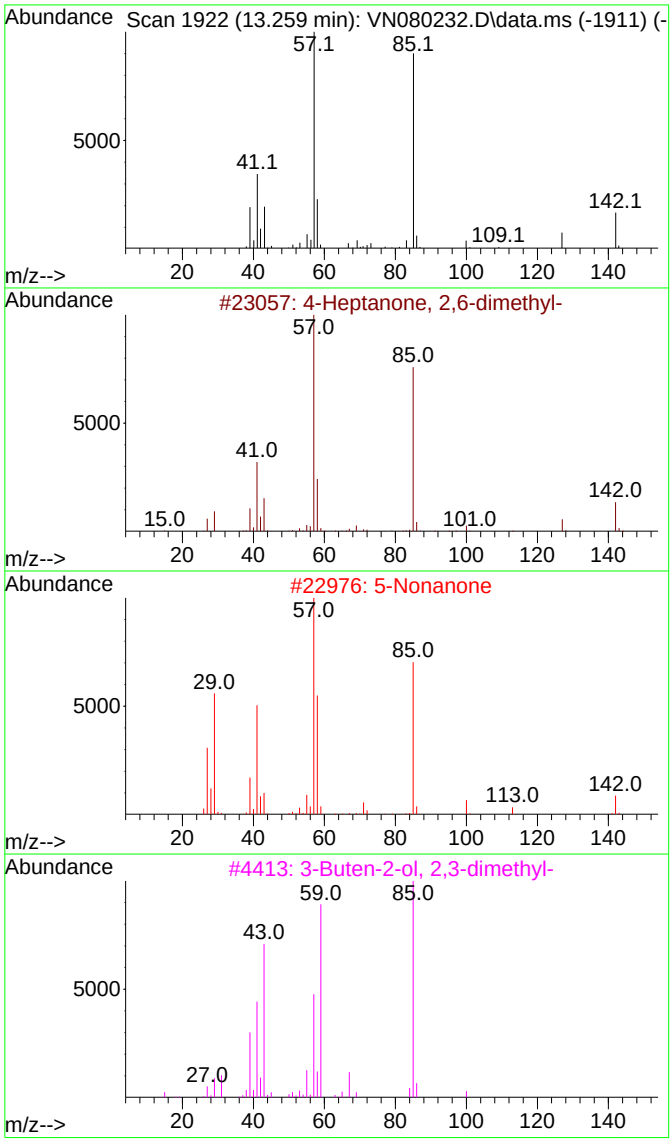
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

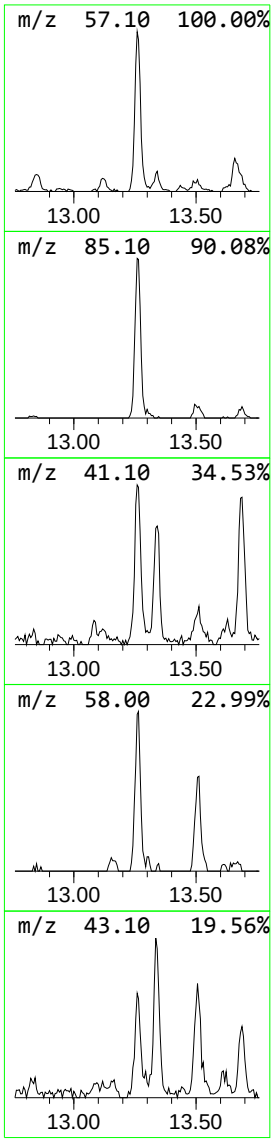
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	9.16 ug/l	172045	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	91
2	5-Nonanone	142	C9H18O	000502-56-7	59
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
4	2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50





