LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

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\82N042524W.M
Title : SW846 8260

Signal : TIC: VN081860.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	rVB	120639	168362	11.97%	1.451%
2	2.312	54	61	66	rBV7	11619	23209	1.65%	0.200%
3	2.512	91	95	102	rVB2	12489	26299	1.87%	0.227%
4	2.665	117	121	125	rVB5	7290	14755	1.05%	0.127%
5	3.783	301	311	325	rBV2	180856	490573	34.89%	4.229%
6	4.430	411	421	430	rBV2	12333	37349	2.66%	0.322%
7	4.712	460	469	470	rBV2	18526	34000	2.42%	0.293%
8	5.512	594	605	614	rBV2	20830	71812	5.11%	0.619%
9	7.224	885	896	908	rBV2	110340	323788	23.03%	2.791%
10	7.483	931	940	951	rBV2	25556	64387	4.58%	0.555%
11	7.783	985	991	997	rVB2	15414	34224	2.43%	0.295%
12	8.171	1047	1057	1061	rBV	164968	413119	29.38%	3.561%
13	8.224	1061	1066	1077	rVB	323069	711843	50.62%	6.136%
14	8.577	1113	1126	1135	rBV2	207959	545557	38.80%	4.703%
15	8.659	1135	1140	1145	rBV3	24222	63076	4.49%	0.544%
16	9.100	1205	1215	1228	rBV	496007	1025471	72.93%	8.840%
17	9.271	1236	1244	1254	rBV3	15924	39690	2.82%	0.342%
18	9.647	1302	1308	1314	rBV5	12430	23594	1.68%	0.203%
19	10.565	1456	1464	1471	rBV	743455	1406138	100.00%	12.121%
20	10.630	1471	1475	1484	rVB	36209	73147	5.20%	0.631%
21	11.865	1671	1685	1696	rBV	668363	1224557	87.09%	10.556%
22	11.965	1696	1702	1707	rVV4	15056	29070	2.07%	0.251%
23	12.029	1707	1713	1716	rVV4	39669	75772	5.39%	0.653%
24	12.065	1716	1719	1728	rVB3	35572	65741	4.68%	0.567%
25	12.165	1728	1736	1740	rBV6	33535	74015	5.26%	0.638%
26	12.206	1740	1743	1749	rVB3	31184	52943	3.77%	0.456%
27	12.418	1765	1779	1787	rBV3	94909	215031	15.29%	1.854%
28	12.635	1810	1816	1822	rBV4	19894	39008	2.77%	0.336%
29	12.700	1822	1827	1832	rVB7	10205	18846	1.34%	0.162%
30	12.847	1844	1852	1860	rBV	519536	929759	66.12%	8.015%
31	13.241	1910	1919	1922	rVV3	49892	103438	7.36%	0.892%
32	13.271	1922	1924	1929	rVB	42934	52857	3.76%	0.456%
33	13.335	1929	1935	1942	rVB	264886	395468	28.12%	3.409%
34	13.435	1947	1952	1956	rBV6	8096	15598	1.11%	0.134%
35	13.488	1956	1961	1964	rBV4	22985	40499	2.88%	0.349%
36	13.529	1964	1968	1976	rVB2	66428	112002	7.97%	0.965%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

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\82N042524W.M
Title : SW846 8260

37	13.635	1980	1986	1990	rBV6	12636	22382	1.59%	0.193%
38	13.688	1992	1995	2000	rVB4	12969	23374	1.66%	0.201%
39	13.794	2004	2013	2020	rBV	620617	1073180	76.32%	9.251%
40	13.871	2020	2026	2034	rVV	489902	805537	57.29%	6.944%
41	13.947	2036	2039	2043	rVV5	13243	21814	1.55%	0.188%
42	14.176	2072	2078	2085	rBV3	30132	56745	4.04%	0.489%
43	14.529	2134	2138	2145	rVB4	19260	31371	2.23%	0.270%
44	14.753	2171	2176	2184	rBV8	19693	50702	3.61%	0.437%
45	15.394	2281	2285	2291	rVV2	23580	40524	2.88%	0.349%
46	15.470	2293	2298	2304	rVB8	10179	23573	1.68%	0.203%
47	15.582	2312	2317	2320	rBV5	10796	18998	1.35%	0.164%
48	15.641	2320	2327	2337	rVB	178539	377416	26.84%	3.253%
49	16.117	2404	2408	2415	rVB7	8946	20212	1.44%	0.174%

