LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071423\
Data File : VN078522.D
Acq On : 14 Jul 2023 15:11
Operator : JC\MD
Sample : 03620-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 713-C

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\82N071023W.M
Title : SW846 8260

Signal : TIC: VN078522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.095	17	24	31	rVB3	89635	144695	6.52%	0.625%
2	2.489	83	91	95	rBV3	28094	54028	2.43%	0.234%
3	2.665	116	121	129	rBV	78236	135715	6.11%	0.587%
4	2.824	143	148	159	rVB4	25782	59404	2.68%	0.257%
5	3.812	308	316	325	rBV4	8436	23030	1.04%	0.100%
6	4.448	414	424	434	rBV2	94853	284871	12.83%	1.231%
7	4.748	464	475	483	rBV5	13332	41514	1.87%	0.179%
8	4.871	485	496	504	rVB4	9767	33617	1.51%	0.145%
9	5.547	597	611	629	rBV2	148517	546639	24.62%	2.362%
10	6.689	793	805	818	rBV5	54362	188036	8.47%	0.813%
11	7.242	888	899	911	rBV3	52243	151961	6.84%	0.657%
12	7.494	926	942	955	rBV	521061	1378802	62.10%	5.959%
13	7.794	986	993	1001	rBV2	56157	142513	6.42%	0.616%
14	8.177	1044	1058	1063	rBV	380016	945243	42.57%	4.085%
15	8.236	1063	1068	1078	rVB	577181	1245970	56.12%	5.385%
16	8.606	1115	1131	1145	rBV3	535991	1788606	80.56%	7.730%
17	8.712	1146	1149	1161	rVV7	10662	38848	1.75%	0.168%
18	8.830	1161	1169	1180	rVB9	17061	70233	3.16%	0.304%
19	9.112	1208	1217	1229	rBV	816177	1716136	77.30%	7.417%
20	9.277	1239	1245	1256	rBV3	23799	55936	2.52%	0.242%
21	9.535	1283	1289	1296	rBV3	19389	41071	1.85%	0.178%
22	9.671	1307	1312	1321	rVB6	10362	33970	1.53%	0.147%
23	10.453	1437	1445	1452	rBV3	19501	34218	1.54%	0.148%
24	10.577	1457	1466	1471	rVV	1192327	2220220	100.00%	9.595%
25	10.635	1471	1476	1488	rVV	684532	1336503	60.20%	5.776%
26	11.271	1579	1584	1588	rBV	35906	64489	2.90%	0.279%
27	11.353	1594	1598	1605	rVB4	19180	35256	1.59%	0.152%
28	11.871	1674	1686	1697	rBV	1171553	2144774	96.60%	9.269%
29	11.971	1697	1703	1711	rVV2	102084	193454	8.71%	0.836%
30	12.076	1711	1721	1732	rVV	266901	526130	23.70%	2.274%
31	12.218	1732	1745	1753	rVB7	31514	85230	3.84%	0.368%
32	12.412	1763	1778	1785	rBV4	305726	702154	31.63%	3.035%
33	12.853	1844	1853	1860	rBV	988756	1767661	79.62%	7.640%
34	12.965	1867	1872	1879	rVB8	9352	22438	1.01%	0.097%
35	13.106	1890	1896	1900	rBV2	24721	50171	2.26%	0.217%
36	13.171	1903	1907	1912	rVB4	20529	40177	1.81%	0.174%

LSC Area Percent Report

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
713-C

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\82N071023W.M
Title : SW846 8260

37	13.347	1932	1937	1947	rVB4	31491	69963	3.15%	0.302%
38	13.447	1947	1954	1956	rBV5	10479	22604	1.02%	0.098%
39	13.488	1956	1961	1965	rVV2	64262	129880	5.85%	0.561%
40	13.535	1965	1969	1975	rVV2	135454	244106	10.99%	1.055%
41	13.588	1975	1978	1983	rVB2	30370	47781	2.15%	0.207%
42	13.800	2006	2014	2021	rBV	1131082	1987696	89.53%	8.591%
43	13.876	2021	2027	2036	rVB	574767	965821	43.50%	4.174%
44	14.000	2044	2048	2052	rVB3	22000	37596	1.69%	0.162%
45	14.182	2072	2079	2086	rBV	361791	614985	27.70%	2.658%
46	14.300	2093	2099	2102	rVB7	11953	22406	1.01%	0.097%
47	14.470	2123	2128	2134	rBV8	17194	28025	1.26%	0.121%
48	14.535	2134	2139	2146	rBV8	10573	27816	1.25%	0.120%
49	14.629	2151	2155	2160	rVV7	17572	28983	1.31%	0.125%
50	14.800	2180	2184	2189	rVB5	20647	32794	1.48%	0.142%
51	15.123	2235	2239	2244	rVB4	26529	49523	2.23%	0.214%
52	15.206	2246	2253	2261	rBV8	23687	59930	2.70%	0.259%
53	15.323	2268	2273	2278	rVB8	13045	26098	1.18%	0.113%
54	15.588	2314	2318	2320	rBV3	18613	24342	1.10%	0.105%
55	15.647	2322	2328	2340	rVB	174517	350969	15.81%	1.517%
56	16.500	2463	2473	2475	rBV7	9087	23258	1.05%	0.101%