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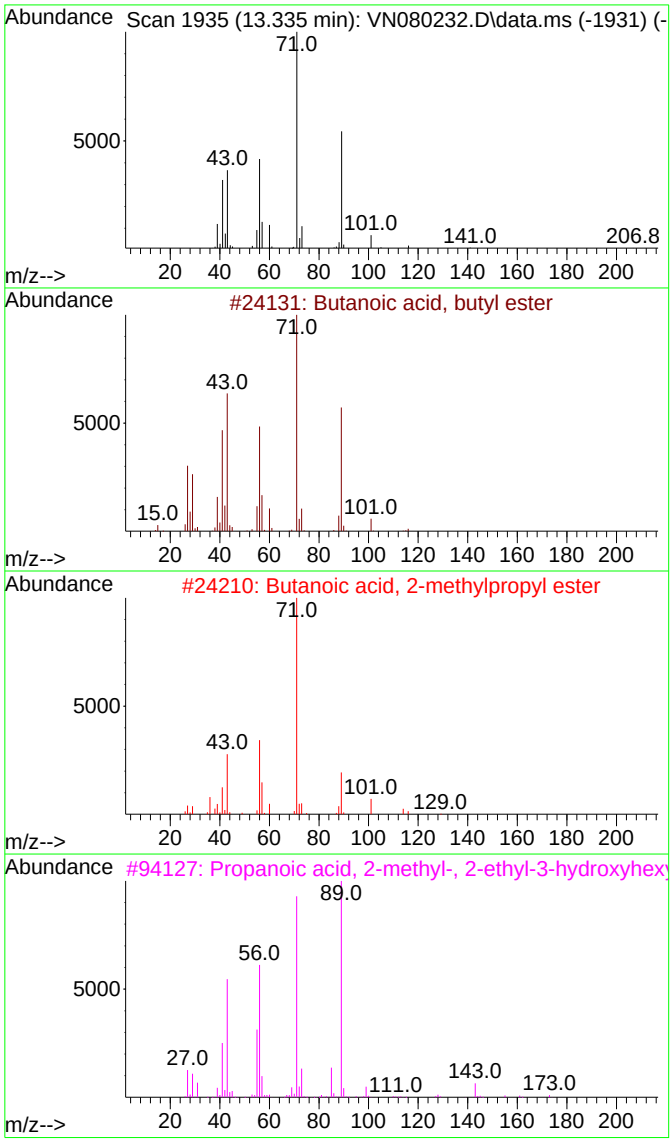
Quant Title : SW846 8260

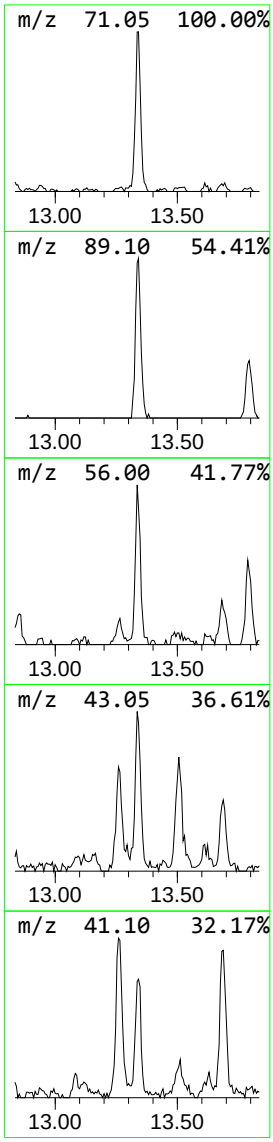
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	5.67 ug/l	106539	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	83
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	64
4	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56
5	Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	53