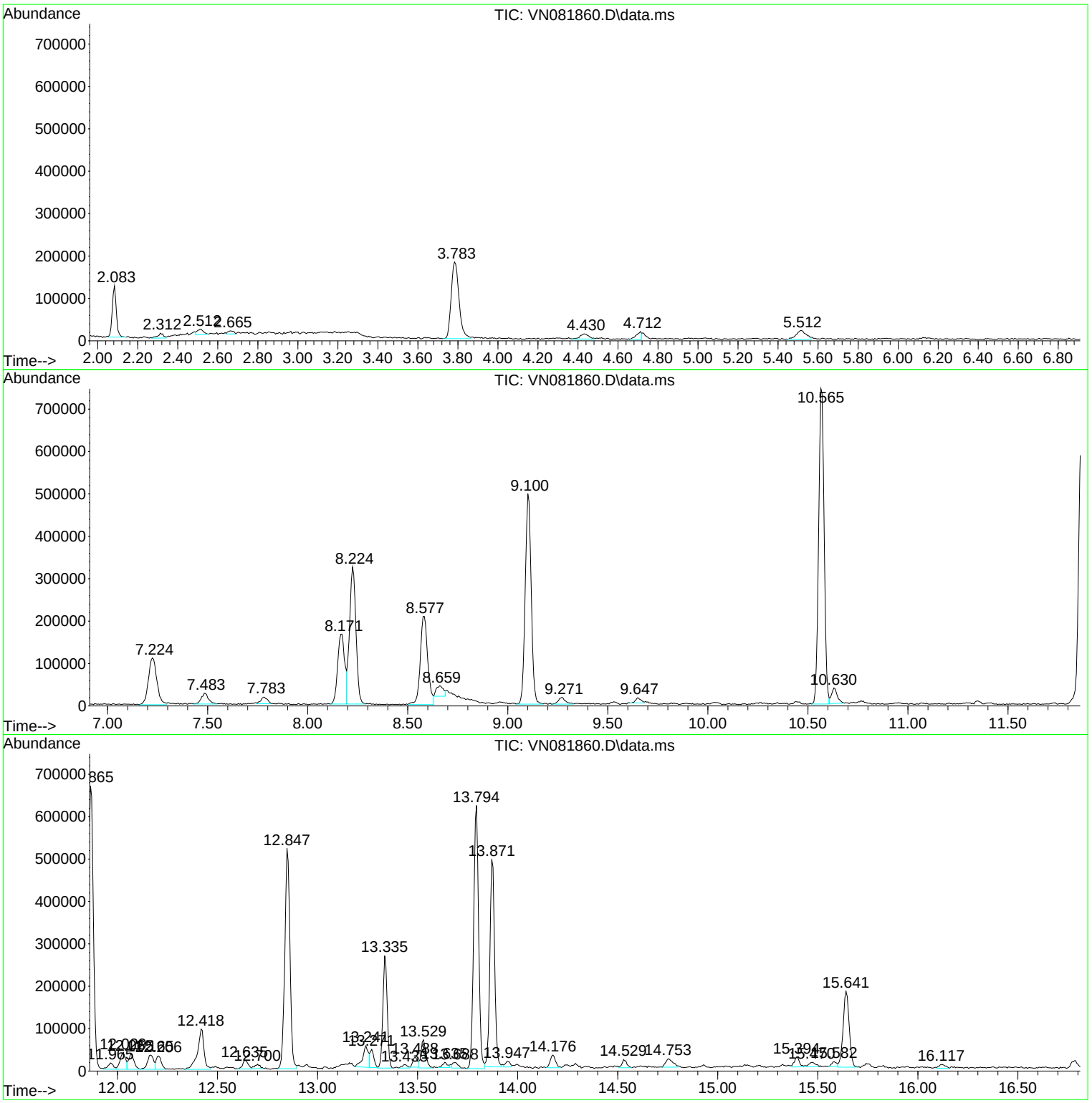
Sum of corrected areas: 11600825

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

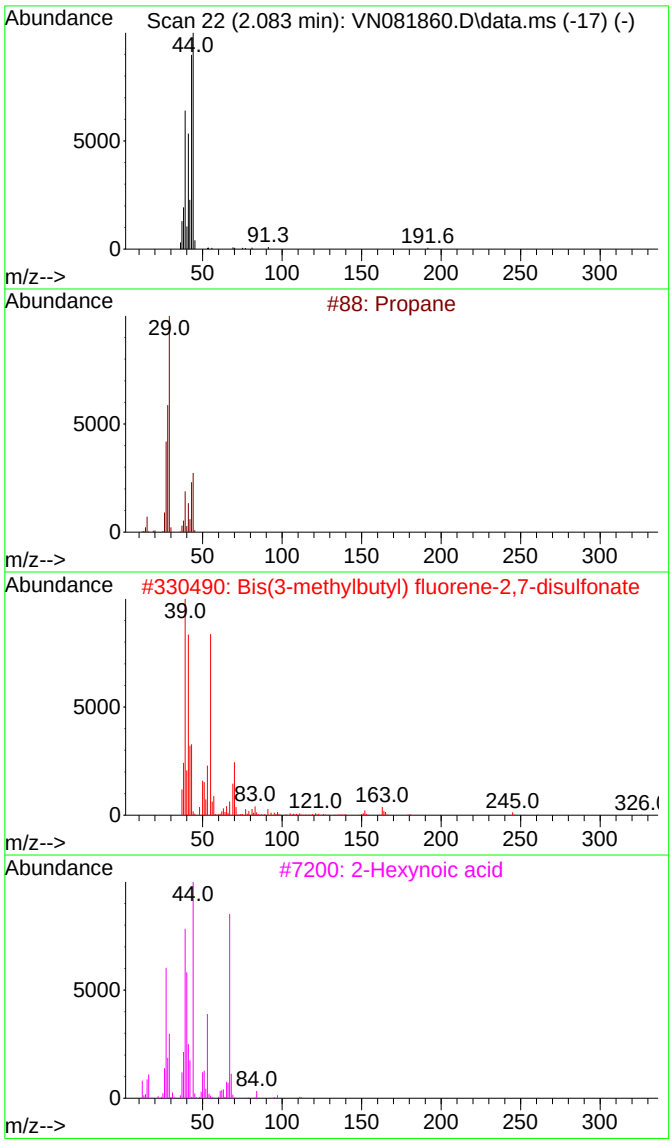
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

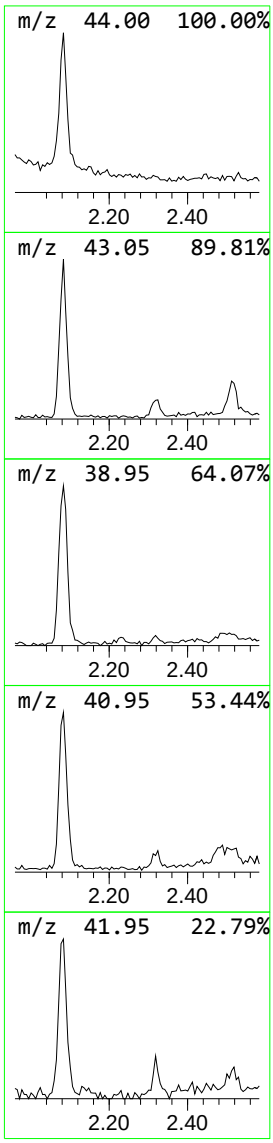
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	11.83 ug/l	168362	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	47
3	2-Hexynoic acid	112	C6H8O2	000764-33-0	39
4	1-Propyne, 3-bromo-	118	C3H3Br	000106-96-7	37
5	2-Butenal, (E)-	70	C4H6O	000123-73-9	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