Sum of corrected areas: 23138289

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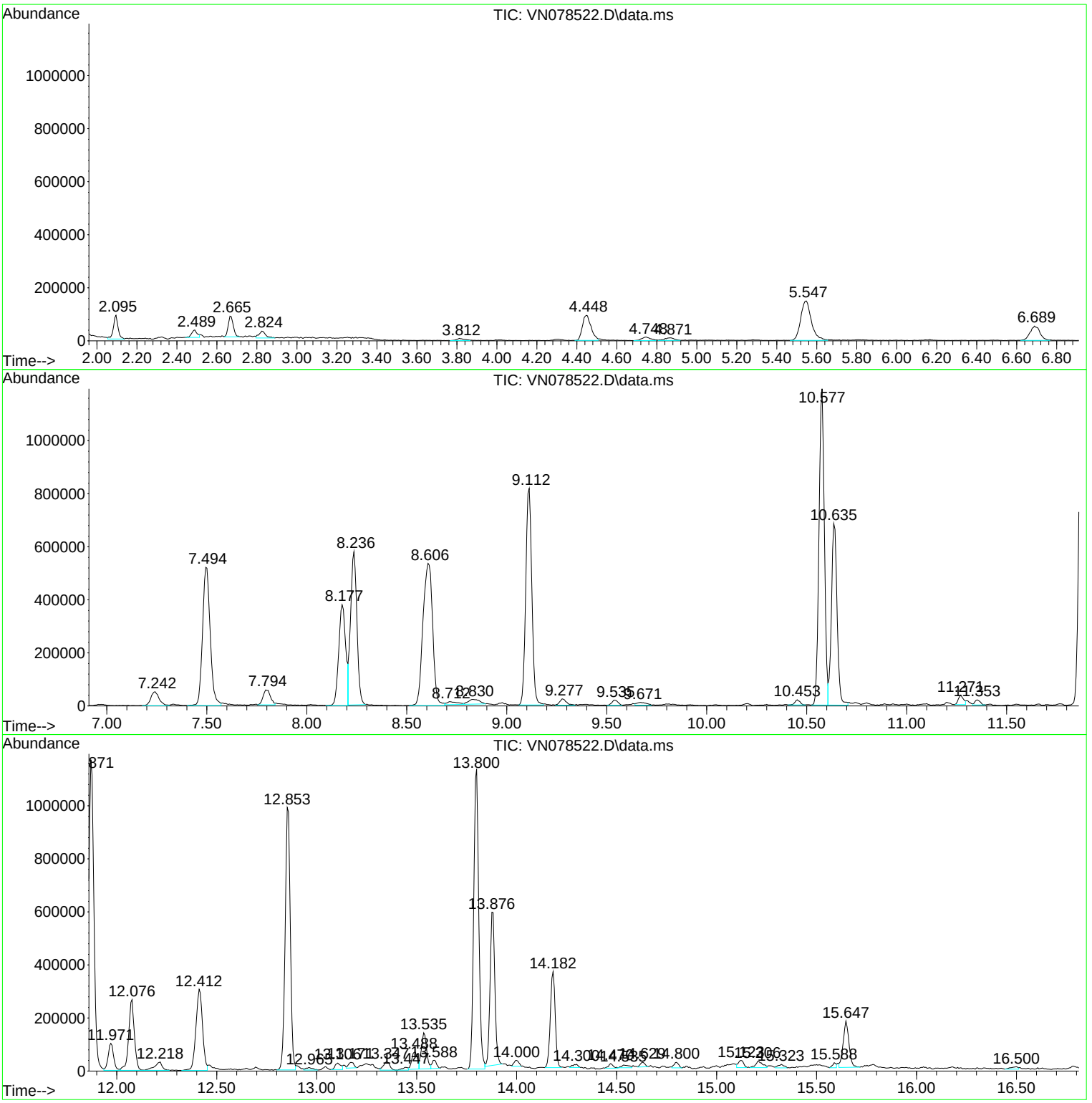
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
713-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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



