LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080249.D
Acq On : 22 Nov 2023 15:55
Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

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: VN080249.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	50	57	66	rVB4	14540	32031	2.41%	0.254%
2	2.871	135	156	157	rBV8	36235	125717	9.44%	0.997%
3	2.889	157	159	161	rVV3	11947	15068	1.13%	0.120%
4	2.924	161	165	166	rVV4	11716	20805	1.56%	0.165%
5	2.942	166	168	174	rVV4	16734	37219	2.80%	0.295%
6	5.042	516	525	533	rBV3	4363	16090	1.21%	0.128%
7	7.224	886	896	906	rBV2	81654	243741	18.31%	1.933%
8	8.165	1046	1056	1061	rBV2	191224	461399	34.65%	3.660%
9	8.224	1061	1066	1079	rVB	279202	619401	46.52%	4.913%
10	8.577	1113	1126	1138	rBV	192077	459952	34.54%	3.648%
11	8.794	1151	1163	1179	rVB4	14429	67020	5.03%	0.532%
12	9.100	1207	1215	1232	rVB	427935	872461	65.52%	6.921%
13	9.282	1238	1246	1260	rBV	188456	419640	31.52%	3.329%
14	9.382	1260	1263	1272	rVB6	7597	15728	1.18%	0.125%
15	9.600	1293	1300	1304	rBV5	12171	23645	1.78%	0.188%
16	9.659	1304	1310	1321	rVB2	15293	37907	2.85%	0.301%
17	10.341	1420	1426	1432	rBV3	8426	17438	1.31%	0.138%
18	10.571	1456	1465	1473	rBV	703188	1331546	100.00%	10.562%
19	10.629	1473	1475	1480	rVB3	12713	19201	1.44%	0.152%
20	10.747	1489	1495	1502	rVB5	24014	47237	3.55%	0.375%
21	10.965	1526	1532	1538	rBV	37182	66495	4.99%	0.527%
22	11.271	1581	1584	1591	rBV5	7791	15709	1.18%	0.125%
23	11.647	1639	1648	1656	rVB3	19374	45190	3.39%	0.358%
24	11.747	1659	1665	1671	rVB2	17490	29326	2.20%	0.233%
25	11.871	1674	1686	1695	rBV	668467	1208880	90.79%	9.589%
26	11.971	1698	1703	1709	rBV3	19042	31831	2.39%	0.252%
27	12.076	1712	1721	1727	rBV	105358	197328	14.82%	1.565%
28	12.400	1763	1776	1784	rBV3	32566	93566	7.03%	0.742%
29	12.482	1787	1790	1796	rVB6	9617	14574	1.09%	0.116%
30	12.623	1810	1814	1820	rVB6	8057	14273	1.07%	0.113%
31	12.800	1842	1844	1847	rVV2	15539	18794	1.41%	0.149%
32	12.853	1847	1853	1863	rVB	572034	994516	74.69%	7.889%
33	13.035	1878	1884	1888	rVB6	10136	21179	1.59%	0.168%
34	13.106	1889	1896	1900	rBV4	26826	60683	4.56%	0.481%
35	13.165	1901	1906	1913	rVV4	84935	166198	12.48%	1.318%
36	13.341	1929	1936	1941	rBV3	14014	30250	2.27%	0.240%

LSC Area Percent Report

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Integration Parameters: RTEINT.P
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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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Peak separation: 5

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

37	13.394	1942	1945	1951	rVB7	8157	14191	1.07%	0.113%
38	13.488	1952	1961	1966	rBV	49513	92845	6.97%	0.736%
39	13.541	1966	1970	1974	rVV6	11210	15372	1.15%	0.122%
40	13.688	1988	1995	1997	rBV5	25928	48336	3.63%	0.383%
41	13.794	2007	2013	2022	rBV	714510	1269763	95.36%	10.072%
42	13.876	2022	2027	2034	rVB	92296	174380	13.10%	1.383%
43	13.988	2043	2046	2049	rBV4	13796	23332	1.75%	0.185%
44	14.106	2061	2066	2073	rBV2	115453	210552	15.81%	1.670%
45	14.329	2100	2104	2110	rVB3	24418	39162	2.94%	0.311%
46	14.441	2117	2123	2128	rBV8	16485	34233	2.57%	0.272%
47	14.506	2128	2134	2141	rBV9	33288	86526	6.50%	0.686%
48	14.629	2150	2155	2158	rBV5	69501	117195	8.80%	0.930%
49	14.664	2158	2161	2166	rVV	61094	83013	6.23%	0.658%
50	14.735	2170	2173	2174	rBV3	26618	27104	2.04%	0.215%
51	14.776	2175	2180	2188	rVB5	96261	249187	18.71%	1.977%
52	14.959	2204	2211	2219	rBV	195046	327219	24.57%	2.596%
53	15.041	2221	2225	2230	rBV5	47702	112406	8.44%	0.892%
54	15.235	2255	2258	2261	rBV5	25378	34050	2.56%	0.270%
55	15.264	2261	2263	2267	rVB5	35719	45180	3.39%	0.358%
56	15.329	2269	2274	2280	rBV10	38001	98015	7.36%	0.777%
57	15.429	2284	2291	2296	rBV10	45625	119570	8.98%	0.948%
58	15.594	2315	2319	2327	rBV5	44643	94502	7.10%	0.750%
59	15.676	2329	2333	2335	rBV4	25617	43519	3.27%	0.345%
60	15.835	2355	2360	2371	rVB	243271	503318	37.80%	3.992%
61	15.970	2371	2383	2386	rBV	56002	200521	15.06%	1.591%
62	16.170	2413	2417	2425	rVB4	95820	187298	14.07%	1.486%
63	16.317	2437	2442	2446	rBV5	54225	110933	8.33%	0.880%
64	16.494	2464	2472	2478	rBV6	78403	276292	20.75%	2.192%
65	16.711	2505	2509	2512	rBV5	40922	76656	5.76%	0.608%

