LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

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: VN080247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	49	57	64	rBV2	15599	35101	1.07%	0.078%
2	2.506	85	94	100	rBV6	15527	48228	1.47%	0.107%
3	2.900	138	161	162	rBV7	40366	165439	5.04%	0.368%
4	2.947	165	169	173	rVV	16328	35489	1.08%	0.079%
5	6.294	727	738	754	rVB4	12636	40849	1.24%	0.091%
6	6.677	789	803	817	rBV5	11695	52072	1.59%	0.116%
7	7.224	884	896	905	rBV	455776	1376537	41.91%	3.061%
8	8.165	1046	1056	1061	rBV2	153693	380037	11.57%	0.845%
9	8.224	1061	1066	1078	rVV	260247	608565	18.53%	1.353%
10	8.441	1094	1103	1110	rBV3	33373	77800	2.37%	0.173%
11	8.571	1113	1125	1138	rBV3	211620	667842	20.33%	1.485%
12	8.965	1185	1192	1201	rVV2	89466	173333	5.28%	0.385%
13	9.100	1208	1215	1228	rVB	343800	723700	22.03%	1.609%
14	9.288	1237	1247	1262	rBV	1302695	2632128	80.14%	5.853%
15	9.600	1286	1300	1306	rBV2	189222	423426	12.89%	0.942%
16	9.659	1306	1310	1320	rVB4	55170	131826	4.01%	0.293%
17	10.153	1385	1394	1397	rBV2	25482	46555	1.42%	0.104%
18	10.206	1397	1403	1416	rVB2	124047	308911	9.41%	0.687%
19	10.341	1418	1426	1441	rVV	128991	292203	8.90%	0.650%
20	10.570	1457	1465	1470	rBV	740879	1397007	42.53%	3.107%
21	10.629	1470	1475	1482	rVV	288815	594385	18.10%	1.322%
22	10.700	1482	1487	1489	rVV3	28522	50414	1.53%	0.112%
23	10.747	1489	1495	1502	rVB	427052	712474	21.69%	1.584%
24	10.912	1518	1523	1527	rBV2	53398	93094	2.83%	0.207%
25	10.965	1527	1532	1536	rVV	148412	263242	8.01%	0.585%
26	11.006	1536	1539	1548	rVV5	49282	127423	3.88%	0.283%
27	11.082	1548	1552	1558	rVB2	36965	65563	2.00%	0.146%
28	11.176	1561	1568	1574	rBV2	71819	131107	3.99%	0.292%
29	11.276	1579	1585	1593	rVV2	84722	172316	5.25%	0.383%
30	11.347	1593	1597	1602	rVV3	37670	65348	1.99%	0.145%
31	11.417	1602	1609	1614	rVV	116871	236031	7.19%	0.525%
32	11.470	1614	1618	1624	rVV2	74039	137848	4.20%	0.307%
33	11.576	1631	1636	1640	rVV	66771	118577	3.61%	0.264%
34	11.647	1640	1648	1659	rVV4	345470	798350	24.31%	1.775%
35	11.747	1659	1665	1671	rVV	270449	444618	13.54%	0.989%
36	11.870	1674	1686	1695	rVV	559232	1125769	34.28%	2.503%

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

37	11.970	1695	1703	1708	rVV2	206213	379121	11.54%	0.843%
38	12.070	1712	1720	1731	rVV2	1762900	3284510	100.00%	7.304%
39	12.159	1731	1735	1740	rVB4	62467	113337	3.45%	0.252%
40	12.294	1752	1758	1764	rVB4	65267	127175	3.87%	0.283%
41	12.400	1764	1776	1783	rBV2	422990	1120363	34.11%	2.491%
42	12.482	1786	1790	1795	rVB3	145019	241863	7.36%	0.538%
43	12.594	1795	1809	1810	rBV7	93766	346412	10.55%	0.770%
44	12.623	1811	1814	1819	rVV	110494	197458	6.01%	0.439%
45	12.712	1822	1829	1830	rVV3	72098	156458	4.76%	0.348%
46	12.747	1831	1835	1836	rVV3	126311	194889	5.93%	0.433%
47	12.770	1836	1839	1841	rVV	199954	286683	8.73%	0.638%
48	12.800	1841	1844	1848	rVV	216317	312148	9.50%	0.694%
49	12.853	1848	1853	1864	rVB2	500996	1102927	33.58%	2.453%
50	12.947	1864	1869	1873	rBV6	33306	63984	1.95%	0.142%
51	13.035	1878	1884	1889	rVB3	111363	225064	6.85%	0.500%
52	13.100	1889	1895	1899	rBV	312082	598022	18.21%	1.330%
53	13.164	1901	1906	1914	rVV2	1024828	1915569	58.32%	4.260%
54	13.229	1914	1917	1923	rVB4	62071	97401	2.97%	0.217%
55	13.341	1927	1936	1942	rBV3	317300	660967	20.12%	1.470%
56	13.394	1942	1945	1951	rVV4	87045	132202	4.03%	0.294%
57	13.488	1955	1961	1966	rVV	504841	838222	25.52%	1.864%
58	13.535	1966	1969	1974	rVV6	54055	101815	3.10%	0.226%
59	13.688	1988	1995	1998	rBV2	224394	446626	13.60%	0.993%
60	13.723	1998	2001	2004	rVV2	148920	218943	6.67%	0.487%
61	13.794	2008	2013	2021	rVV2	643713	1363475	41.51%	3.032%
62	13.876	2021	2027	2033	rVB2	380135	765338	23.30%	1.702%
63	13.953	2035	2040	2043	rBV4	101868	170459	5.19%	0.379%
64	13.988	2043	2046	2049	rVV2	87782	115285	3.51%	0.256%
65	14.023	2049	2052	2058	rVB2	135226	216882	6.60%	0.482%
66	14.106	2061	2066	2073	rBV	865923	1468728	44.72%	3.266%
67	14.247	2083	2090	2092	rBV5	143202	292561	8.91%	0.651%
68	14.335	2100	2105	2109	rVB	232133	353920	10.78%	0.787%
69	14.441	2117	2123	2127	rBV3	146788	273924	8.34%	0.609%
70	14.511	2128	2135	2142	rBV6	216963	492634	15.00%	1.096%
71	14.582	2142	2147	2149	rBV5	137261	236665	7.21%	0.526%
72	14.629	2150	2155	2158	rBV4	384584	627092	19.09%	1.395%
73	14.664	2158	2161	2165	rVB	423790	585410	17.82%	1.302%
74	14.735	2170	2173	2176	rVV3	181307	292307	8.90%	0.650%
75	14.776	2176	2180	2187	rVV3	491682	1143062	34.80%	2.542%
76	14.841	2187	2191	2197	rVB5	180864	325610	9.91%	0.724%