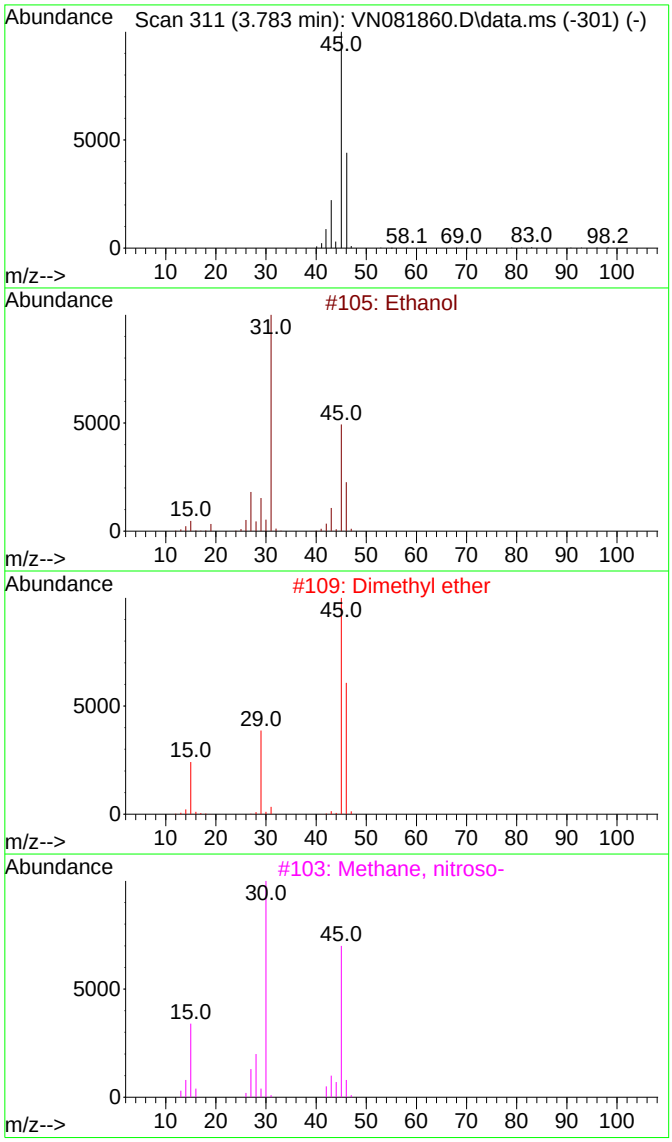
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

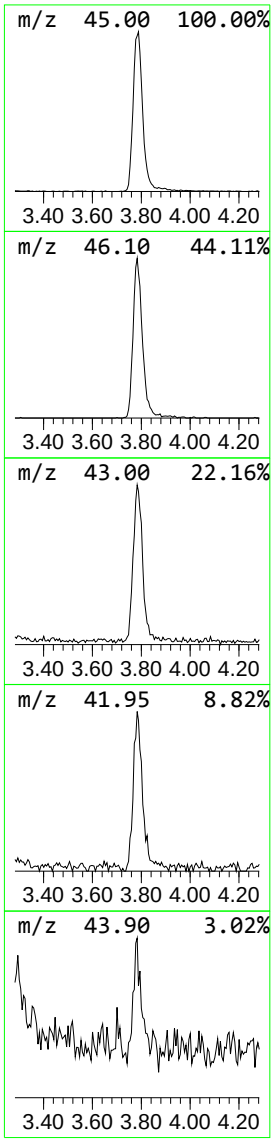
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	34.46 ug/l	490573	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	78
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4
5	Formic acid	46	CH2O2	000064-18-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