Sum of corrected areas: 12606708

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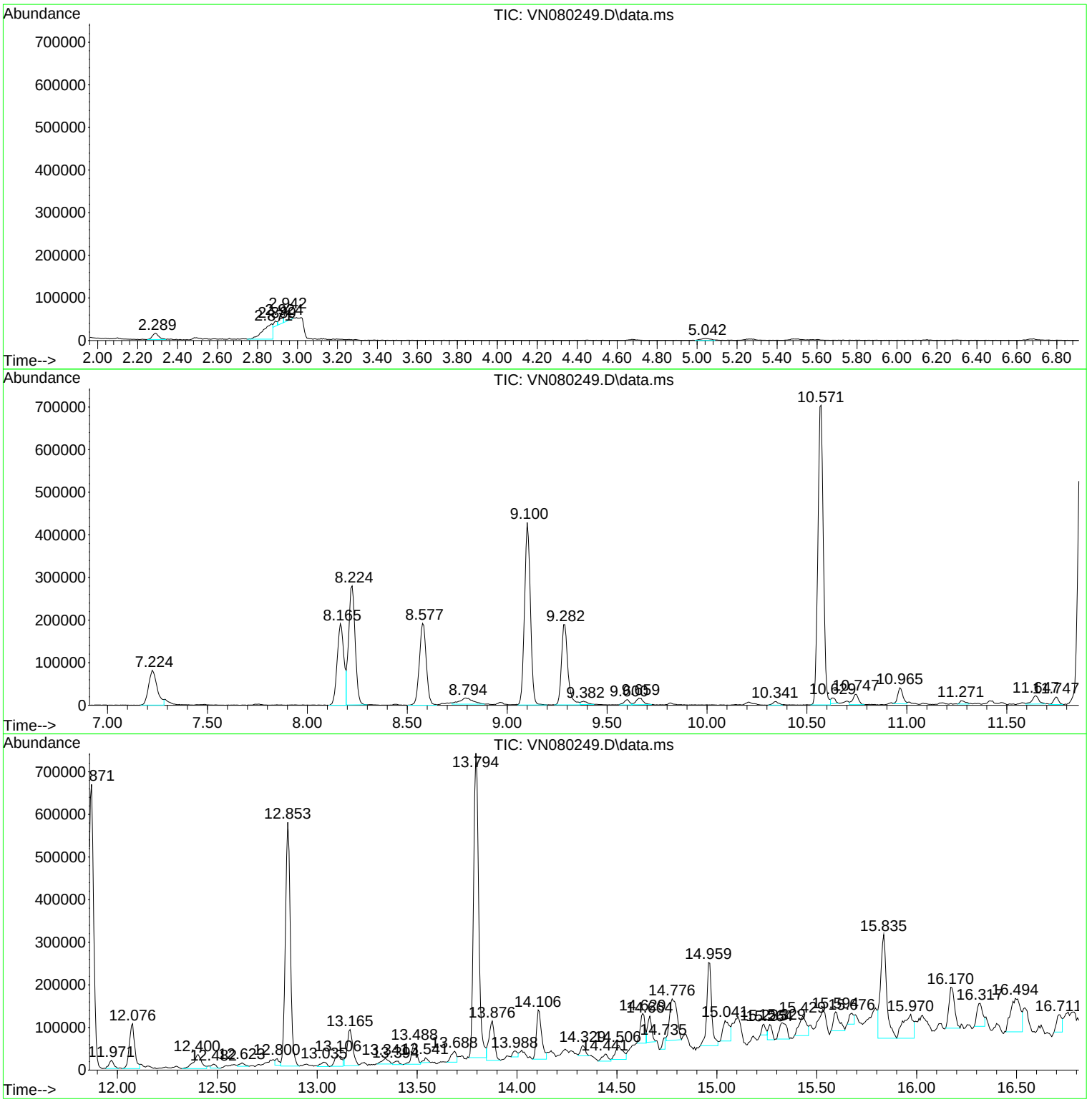
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

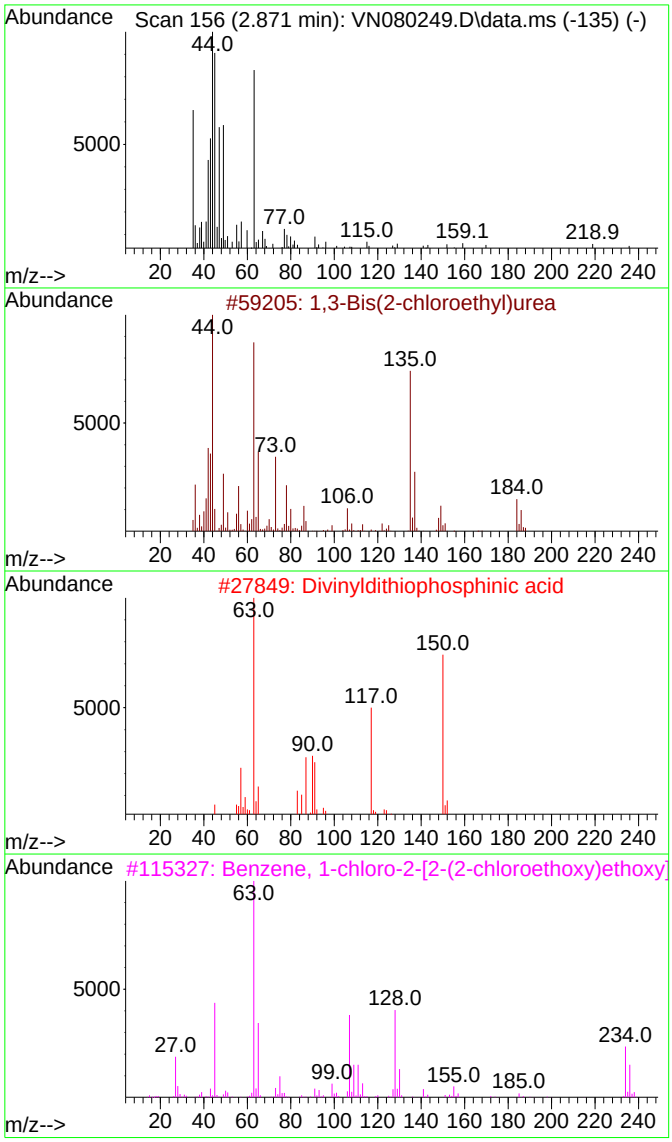
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