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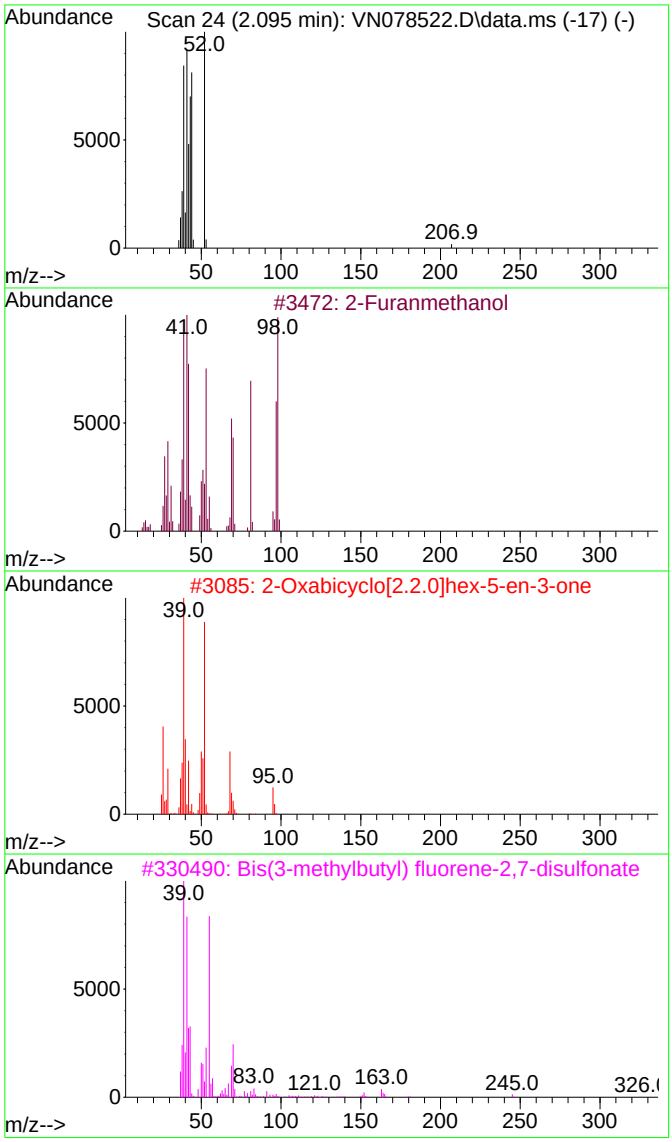
Quant Title : SW846 8260

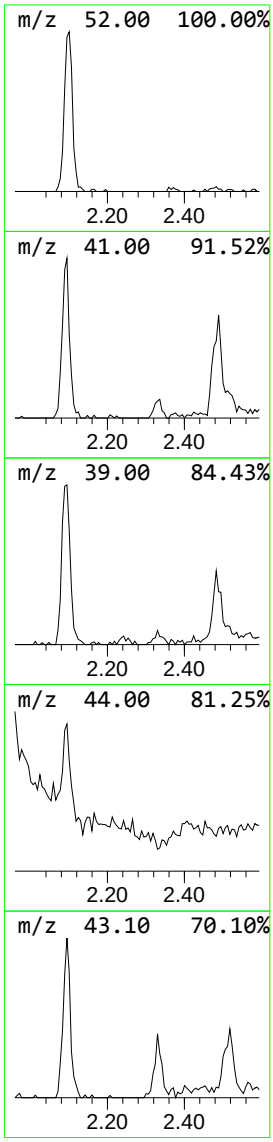
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown2.095 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.095	5.81 ug/l	144695	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanol	98	C5H6O2	000098-00-0	43
2	2-Oxabicyclo[2.2.0]hex-5-en-3-one	96	C5H4O2	022980-23-0	40
3	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	38
4	3-Butenoic acid	86	C4H6O2	000625-38-7	37
5	2-Butenal	70	C4H6O	004170-30-3	32





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
713-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

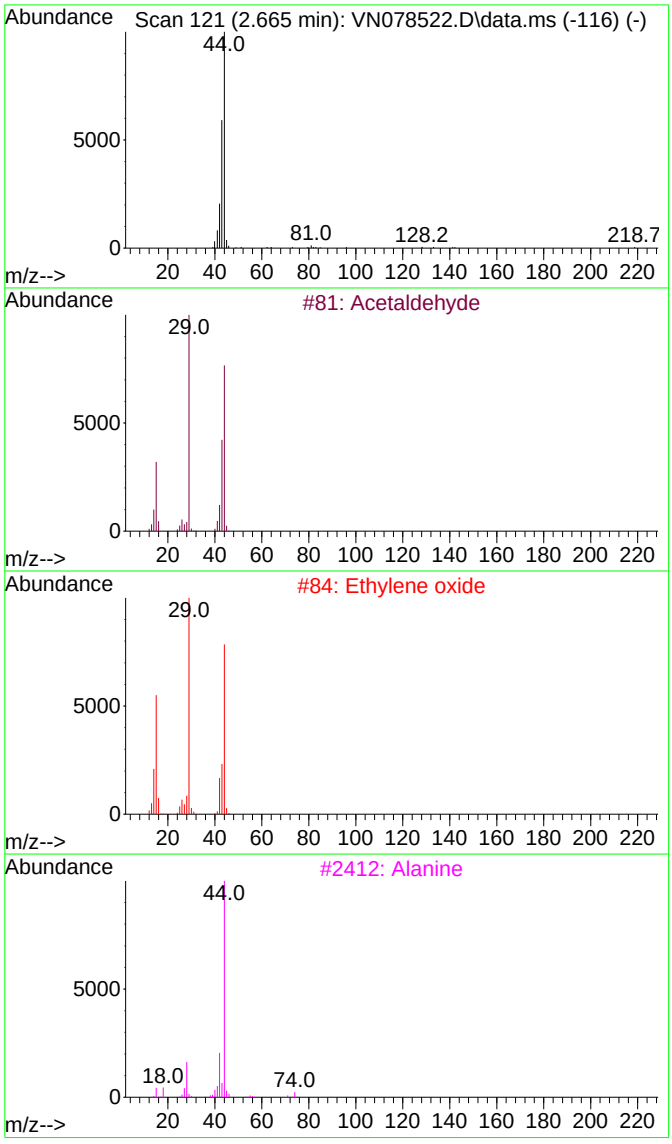
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