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Title : SW846 8260

77	14.964	2203	2212	2220	rBV	947365	1557715	47.43%	3.464%
78	15.041	2220	2225	2230	rBV3	248912	555398	16.91%	1.235%
79	15.235	2254	2258	2261	rBV5	132974	219546	6.68%	0.488%
80	15.264	2261	2263	2268	rVB4	172613	238920	7.27%	0.531%
81	15.347	2269	2277	2282	rBV4	240242	594939	18.11%	1.323%
82	15.535	2302	2309	2314	rVB6	203278	543525	16.55%	1.209%
83	15.594	2314	2319	2326	rBV4	205208	445865	13.57%	0.992%
84	15.835	2356	2360	2371	rVB	721959	1366425	41.60%	3.039%
85	15.941	2372	2378	2379	rBV4	105446	213557	6.50%	0.475%
86	16.176	2413	2418	2425	rBV2	431319	801848	24.41%	1.783%
87	16.317	2437	2442	2452	rVB4	279708	713128	21.71%	1.586%
88	16.488	2464	2471	2479	rBV3	266628	902226	27.47%	2.006%
89	16.717	2505	2510	2512	rBV2	92708	176477	5.37%	0.392%

Sum of corrected areas: 44968687

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MSVOA_N
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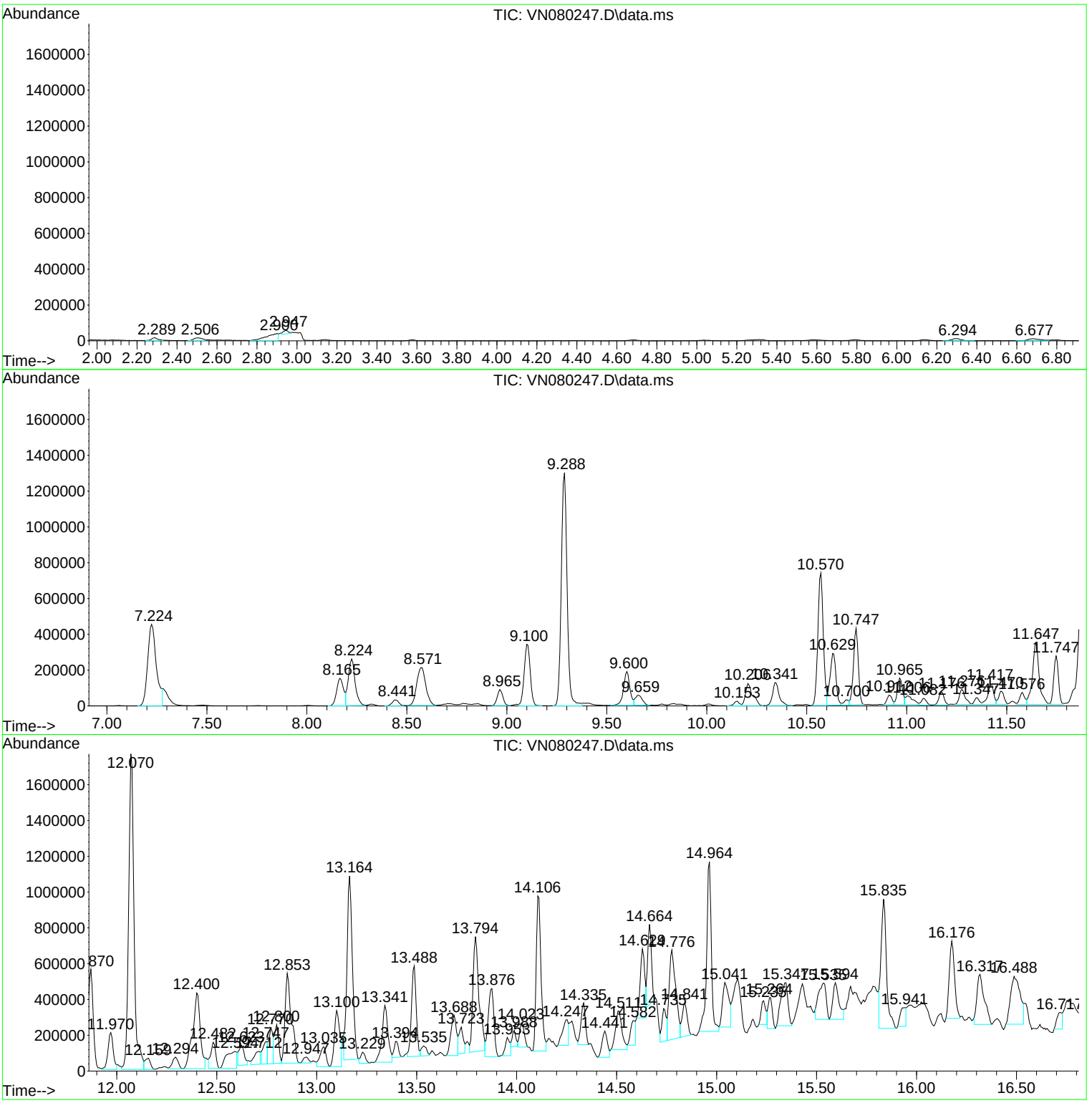
1109

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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Quant Title : SW846 8260