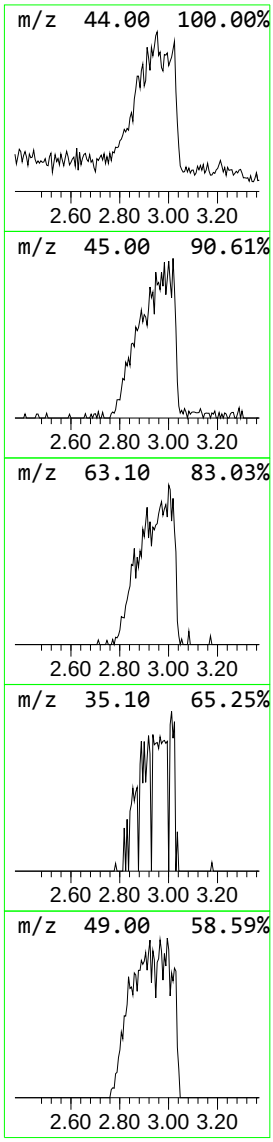
****

Peak Number 1 unknown2.871 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.871	10.15 ug/l	125717	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Bis(2-chloroethyl)urea	184	C5H10Cl2N2O	002214-72-4	25
2	Divinyldithiophosphinic acid	150	C4H7PS2	085417-00-1	23
3	Benzene, 1-chloro-2-[2-(2-chloro...	234	C10H12Cl2O2	007501-11-3	10
4	Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	10
5	Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	10





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

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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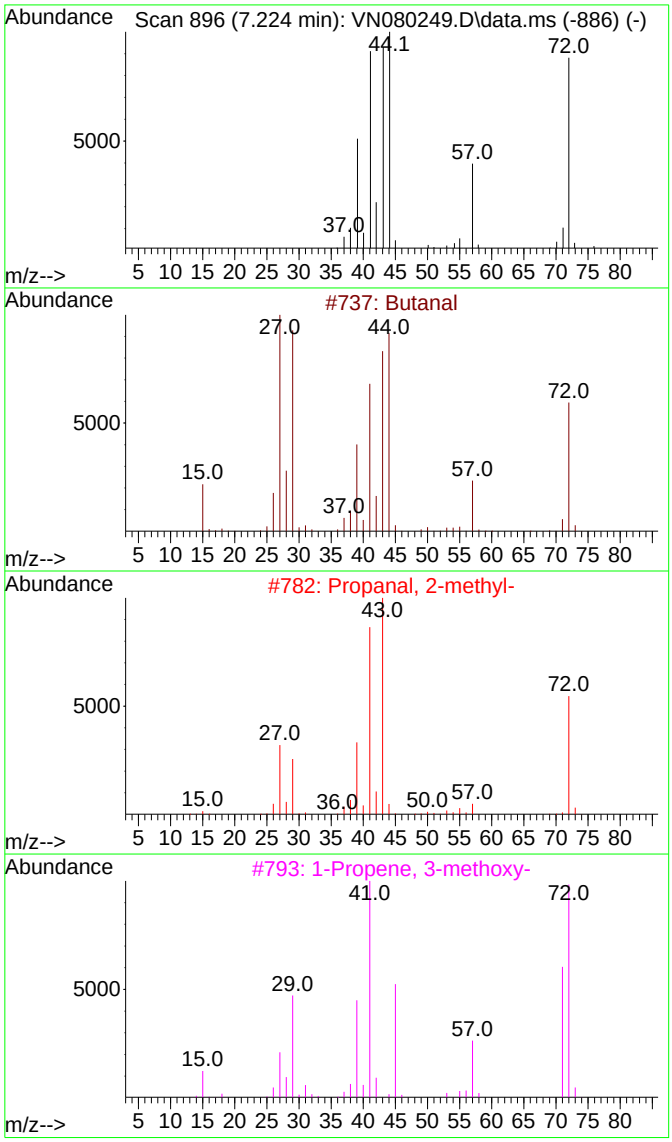
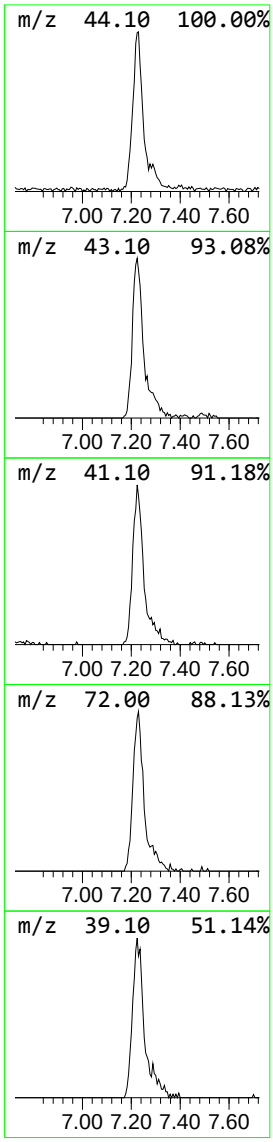
Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	19.68 ug/l	243741	Pentafluorobenzene	8.224

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	43
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	32
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	28





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Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