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Data File : VN080232.D
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MSVOA_N
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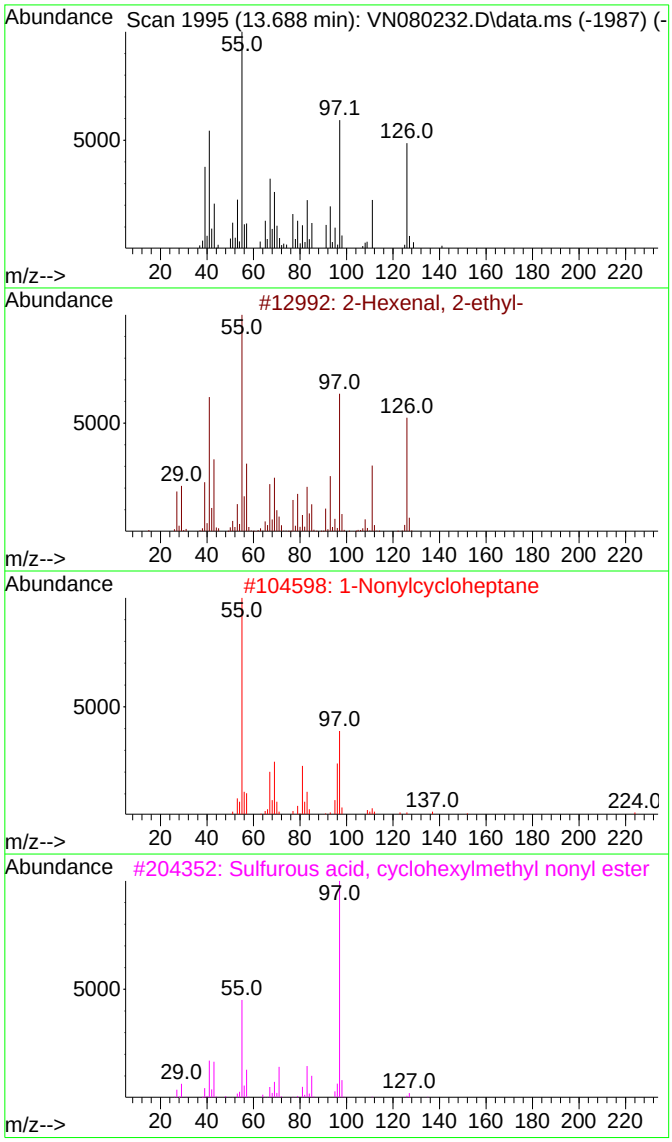
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

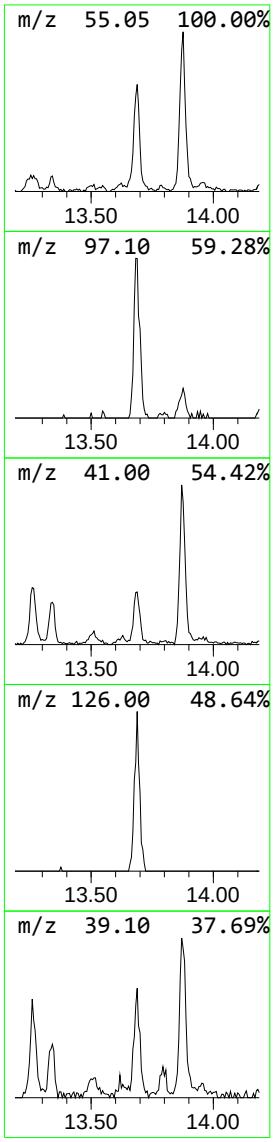
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Hexenal, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	9.71 ug/l	182452	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	91
2	1-Nonylcycloheptane	224	C16H32	1000371-47-7	35
3	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	35
4	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	35
5	2-Heptenal, 2-methyl-	126	C8H14O	030567-26-1	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112123\
Data File : VN080232.D
Acq On : 21 Nov 2023 15:16
Operator : JC\MD
Sample : 05482-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