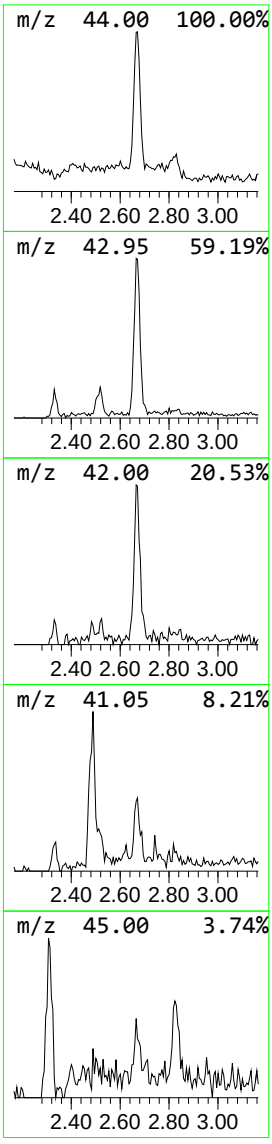
****

Peak Number 2 Acetaldehyde Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.665	5.45 ug/l	135715	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Ethylene oxide	44	C2H4O	000075-21-8	9
3	Alanine	89	C3H7NO2	000056-41-7	9
4	2-Methanesulfonylethanamine	123	C3H9NO2S	049773-20-8	9
5	Propane	44	C3H8	000074-98-6	5





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Instrument :
MSVOA_N
ClientSampleId :
713-C

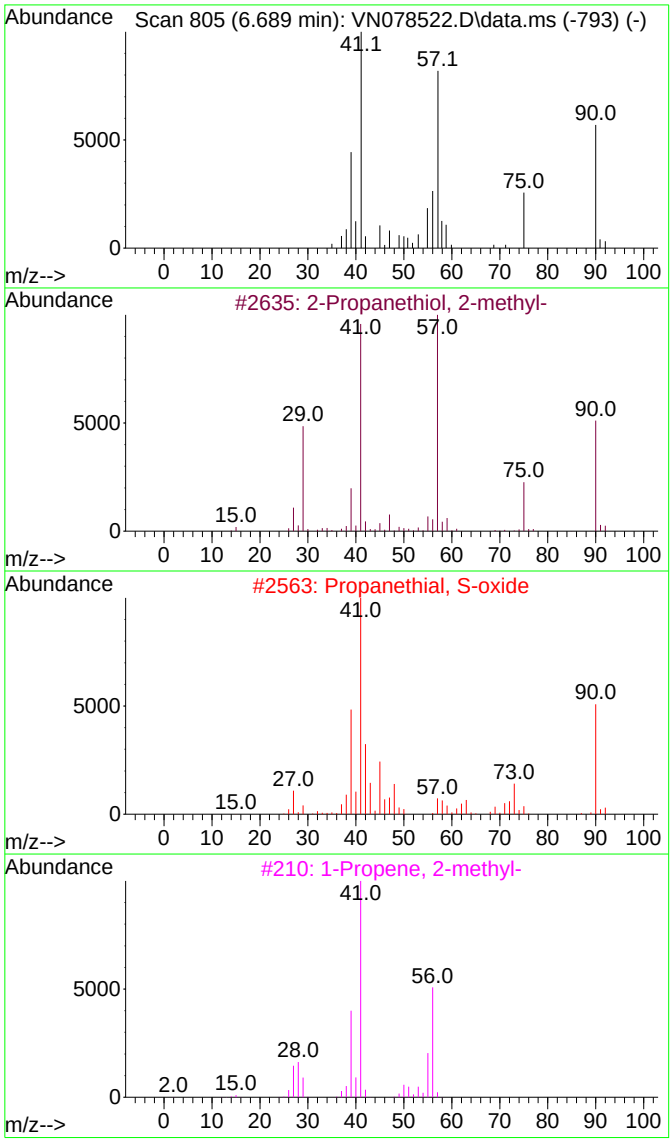
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