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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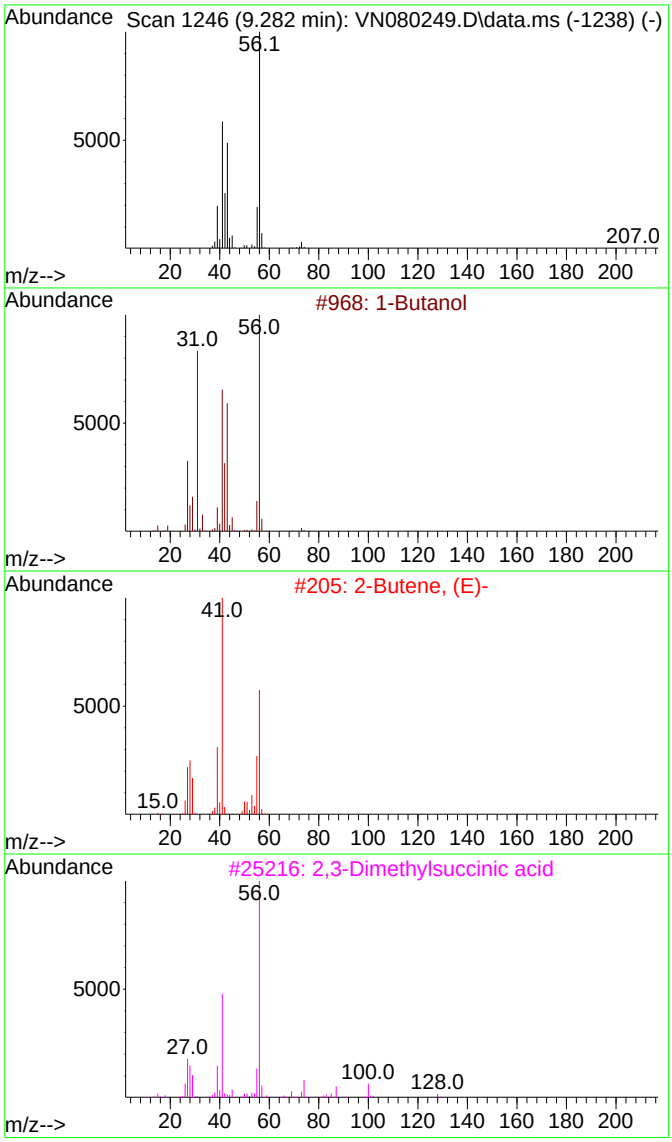
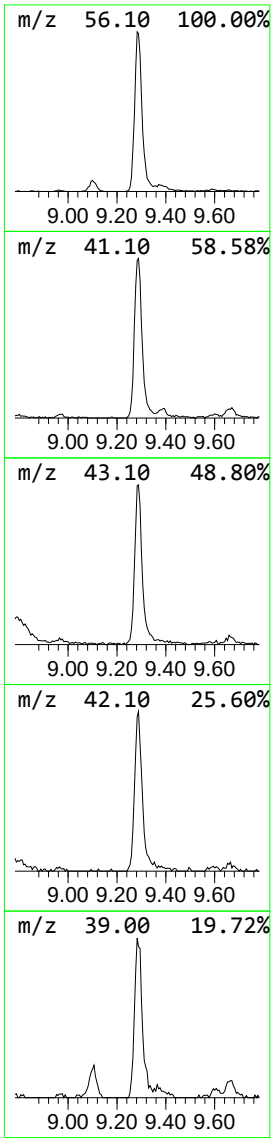
Peak Number 3 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.282	24.05 ug/l	419640	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	2-Butene, (E)-	56	C4H8	000624-64-6	47
3	2,3-Dimethylsuccinic acid	146	C6H10O4	013545-04-5	42
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	39





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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

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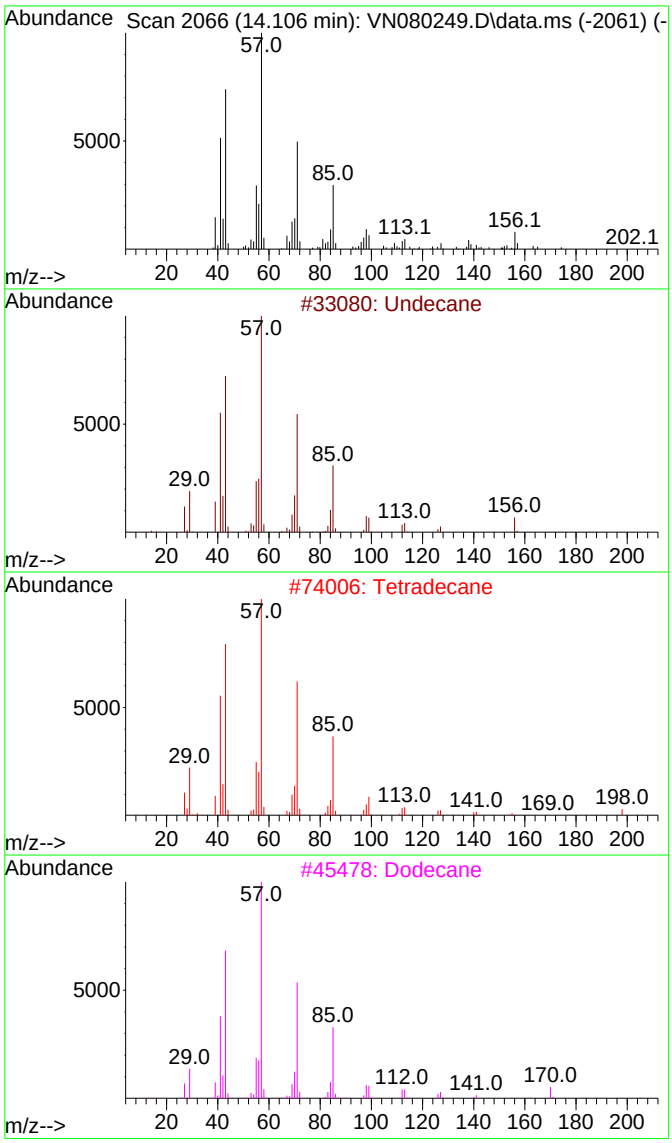
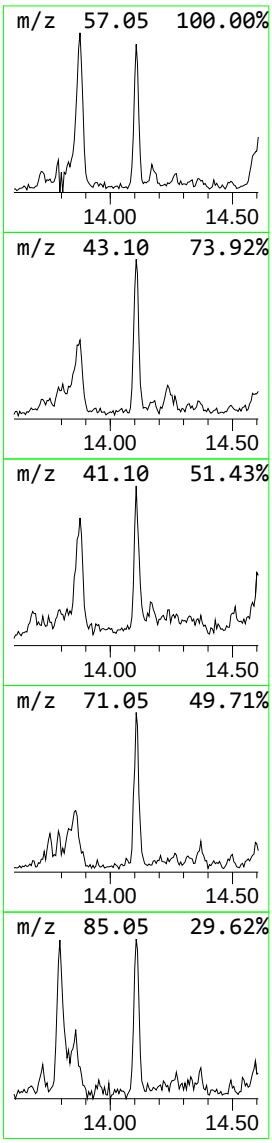
Peak Number 4 Undecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	8.29 ug/l	210552	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Tetradecane	198	C14H30	000629-59-4	86
3	Dodecane	170	C12H26	000112-40-3	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	80