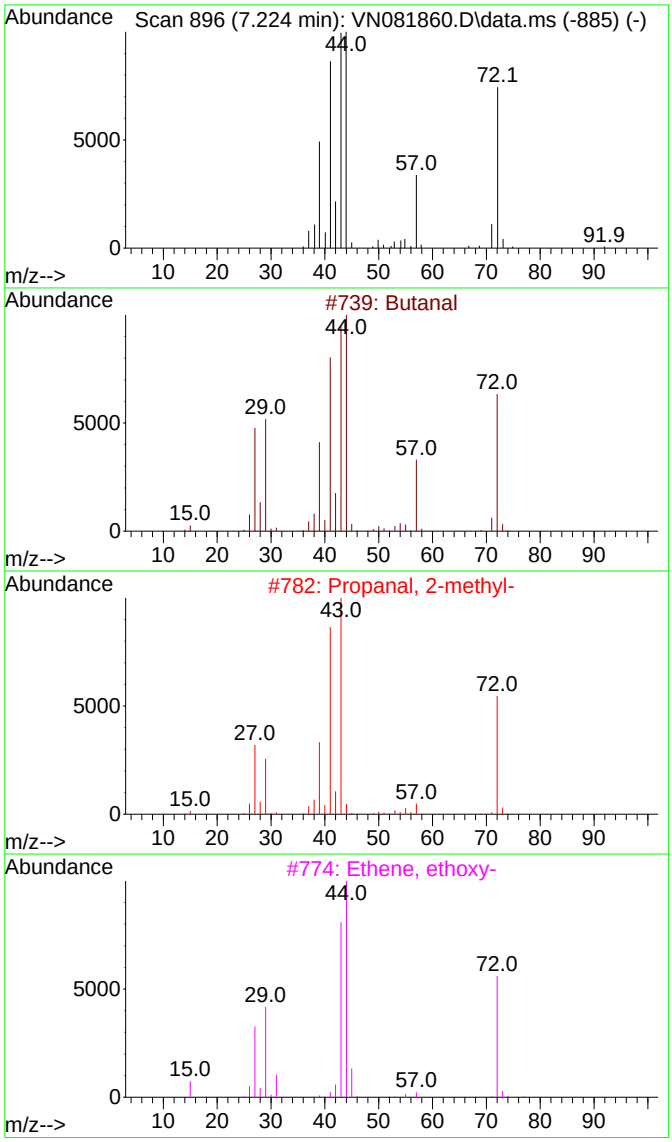
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

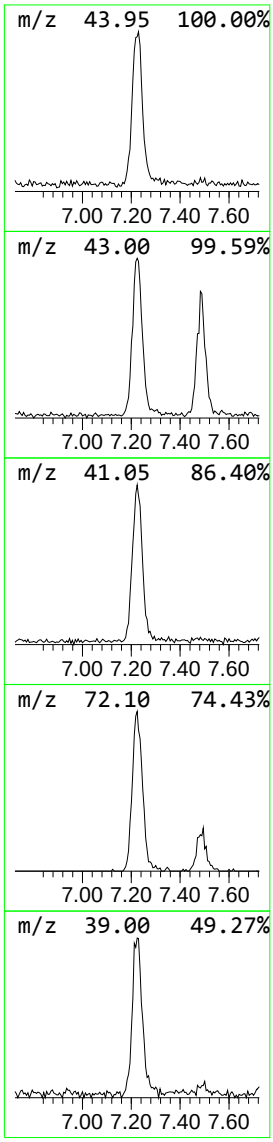
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	22.74 ug/l	323788	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5	Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