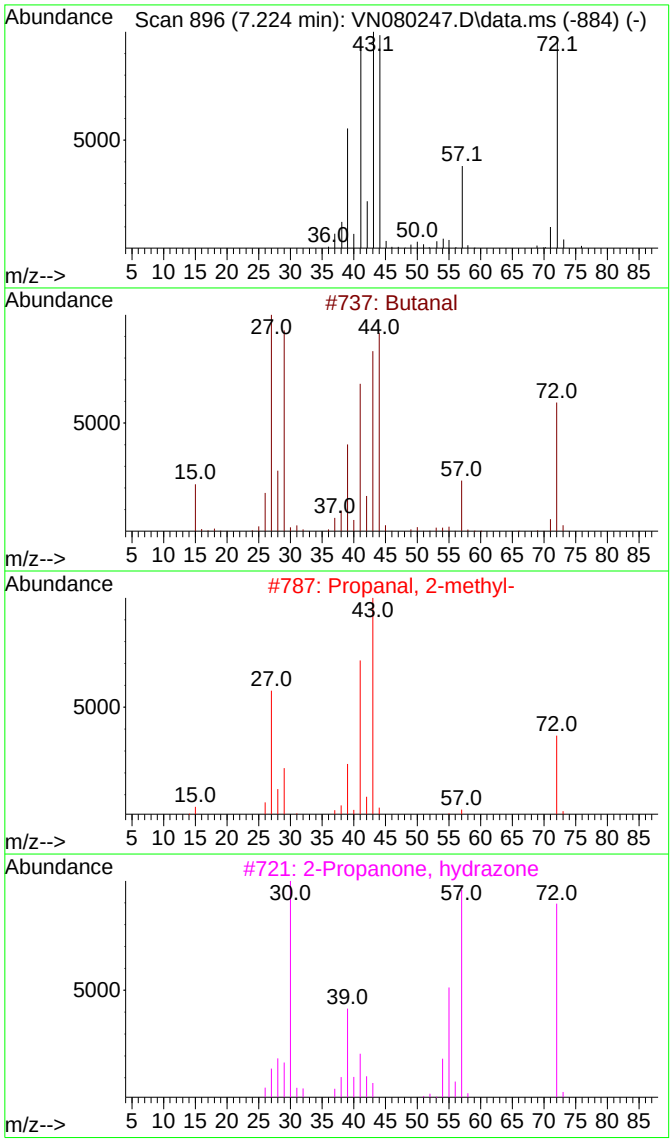
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

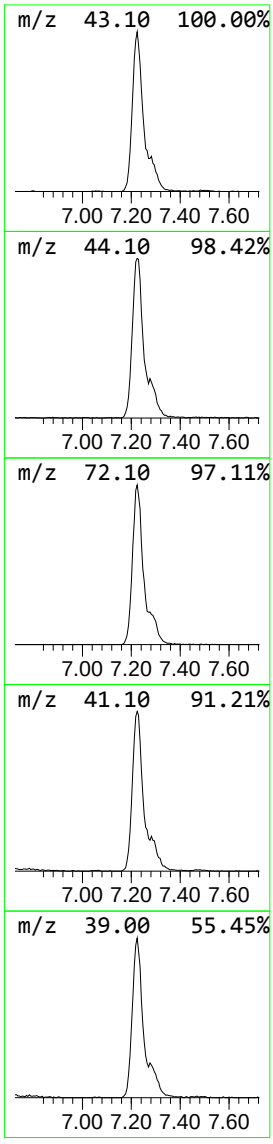
****

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	113.10 ug/l	1376540	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	80
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
4	Propane	44	C3H8	000074-98-6	35
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32





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

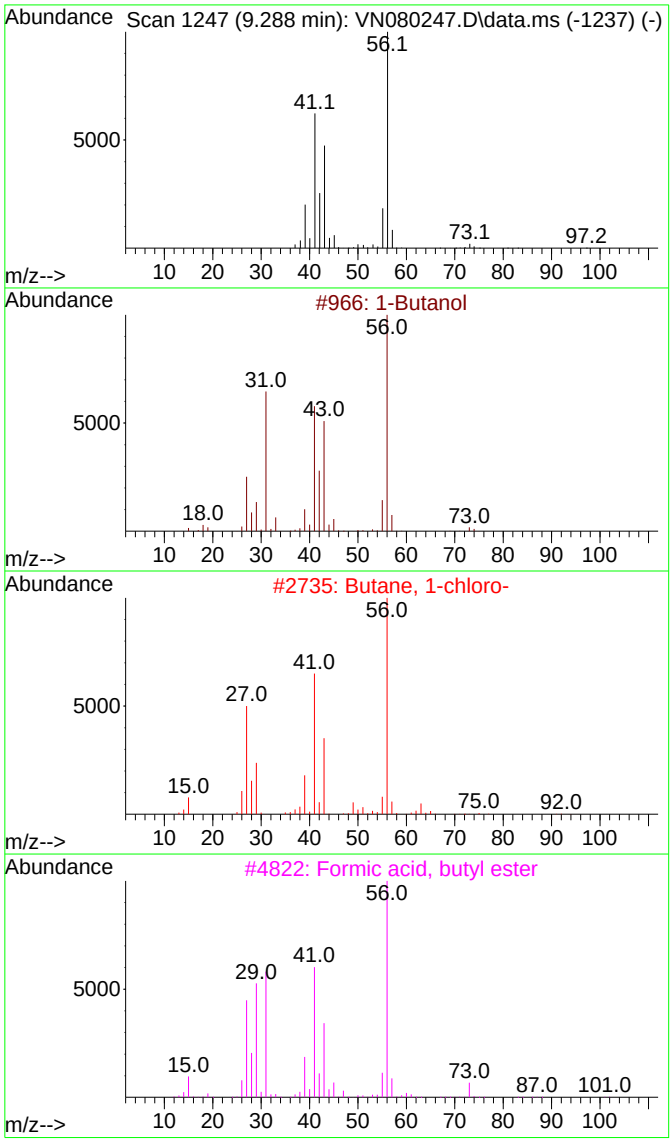
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

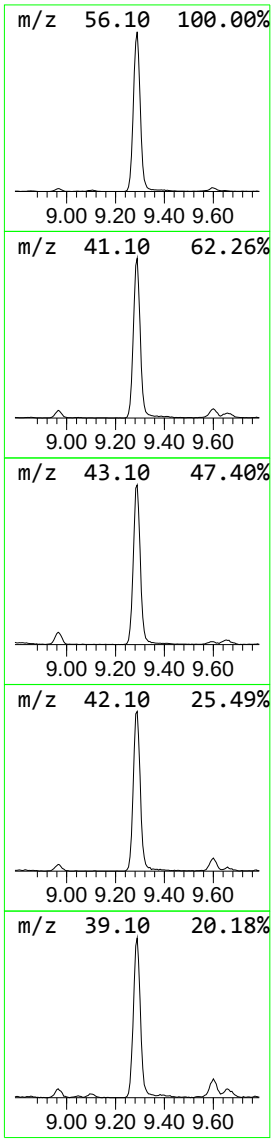
****

Peak Number 2 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.288	181.85 ug/l	2632130	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
3	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9