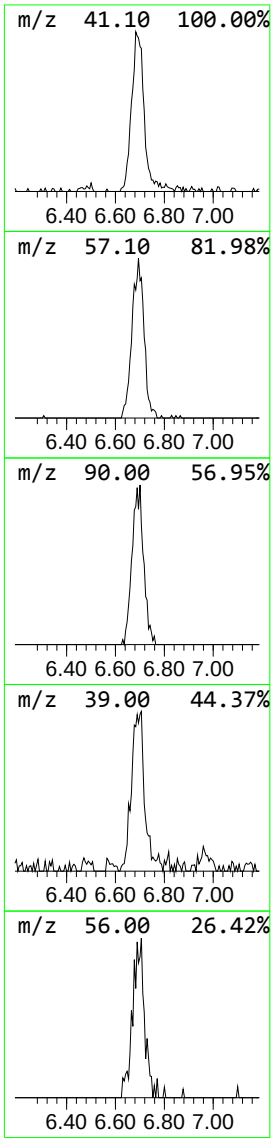
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown6.689 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.689	7.55 ug/l	188036	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	49
2	Propanethial, S-oxide	90	C3H6OS	032157-29-2	35
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	25
4	Nitroxide, bis(1,1-dimethylethyl)	144	C8H18NO	002406-25-9	23
5	2-Butene	56	C4H8	000107-01-7	22





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
713-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

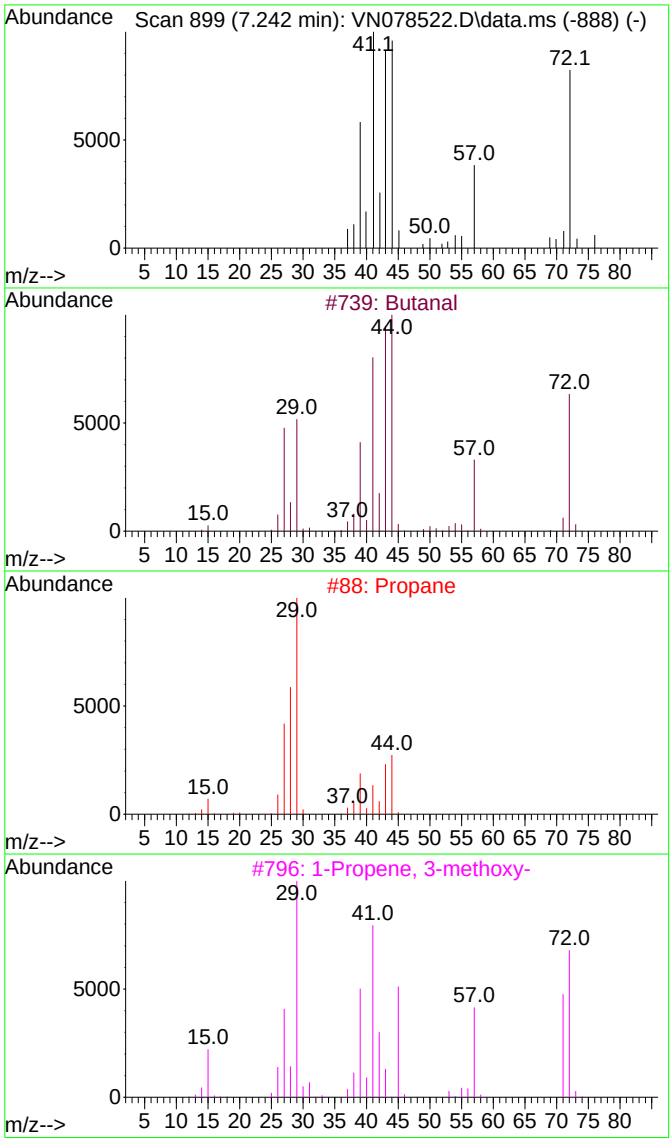
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

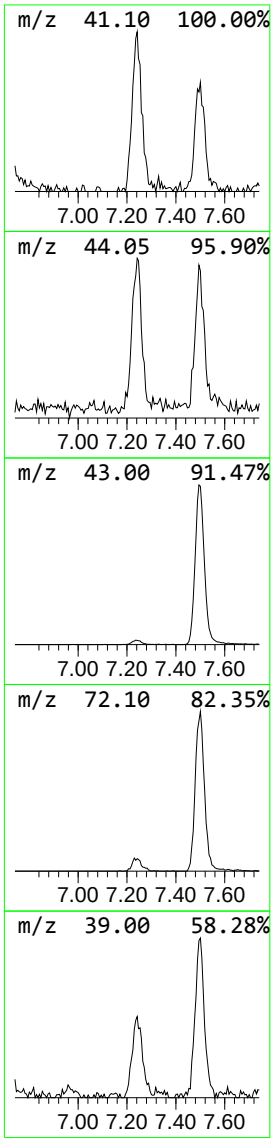
****

Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.242	6.10 ug/l	151961	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	90
2	Propane	44	C3H8	000074-98-6	43
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	27