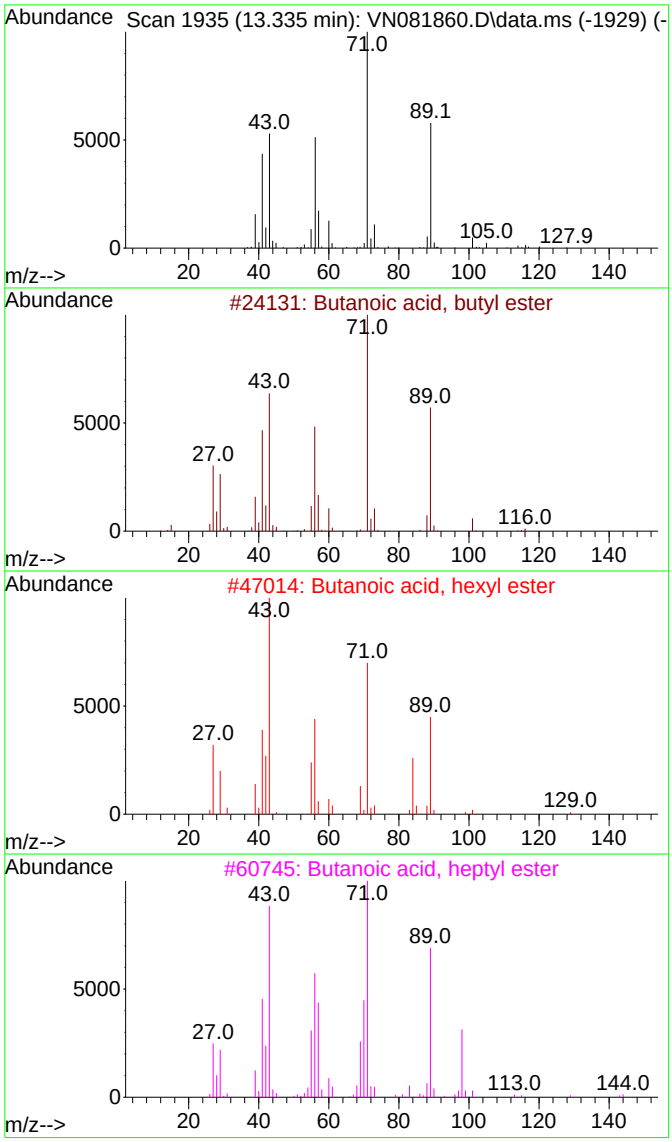
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

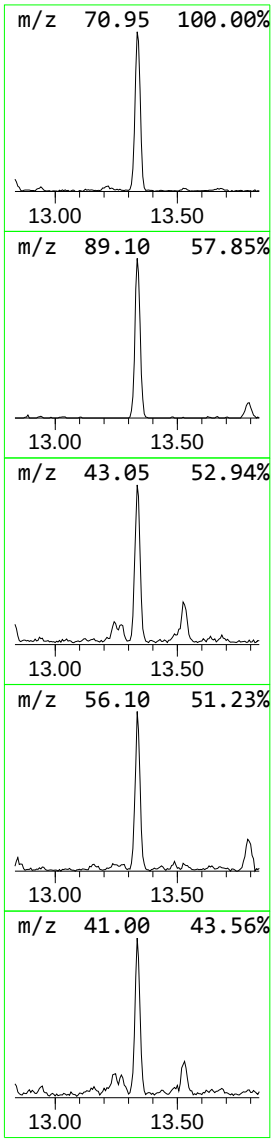
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	18.43 ug/l	395468	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	78
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	78
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