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

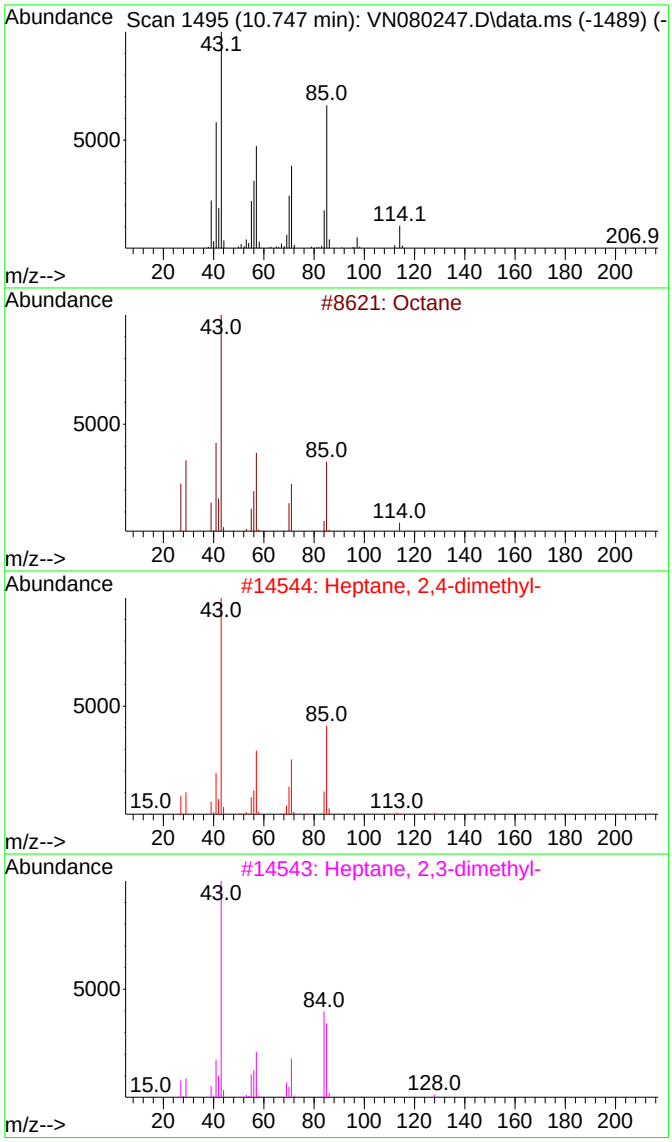
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

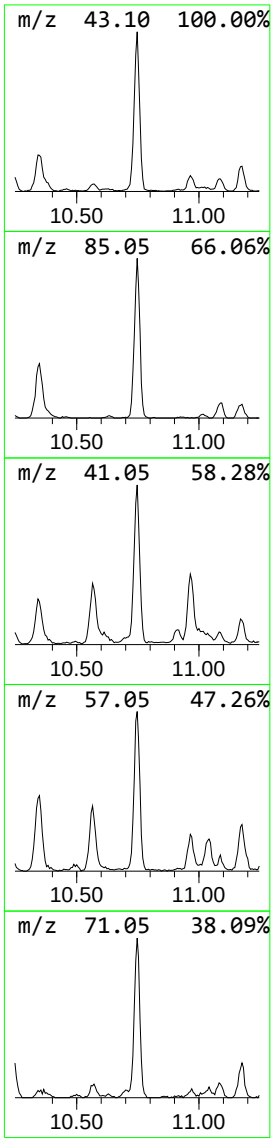
****

Peak Number 3 Octane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.747	31.64 ug/l	712474	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	91
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53
4	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	47
5	2-Ethylpiperazine	114	C6H14N2	013961-37-0	47





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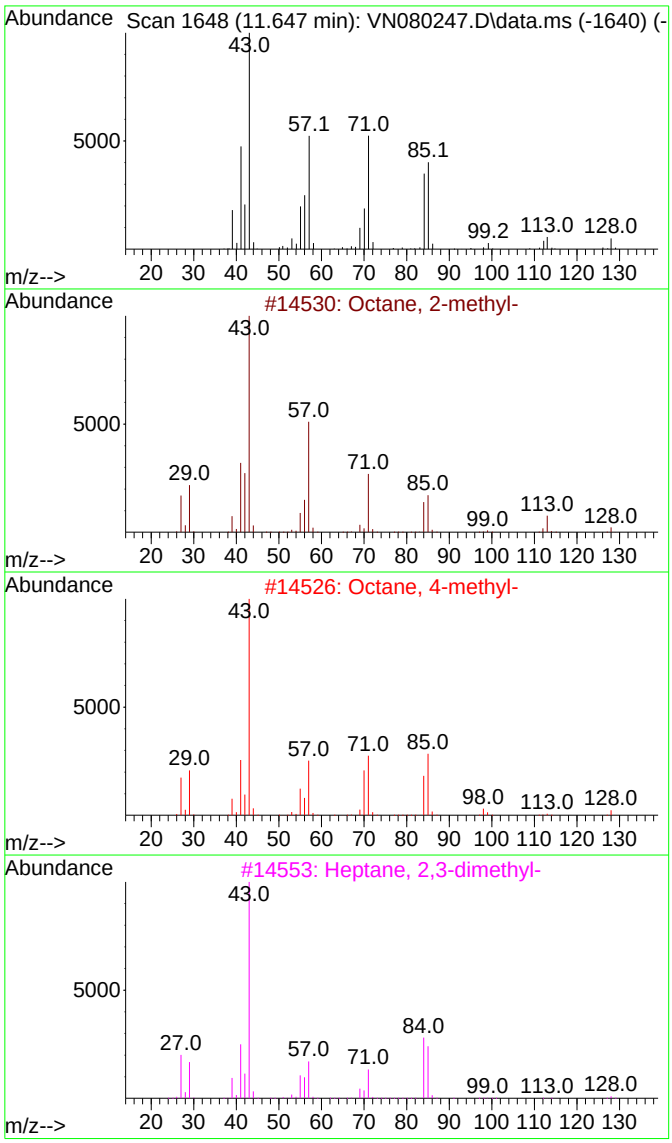
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