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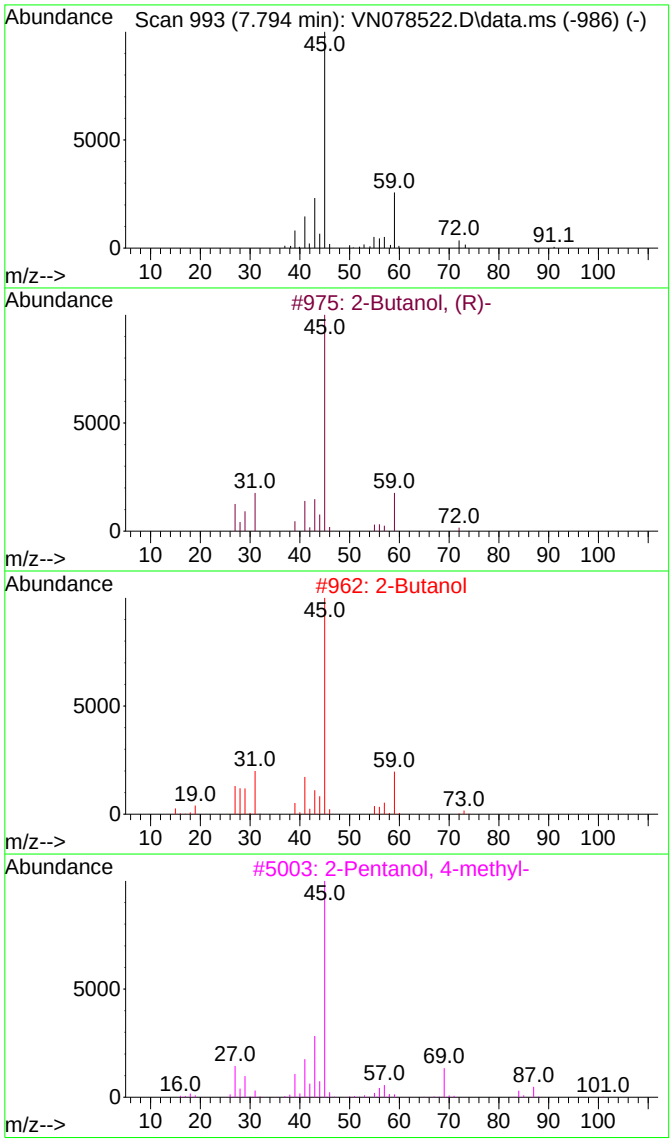
Quant Title : SW846 8260

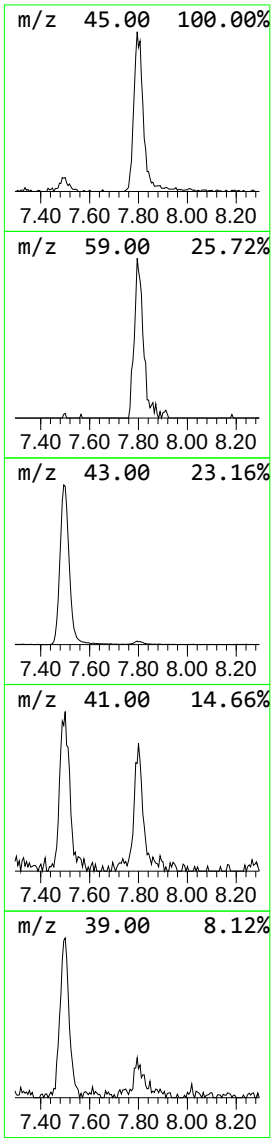
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanol, (R)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.794	5.72 ug/l	142513	Pentafluorobenzene	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
2	2-Butanol	74	C4H10O	000078-92-2	83
3	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	45
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	42
5	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	40





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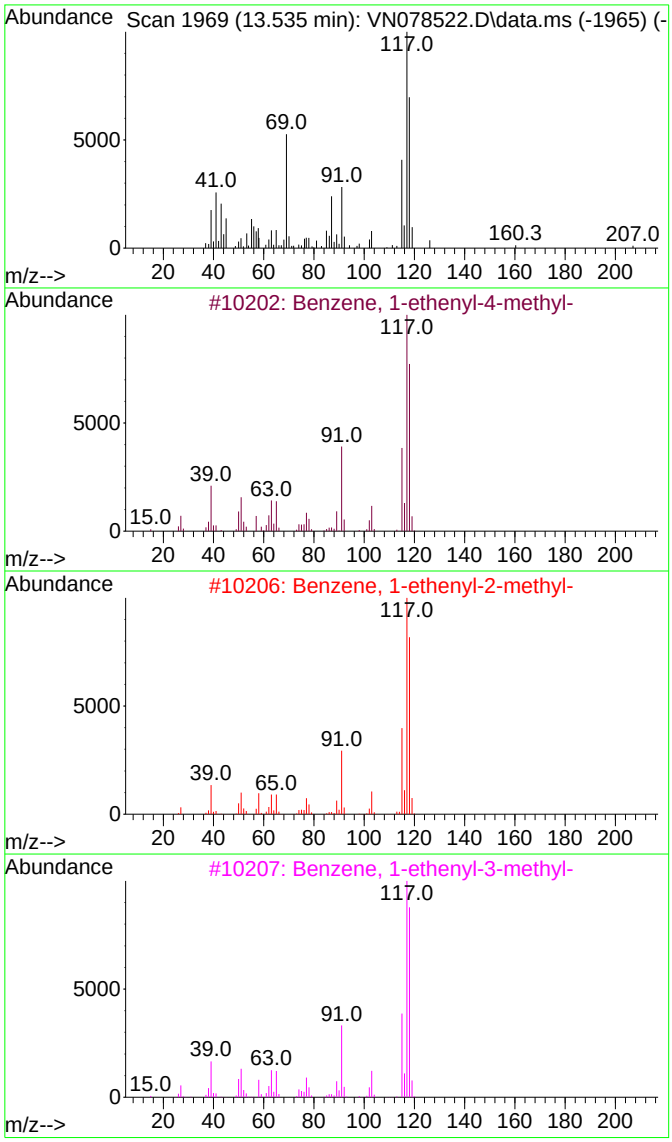
Quant Title : SW846 8260