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

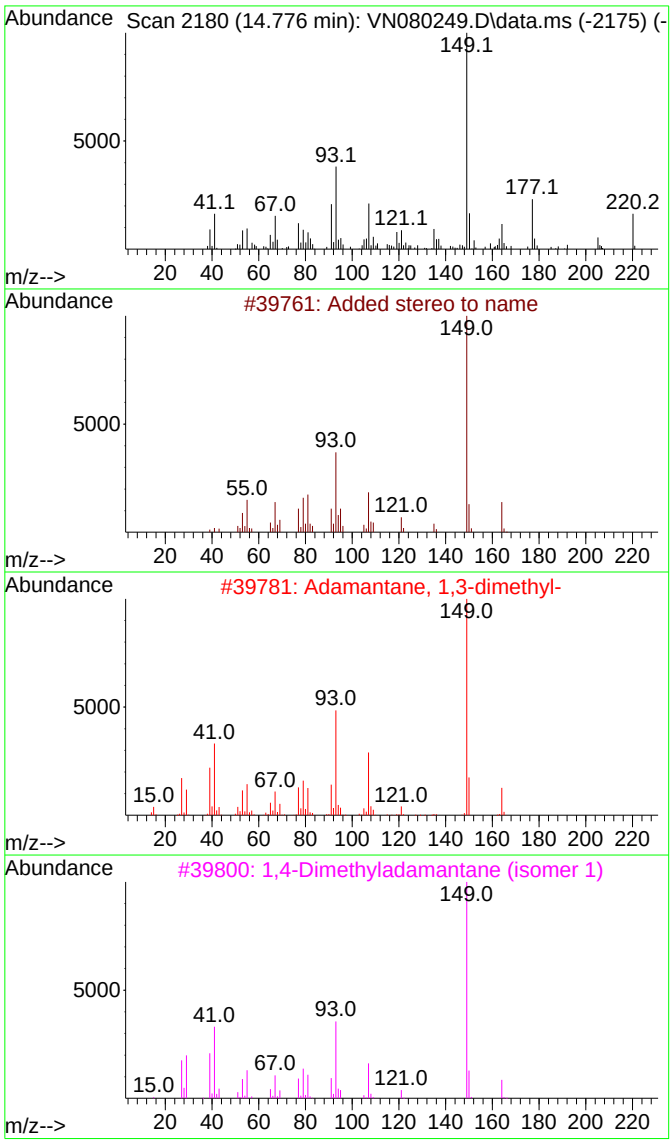
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

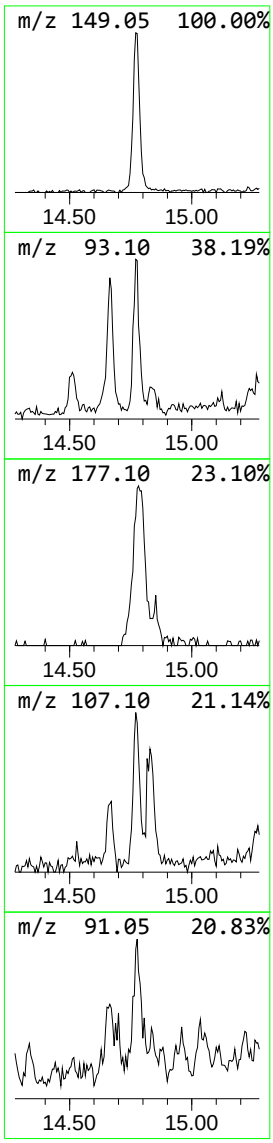
****

Peak Number 5 Adamantane, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.776	9.81 ug/l	249187	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name	164	C12H20	024145-89-9	72
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	68
3	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	64
4	Adamantane, 1-isothiocyanato-3-m...	207	C12H17NS	136860-48-5	62
5	3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	50





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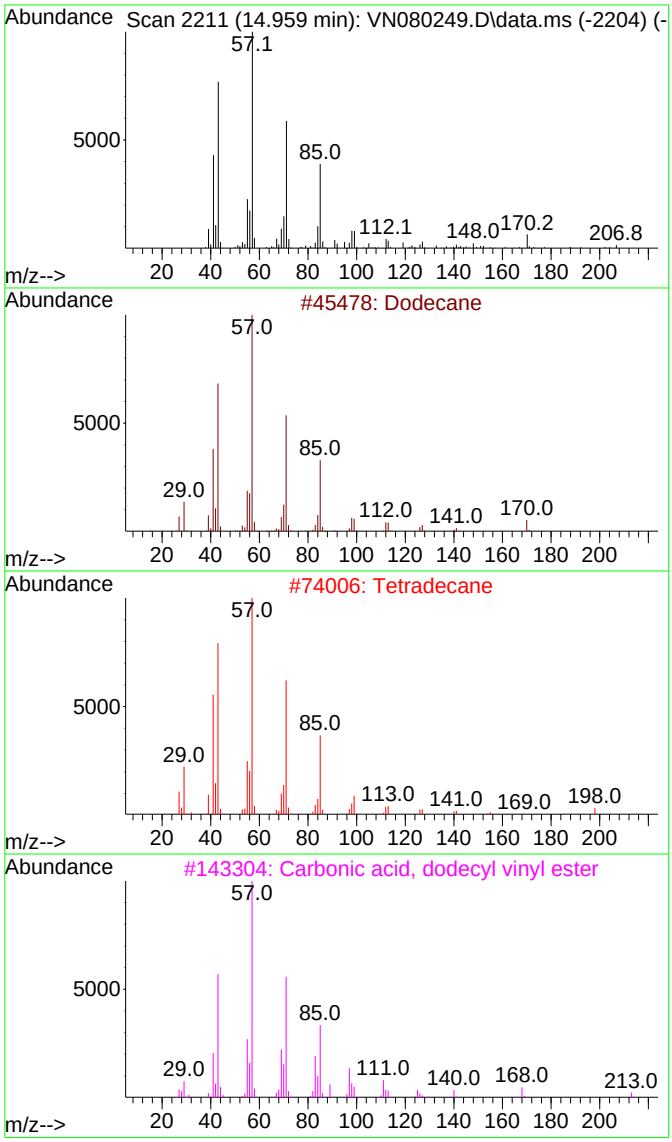
Quant Title : SW846 8260