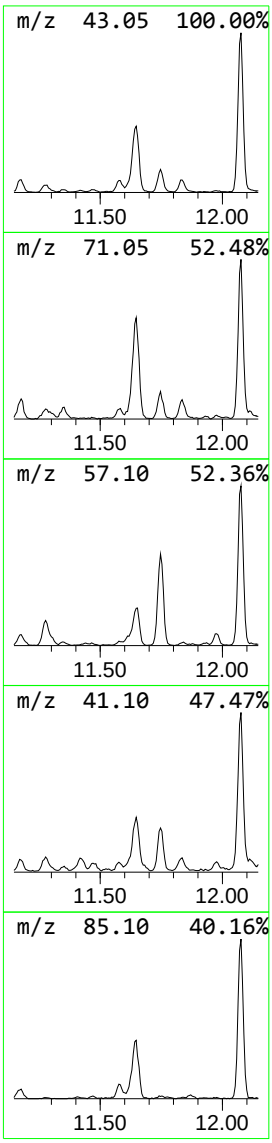
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.647	35.46 ug/l	798350	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	74
2	Octane, 4-methyl-	128	C9H20	002216-34-4	64
3	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	59
4	(2-Piperidin-3-ylethyl)amine	128	C7H16N2	089850-94-2	50
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50





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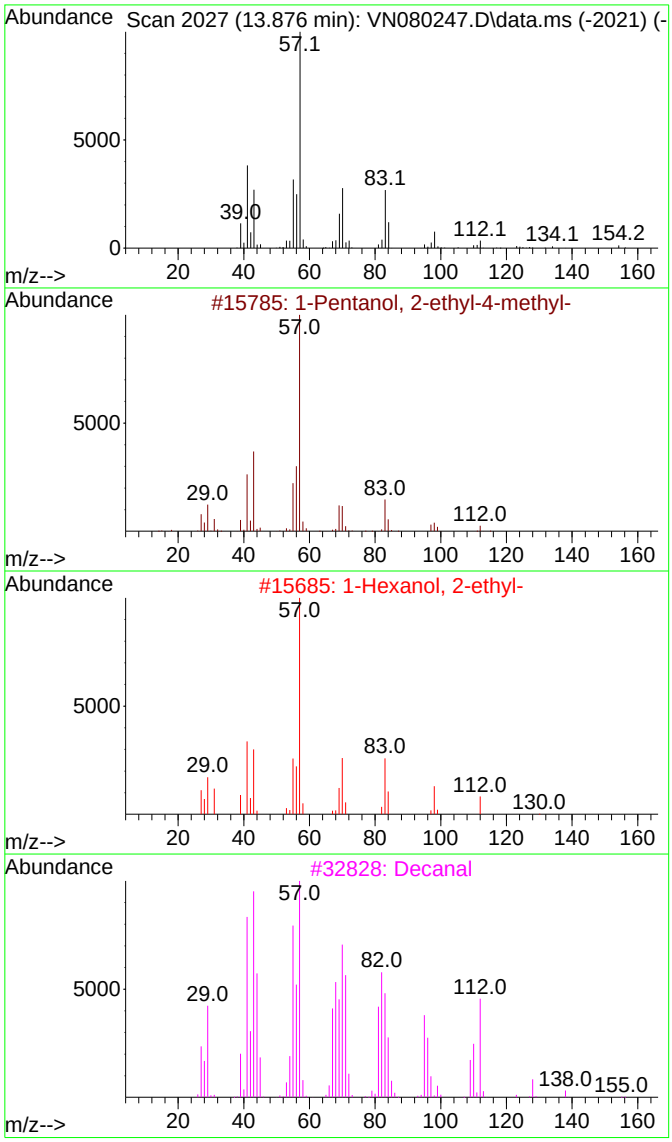
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

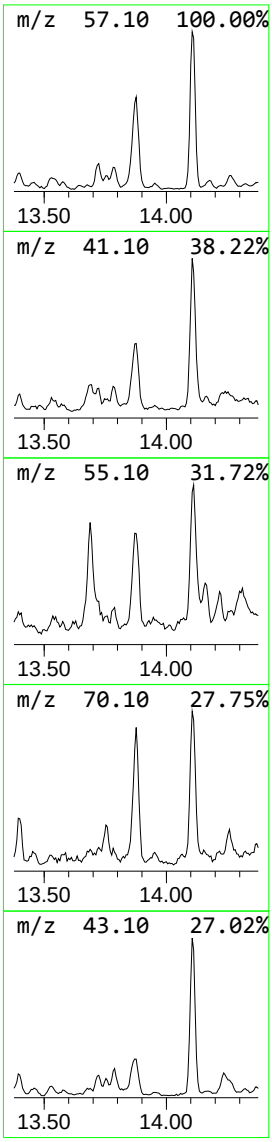
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Pentanol, 2-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	28.07 ug/l	765338	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3	Decanal	156	C10H20O	000112-31-2	53
4	1-Decene, 3,4-dimethyl-	168	C12H24	050871-03-9	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