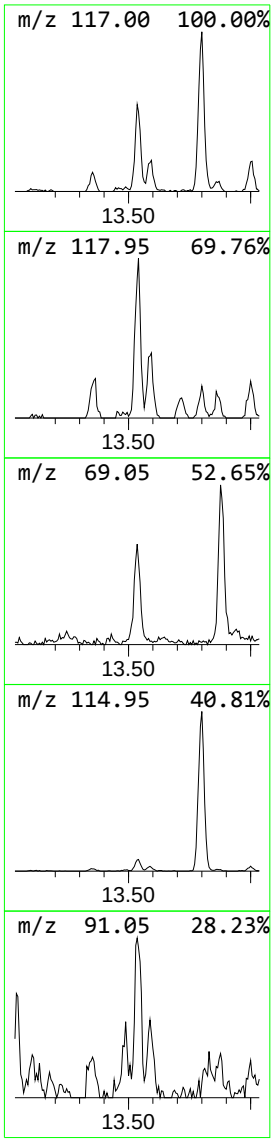
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethenyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.535	6.14 ug/l	244106	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	86
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
3	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	70
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	70
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70





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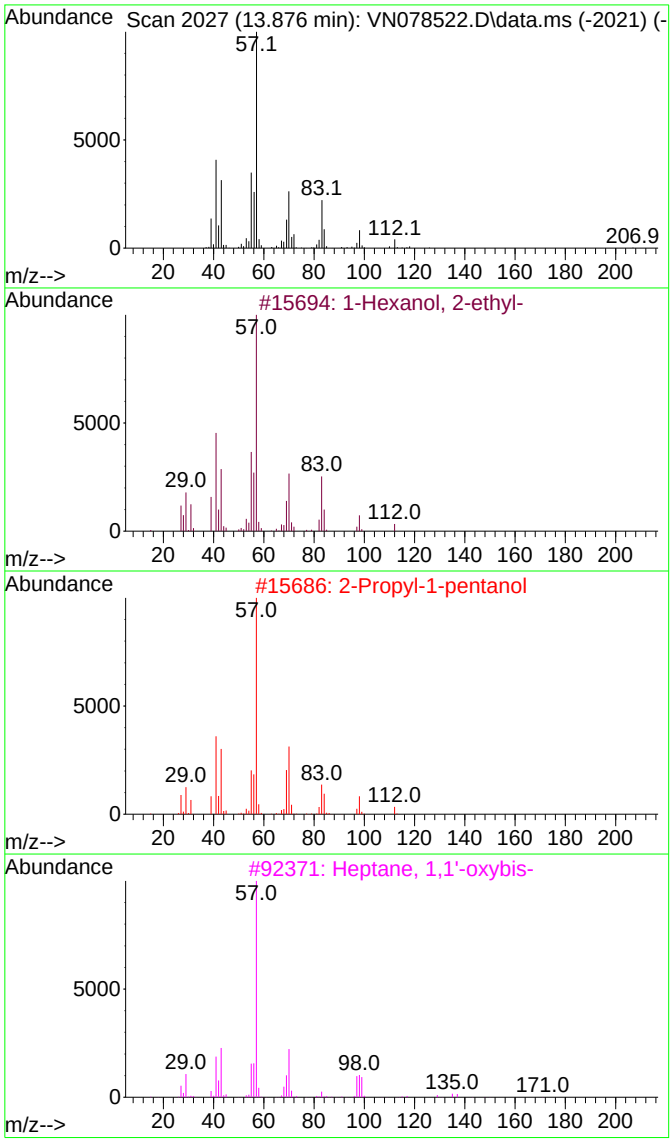
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

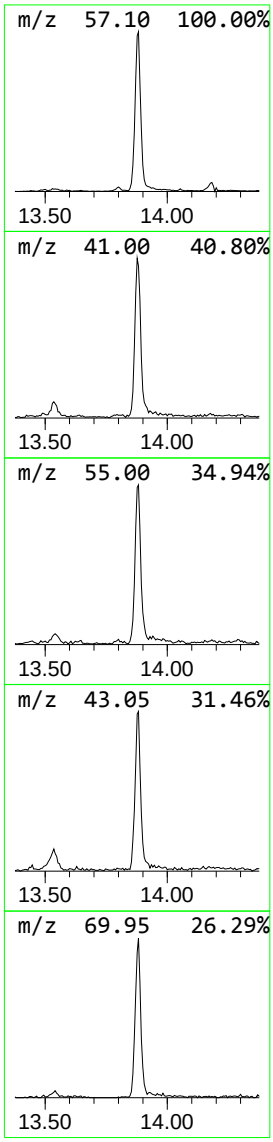
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	24.30 ug/l	965821	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	47