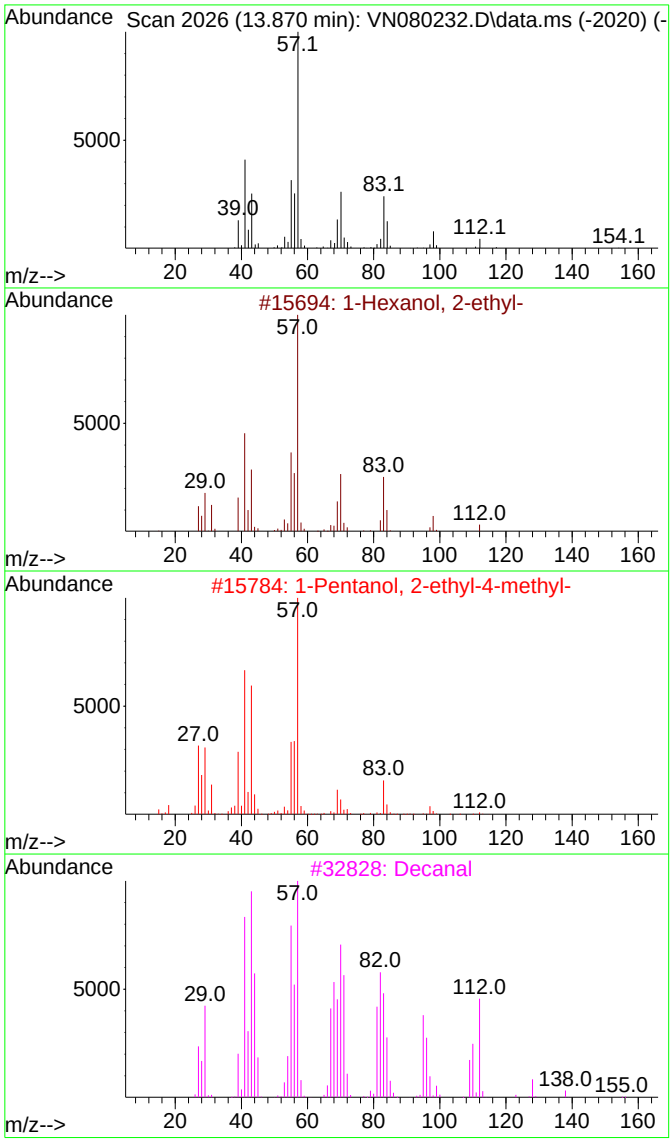
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

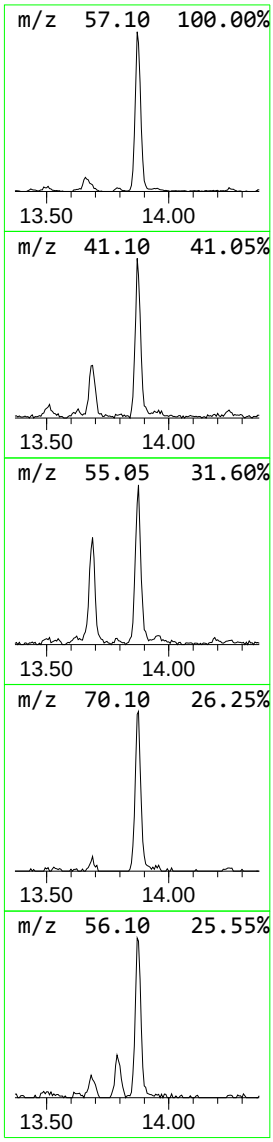
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	20.11 ug/l	377626	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	59
3	Decanal	156	C10H20O	000112-31-2	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112123\
Data File : VN080232.D
Acq On : 21 Nov 2023 15:16
Operator : JC\MD
Sample : 05482-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.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	2.665	20.5	ug/l	210205	1	8.230	512490	50.0
Propanal	4.289	21.1	ug/l	215955	1	8.230	512490	50.0
Butanal	7.224	92.9	ug/l	952491	1	8.230	512490	50.0
Pentanal	9.659	7.6	ug/l	102796	2	9.100	675531	50.0
2-Pentanol, 4-m...	11.206	7.8	ug/l	148324	3	11.871	946406	50.0
4-Heptanone, 2,...	13.259	9.2	ug/l	172045	4	13.794	939081	50.0
Butanoic acid, ...	13.335	5.7	ug/l	106539	4	13.794	939081	50.0
2-Hexenal, 2-et...	13.688	9.7	ug/l	182452	4	13.794	939081	50.0
1-Hexanol, 2-et...	13.870	20.1	ug/l	377626	4	13.794	939081	50.0