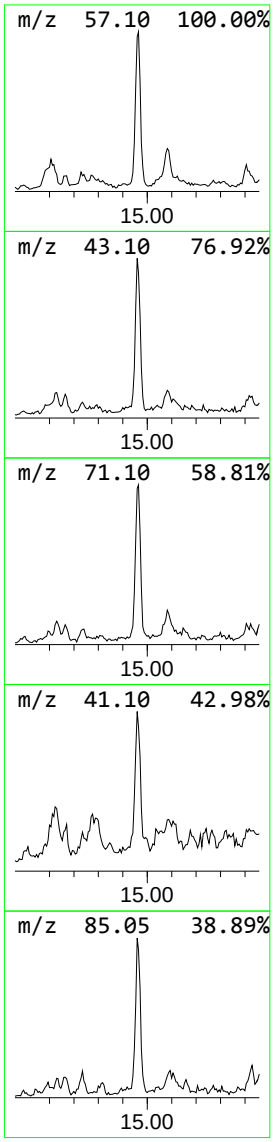
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	12.89 ug/l	327219	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Tetradecane	198	C14H30	000629-59-4	91
3	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tridecane	184	C13H28	000629-50-5	86





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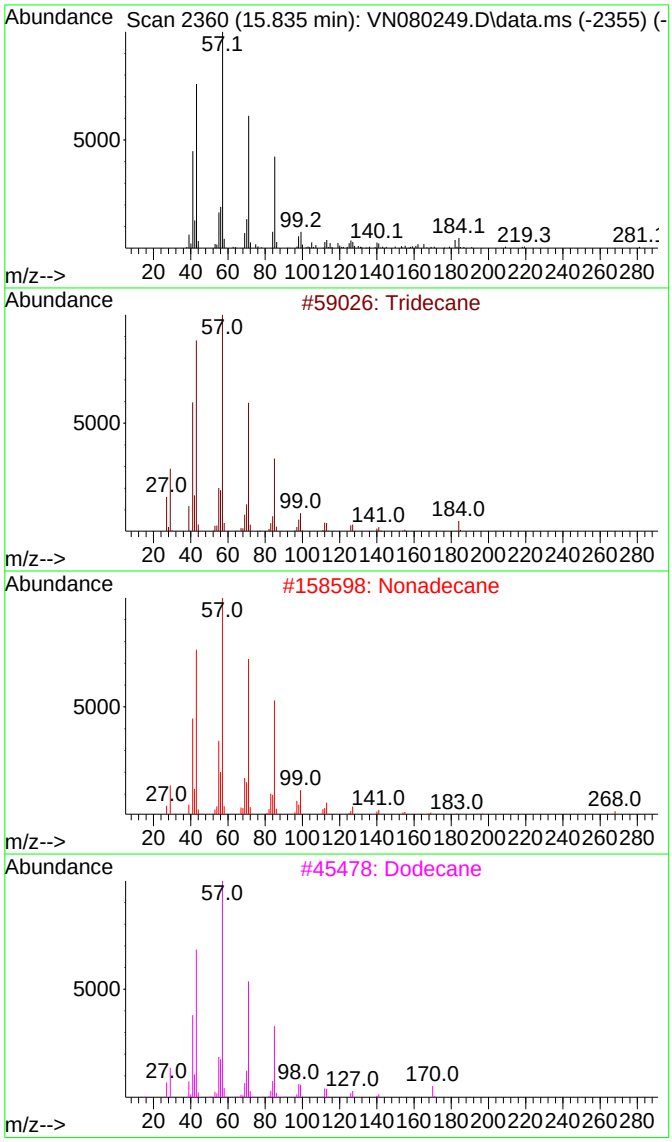
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

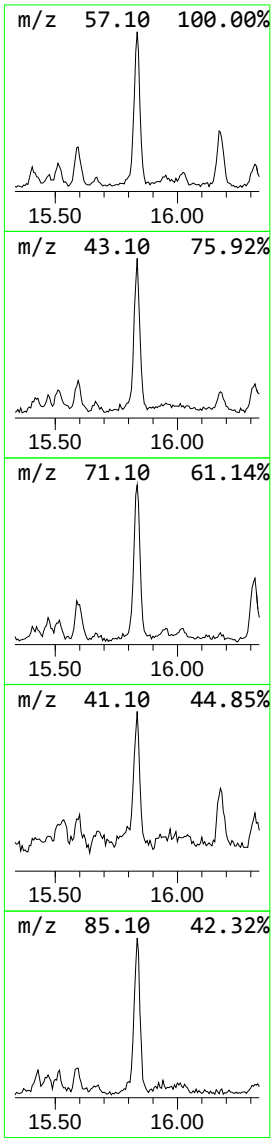
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	19.82 ug/l	503318	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Nonadecane	268	C19H40	000629-92-5	86
3	Dodecane	170	C12H26	000112-40-3	86
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
5	Tetradecane	198	C14H30	000629-59-4	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080249.D
Acq On : 22 Nov 2023 15:55
Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