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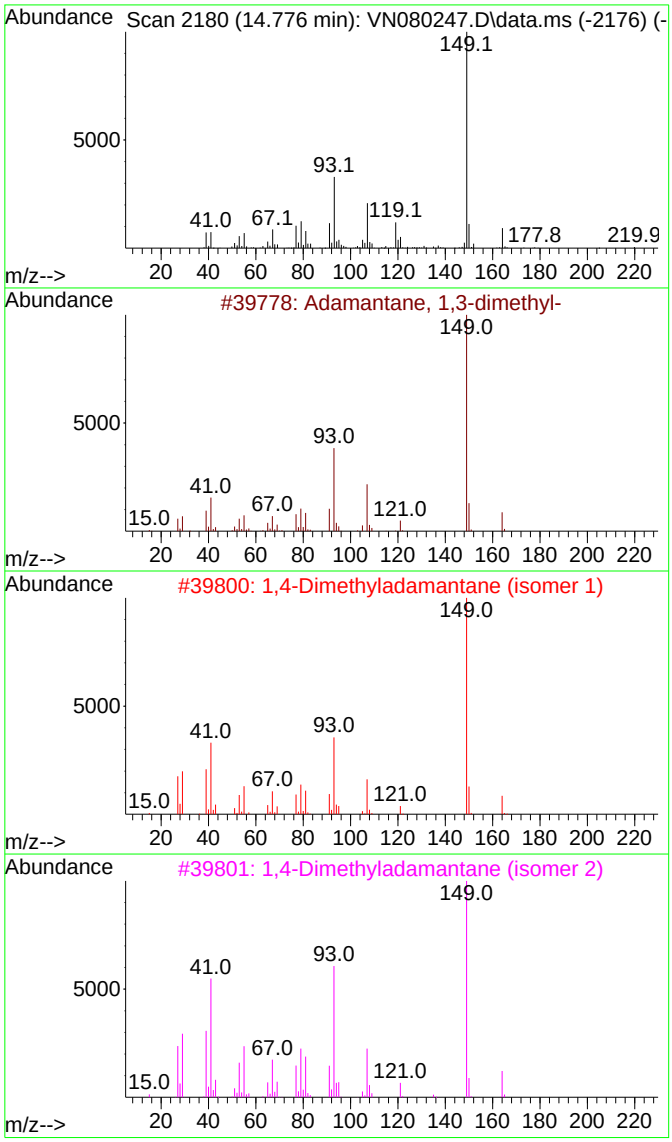
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

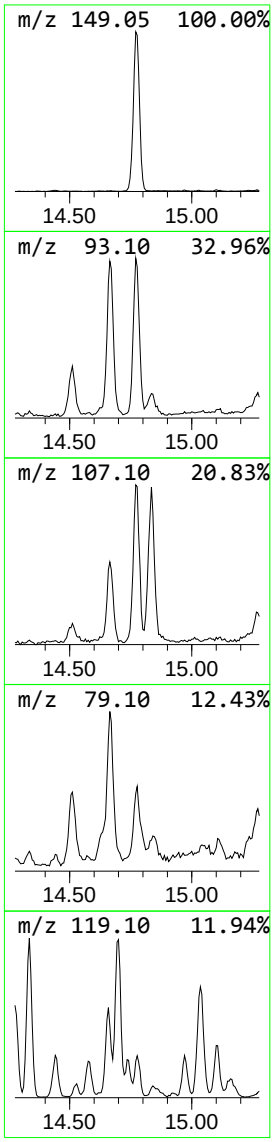
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Adamantane, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.776	41.92 ug/l	1143060	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	95
2	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	94
3	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	87
4	Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	64
5	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

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

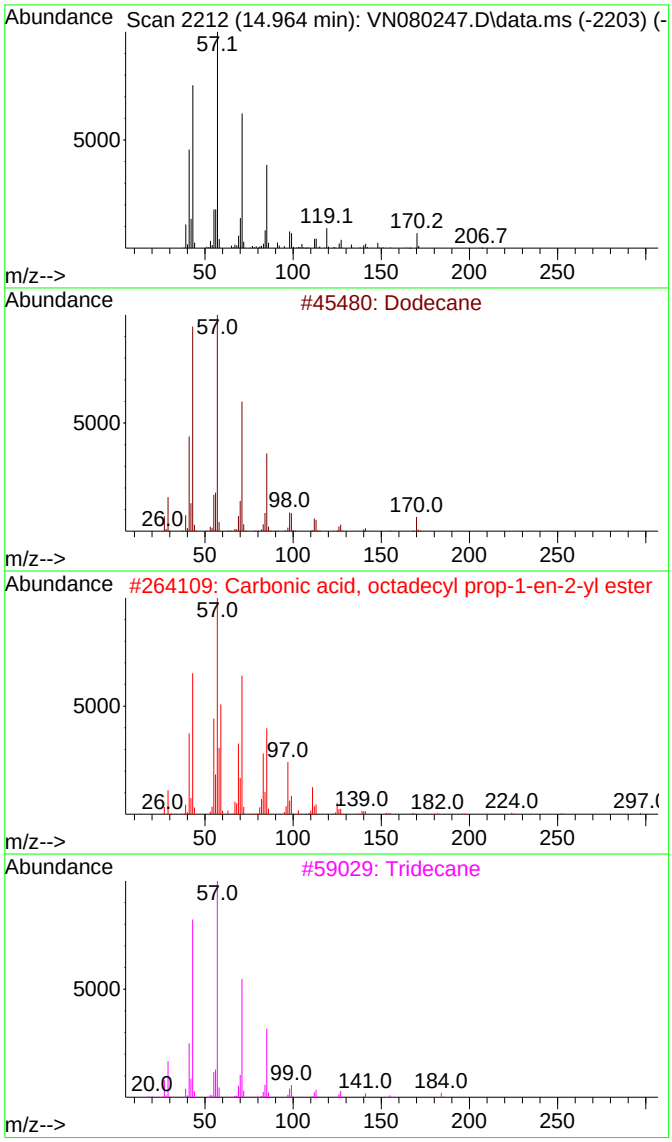
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

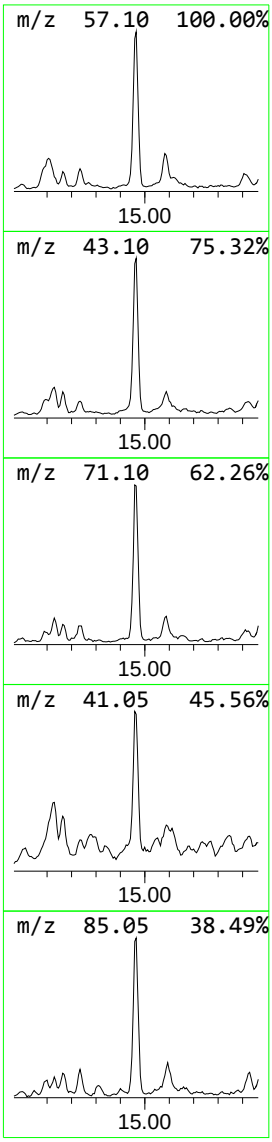
****

Peak Number 7 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	57.12 ug/l	1557720	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