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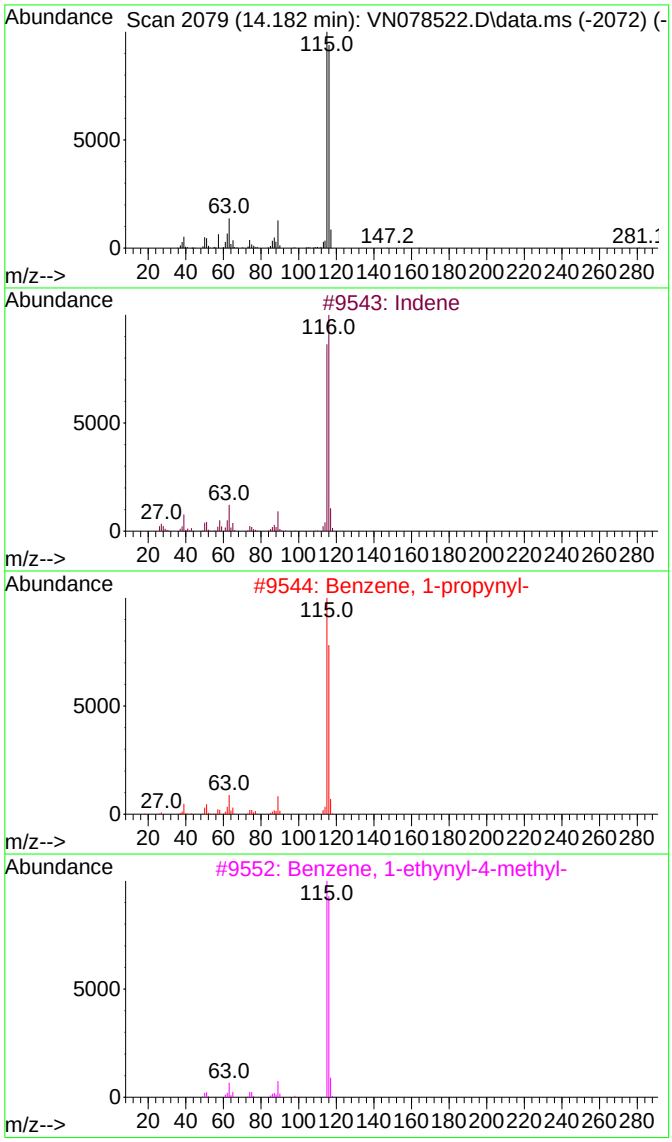
Quant Title : SW846 8260

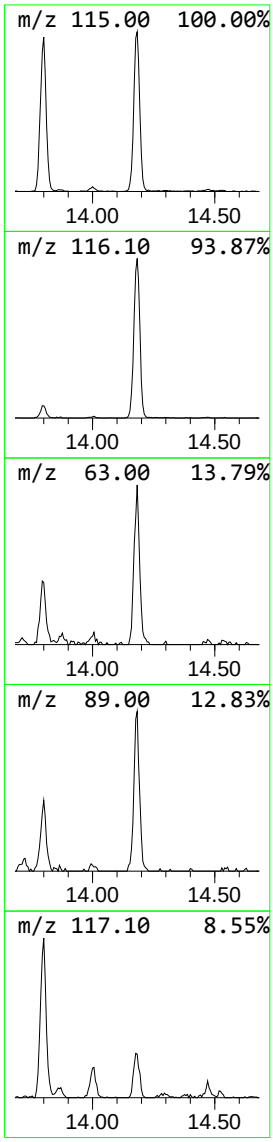
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	15.47 ug/l	614985	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	94
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071423\
Data File : VN078522.D
Acq On : 14 Jul 2023 15:11
Operator : JC\MD
Sample : 03620-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
713-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.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
unknown2.095	2.095	5.8	ug/l	144695	1	8.236	1245970	50.0
Acetaldehyde	2.665	5.5	ug/l	135715	1	8.236	1245970	50.0
unknown6.689	6.689	7.5	ug/l	188036	1	8.236	1245970	50.0
Butanal	7.242	6.1	ug/l	151961	1	8.236	1245970	50.0
2-Butanol, (R)-	7.794	5.7	ug/l	142513	1	8.236	1245970	50.0
Benzene, 1-ethe...	13.535	6.1	ug/l	244106	4	13.800	1987700	50.0
1-Hexanol, 2-et...	13.876	24.3	ug/l	965821	4	13.800	1987700	50.0
Indene	14.182	15.5	ug/l	614985	4	13.800	1987700	50.0