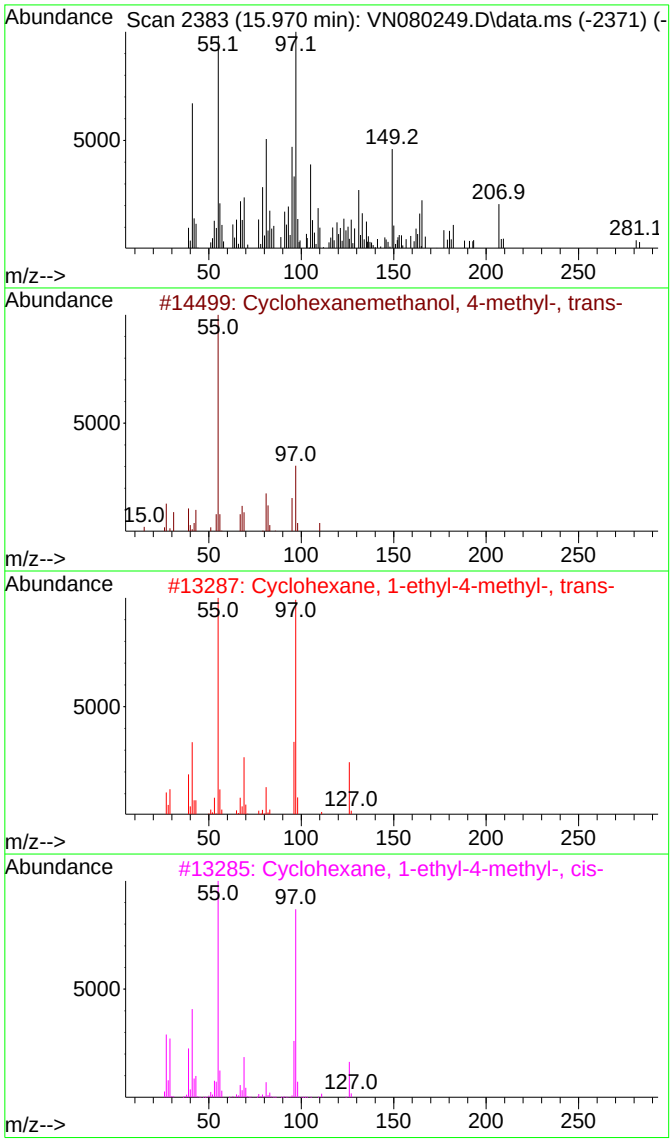
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

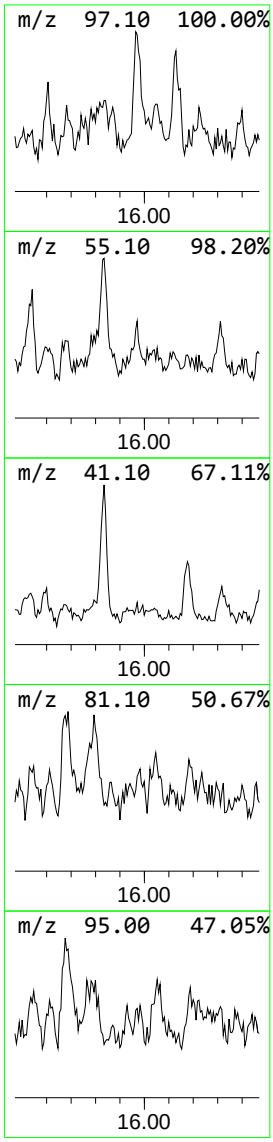
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown15.970 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.970	7.90 ug/l	200521	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	35
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	30
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	30
4	3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	27
5	1-Methylpyrazol-3-amine	97	C4H7N3	001904-31-0	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080249.D
Acq On : 22 Nov 2023 15:55
Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

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

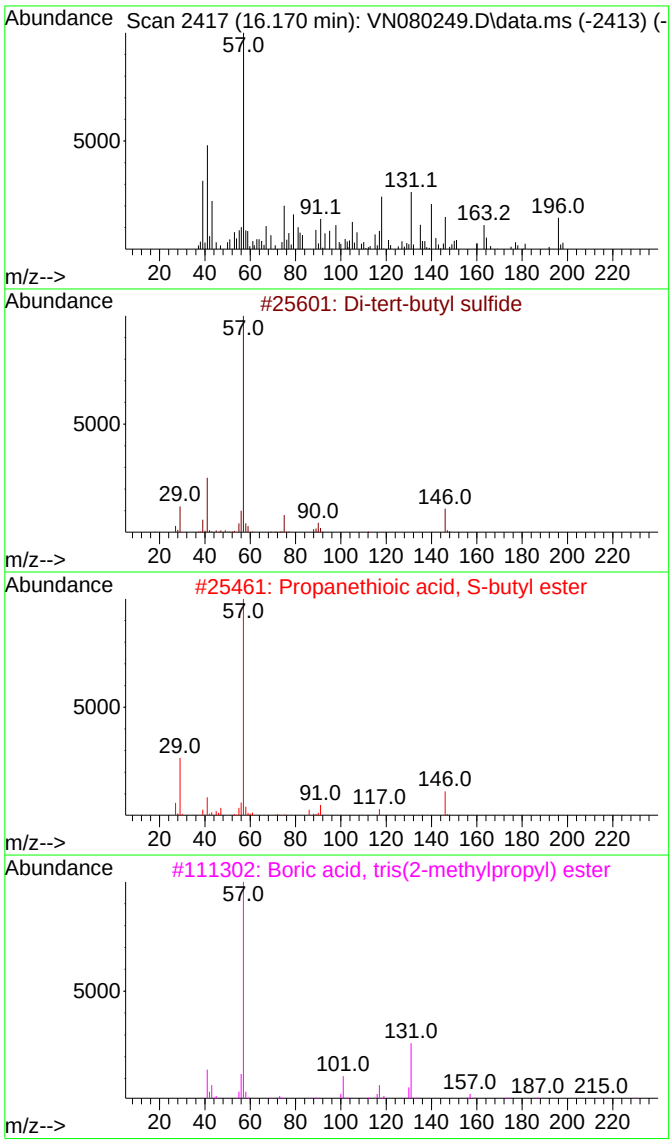
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