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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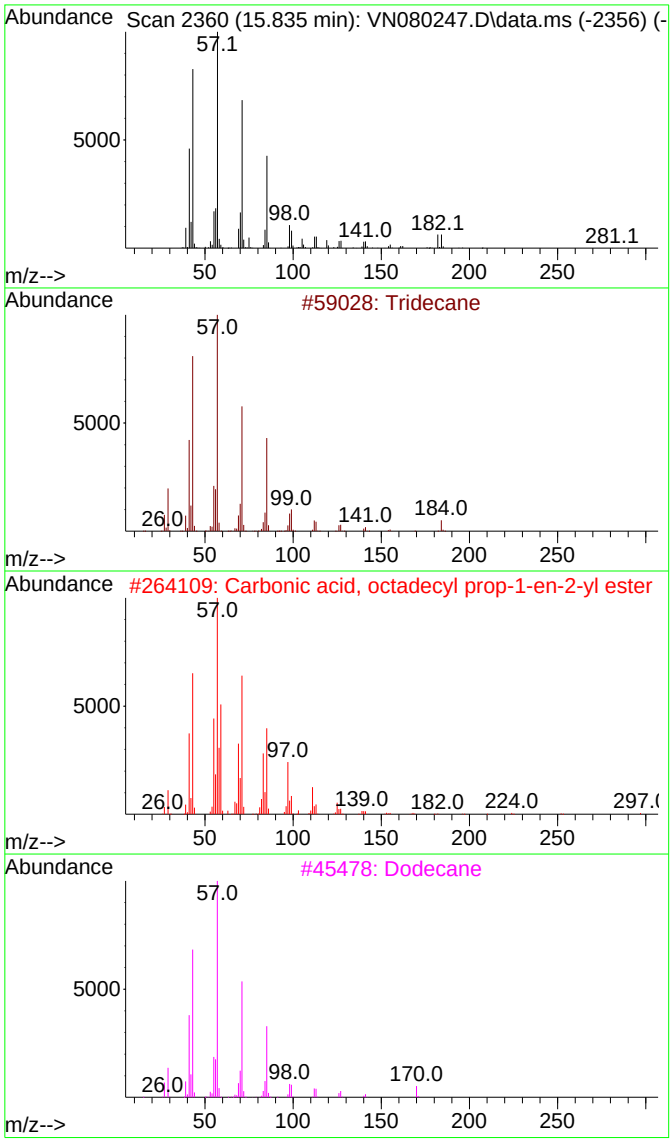
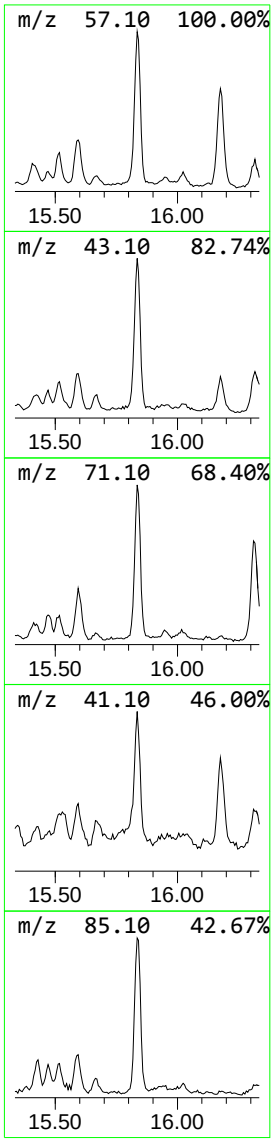
Peak Number 8 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	50.11 ug/l	1366430	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
3	Dodecane	170	C12H26	000112-40-3	86
4	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	80
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

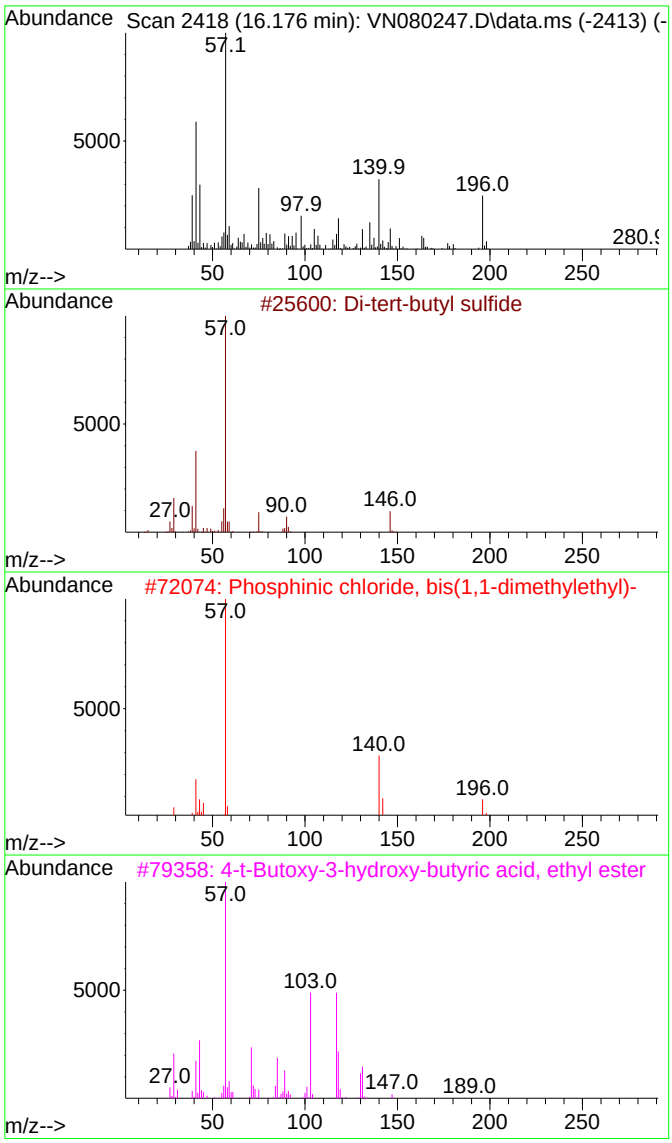
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