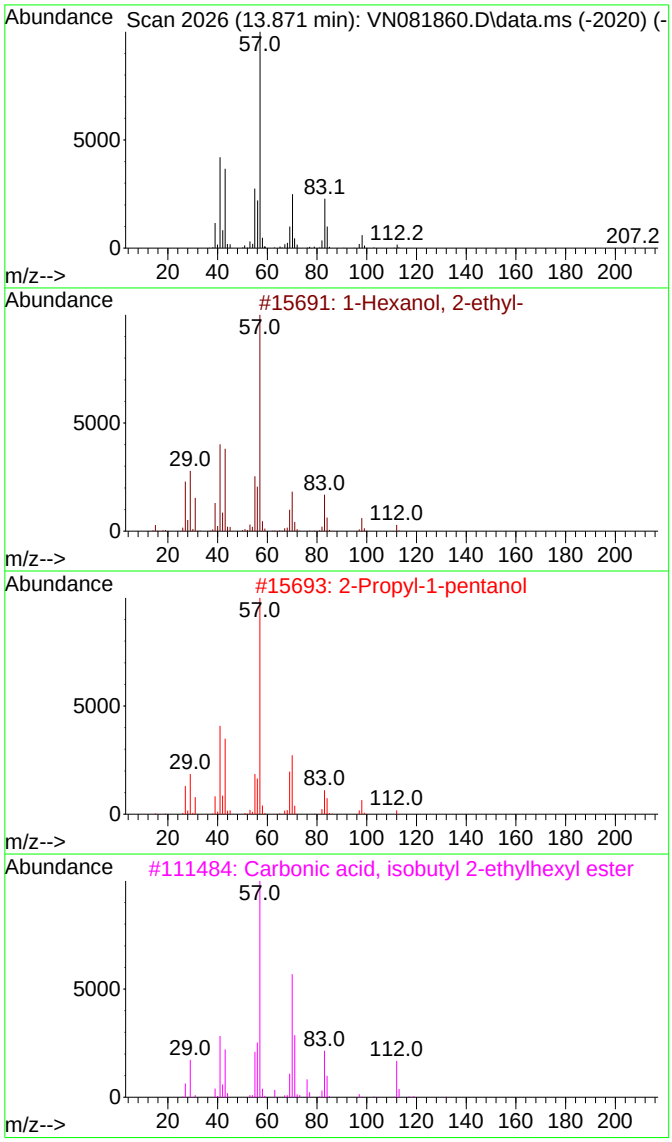
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

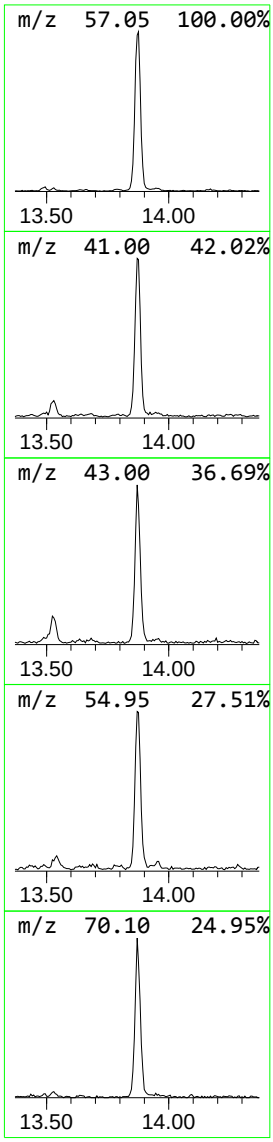
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	37.53 ug/l	805537	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	64
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081860.D
Acq On : 25 Apr 2024 19:04
Operator : JC\MD
Sample : P2257-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
416A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.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	2.083	11.8	ug/l	168362	1	8.224	711843	50.0
Ethanol	3.783	34.5	ug/l	490573	1	8.224	711843	50.0
Butanal	7.224	22.7	ug/l	323788	1	8.224	711843	50.0
Butanoic acid, ...	13.335	18.4	ug/l	395468	4	13.794	1073180	50.0
1-Hexanol, 2-et...	13.871	37.5	ug/l	805537	4	13.794	1073180	50.0