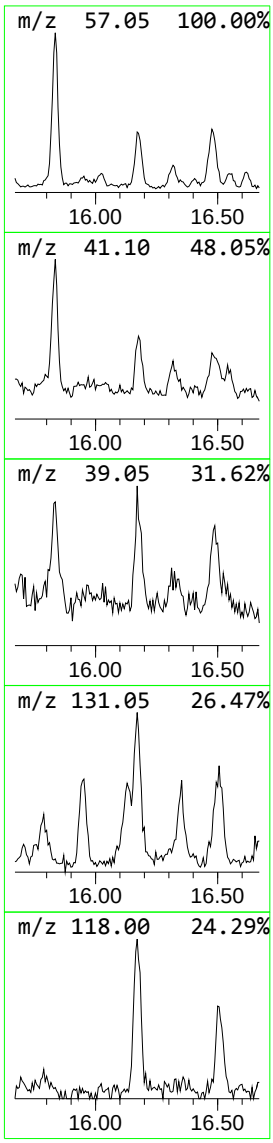
****

Peak Number 9 unknown16.170 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	7.38 ug/l	187298	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	11
2	Propanethioic acid, S-butyl ester	146	C7H14OS	002432-44-2	11
3	Boric acid, tris(2-methylpropyl)...	230	C12H27BO3	013195-76-1	10
4	Phosphinic chloride, bis(1,1-dim...	196	C8H18ClOP	000677-74-7	10
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080249.D
Acq On : 22 Nov 2023 15:55
Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

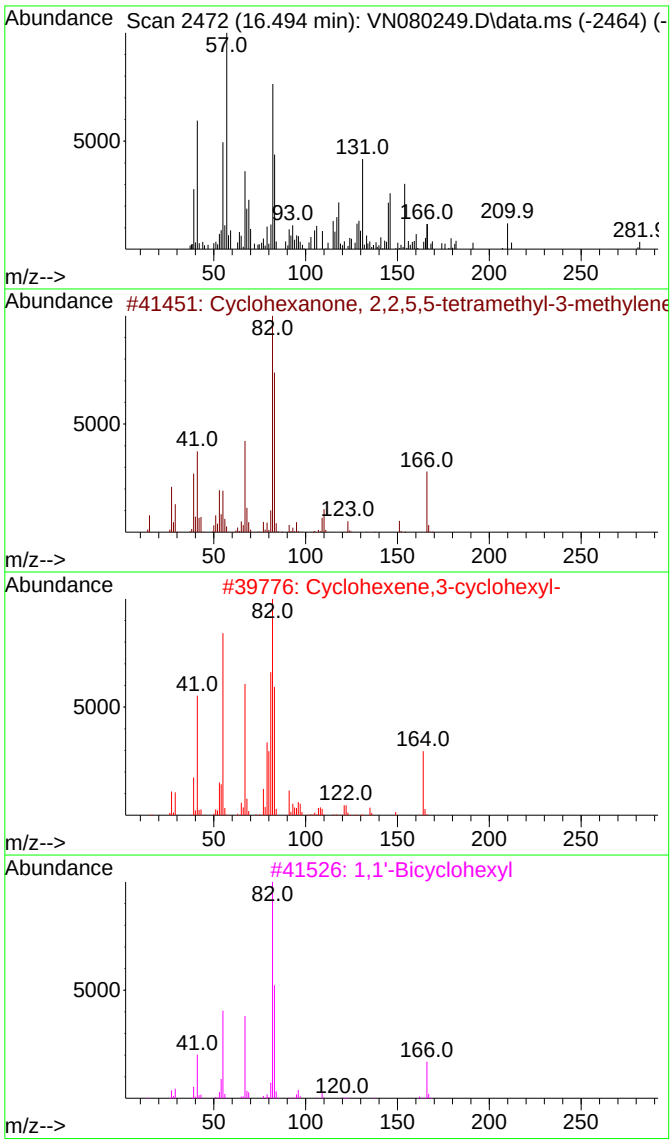
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

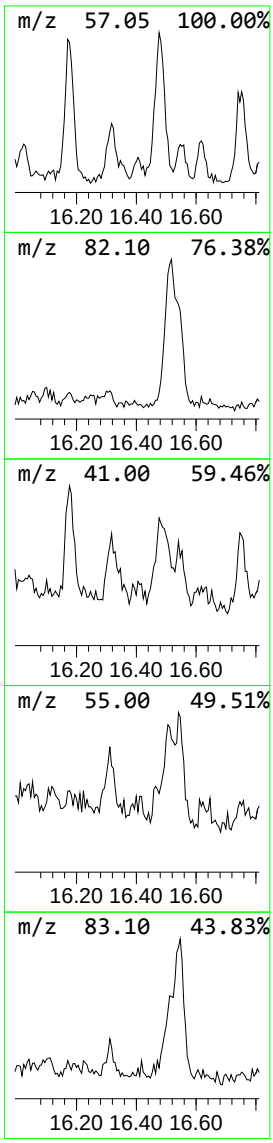
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.494 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.494	10.88 ug/l	276292	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,2,5,5-tetrameth...	166	C11H18O	035505-97-6	43
2	Cyclohexene,3-cyclohexyl-	164	C12H20	001808-09-9	38
3	1,1'-Bicyclohexyl	166	C12H22	000092-51-3	38
4	Carbonic acid, 2,2,2-trichloroet...	274	C9H13Cl3O3	1000357-89-5	35
5	Succinic acid, dodec-2-en-1-yl t...	366	C22H38O4	1000391-12-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080249.D
Acq On : 22 Nov 2023 15:55
Operator : JC\MD
Sample : 05518-05
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1110

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
unknown2.871	2.871	10.2	ug/l	125717	1	8.224	619401	50.0
Butanal	7.224	19.7	ug/l	243741	1	8.224	619401	50.0
1-Butanol	9.282	24.1	ug/l	419640	2	9.100	872461	50.0
Undecane	14.106	8.3	ug/l	210552	4	13.794	1269760	50.0
Adamantane, 1,3...	14.776	9.8	ug/l	249187	4	13.794	1269760	50.0
Dodecane	14.959	12.9	ug/l	327219	4	13.794	1269760	50.0
Tridecane	15.835	19.8	ug/l	503318	4	13.794	1269760	50.0
unknown15.970	15.970	7.9	ug/l	200521	4	13.794	1269760	50.0
unknown16.170	16.170	7.4	ug/l	187298	4	13.794	1269760	50.0
unknown16.494	16.494	10.9	ug/l	276292	4	13.794	1269760	50.0