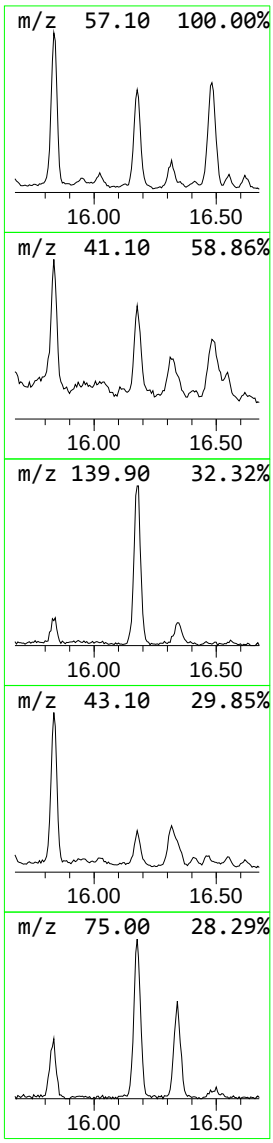
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 unknown16.176 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.176	29.40 ug/l	801848	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	10
2	Phosphinic chloride, bis(1,1-dim...	196	C8H18ClOP	000677-74-7	9
3	4-t-Butoxy-3-hydroxy-butyric aci...	204	C10H20O4	1010192-41-5	9
4	2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	9
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

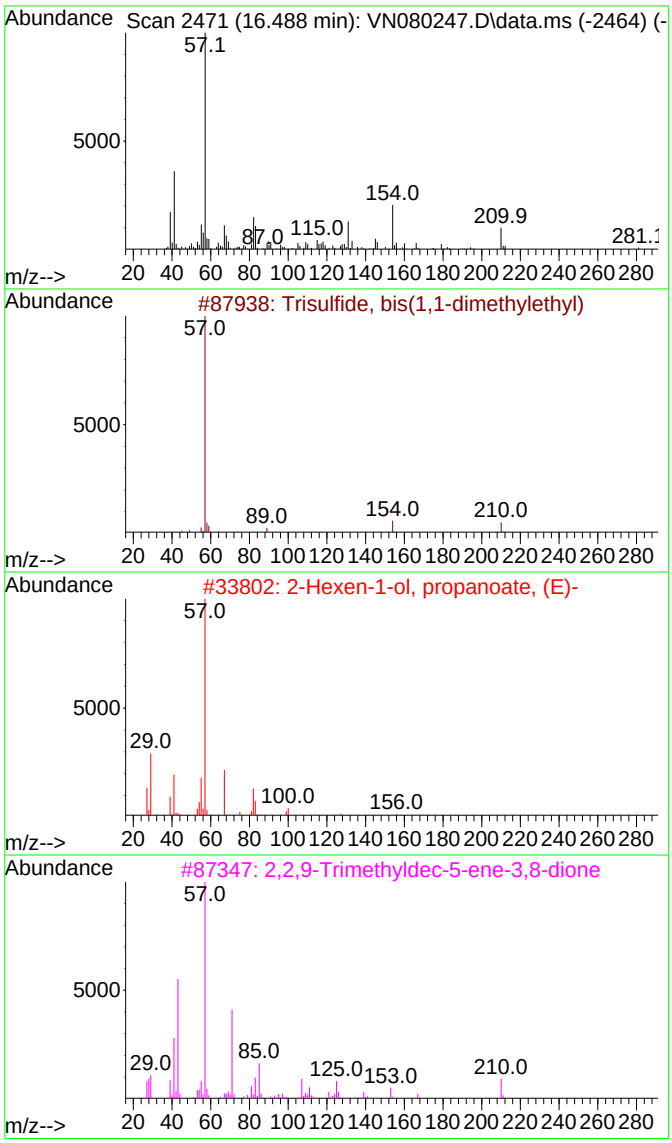
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

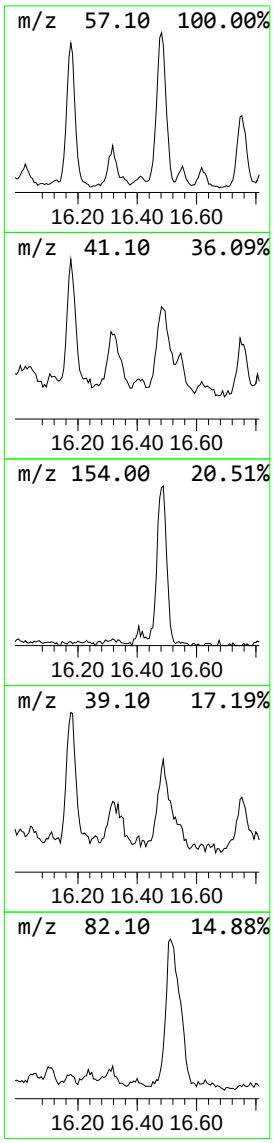
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.488 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	33.09 ug/l	902226	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	25
2	2-Hexen-1-ol, propanoate, (E)-	156	C9H16O2	053398-80-4	22
3	2,2,9-Trimethyldec-5-ene-3,8-dione	210	C13H22O2	083040-81-7	17
4	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	14
5	N-1-Butenyl-N-(1,2,2-trimethylpr...	211	C13H25NO	1000431-10-5	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080247.D
Acq On : 22 Nov 2023 15:07
Operator : JC\MD
Sample : 05518-04
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

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
Butanal	7.224	113.1	ug/l	1376540	1	8.224	608565	50.0
1-Butanol	9.288	181.8	ug/l	2632130	2	9.106	723700	50.0
Octane	10.747	31.6	ug/l	712474	3	11.870	1125770	50.0
Octane, 2-methyl-	11.647	35.5	ug/l	798350	3	11.870	1125770	50.0
1-Pentanol, 2-e...	13.876	28.1	ug/l	765338	4	13.794	1363480	50.0
Adamantane, 1,3...	14.776	41.9	ug/l	1143060	4	13.794	1363480	50.0
Dodecane	14.964	57.1	ug/l	1557720	4	13.794	1363480	50.0
Tridecane	15.835	50.1	ug/l	1366430	4	13.794	1363480	50.0
unknown16.176	16.176	29.4	ug/l	801848	4	13.794	1363480	50.0
unknown16.488	16.488	33.1	ug/l	902226	4	13.794	1363480	50.0