LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071107.D
Acq On : 28 Feb 2022 20:20
Operator : JC\MD
Sample : N1689-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-43

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\82N021522W.M
Title : SW846 8260

Signal : TIC: VN071107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	36	43	49	rBV3	105358	251667	4.96%	0.677%
2	2.440	73	77	85	rVB2	51679	88296	1.74%	0.237%
3	3.128	185	194	204	rVB	189555	434566	8.56%	1.169%
4	3.516	251	260	273	rVB4	51101	164704	3.24%	0.443%
5	3.999	331	342	354	rVB2	42709	120548	2.37%	0.324%
6	4.287	377	391	409	rBV	40324	137153	2.70%	0.369%
7	5.087	515	527	531	rBV2	24733	88185	1.74%	0.237%
8	5.181	533	543	561	rVV6	59330	321097	6.32%	0.864%
9	5.622	602	618	633	rBV4	63594	229811	4.53%	0.618%
10	5.928	660	670	683	rVB6	15563	57209	1.13%	0.154%
11	6.463	753	761	772	rVB6	28802	91709	1.81%	0.247%
12	6.610	775	786	795	rBV4	29094	92835	1.83%	0.250%
13	6.904	826	836	846	rBV4	26059	71594	1.41%	0.193%
14	7.145	863	877	886	rBV2	176003	530498	10.45%	1.427%
15	7.845	988	996	1002	rVB2	53621	123260	2.43%	0.332%
16	8.016	1015	1025	1030	rBV	613473	1480985	29.17%	3.983%
17	8.081	1030	1036	1047	rVV	1390027	3336862	65.72%	8.974%
18	8.169	1047	1051	1063	rVB6	36522	102576	2.02%	0.276%
19	8.434	1087	1096	1111	rBV2	777382	2157987	42.50%	5.804%
20	8.575	1113	1120	1126	rVV7	44498	146634	2.89%	0.394%
21	8.634	1127	1130	1137	rVV4	43630	112094	2.21%	0.301%
22	8.704	1137	1142	1152	rVV5	35127	99028	1.95%	0.266%
23	8.963	1177	1186	1200	rBV	1834936	3965690	78.10%	10.666%
24	9.198	1219	1226	1229	rBV3	38732	84018	1.65%	0.226%
25	9.245	1229	1234	1243	rVB	70720	147525	2.91%	0.397%
26	9.451	1253	1269	1277	rBV6	99965	318276	6.27%	0.856%
27	9.875	1337	1341	1349	rVB3	29290	57636	1.14%	0.155%
28	9.969	1349	1357	1361	rBV3	82092	162936	3.21%	0.438%
29	10.016	1361	1365	1377	rVV6	62967	143543	2.83%	0.386%
30	10.316	1410	1416	1422	rBV2	83237	165648	3.26%	0.446%
31	10.439	1428	1437	1446	rBV	2729445	5077522	100.00%	13.656%
32	10.639	1460	1471	1476	rBV4	67425	149532	2.94%	0.402%
33	10.710	1476	1483	1490	rVB2	54601	108089	2.13%	0.291%
34	10.857	1499	1508	1518	rVB	94541	206193	4.06%	0.555%
35	11.128	1547	1554	1558	rBV3	30286	57249	1.13%	0.154%
36	11.739	1650	1658	1670	rVV	2367367	4257807	83.86%	11.451%

LSC Area Percent Report

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Title : SW846 8260

37	11.839	1670	1675	1684	rVV	163172	296283	5.84%	0.797%
38	11.957	1688	1695	1707	rVB	93234	187121	3.69%	0.503%
39	12.574	1794	1800	1806	rBV	43241	70944	1.40%	0.191%
40	12.727	1818	1826	1837	rBV	1872969	3194520	62.91%	8.592%
41	12.916	1852	1858	1864	rBV	33383	54695	1.08%	0.147%
42	13.010	1866	1874	1879	rBV	44100	73807	1.45%	0.199%
43	13.216	1903	1909	1918	rBV	125233	212446	4.18%	0.571%
44	13.363	1928	1934	1942	rVB	316582	504356	9.93%	1.356%
45	13.669	1979	1986	1999	rBV	1828004	3258755	64.18%	8.764%
46	13.833	2008	2014	2017	rBV	126210	219165	4.32%	0.589%
47	13.874	2017	2021	2025	rVV	283757	455882	8.98%	1.226%
48	13.916	2025	2028	2036	rVB3	53725	94542	1.86%	0.254%
49	13.998	2036	2042	2046	rBV	35375	55814	1.10%	0.150%
50	14.063	2047	2053	2059	rBV	69834	114520	2.26%	0.308%
51	14.127	2059	2064	2067	rBV	60856	105921	2.09%	0.285%
52	14.210	2073	2078	2084	rBV	180428	285515	5.62%	0.768%
53	14.274	2084	2089	2092	rVV	65487	102909	2.03%	0.277%
54	14.321	2092	2097	2104	rVB2	400099	659505	12.99%	1.774%
55	14.457	2114	2120	2126	rVB2	95207	156089	3.07%	0.420%
56	14.533	2126	2133	2136	rBV	148066	238886	4.70%	0.642%
57	14.574	2136	2140	2145	rVB	151041	232177	4.57%	0.624%
58	14.804	2174	2179	2185	rVV2	101601	176200	3.47%	0.474%
59	14.927	2192	2200	2206	rBV3	315760	630149	12.41%	1.695%
60	14.986	2206	2210	2216	rVB4	26294	57100	1.12%	0.154%
61	15.080	2220	2226	2234	rBV4	36936	74293	1.46%	0.200%
62	15.186	2234	2244	2249	rBV2	82991	221403	4.36%	0.595%
63	15.310	2256	2265	2272	rVB2	120070	307704	6.06%	0.828%

Sum of corrected areas: 37181663

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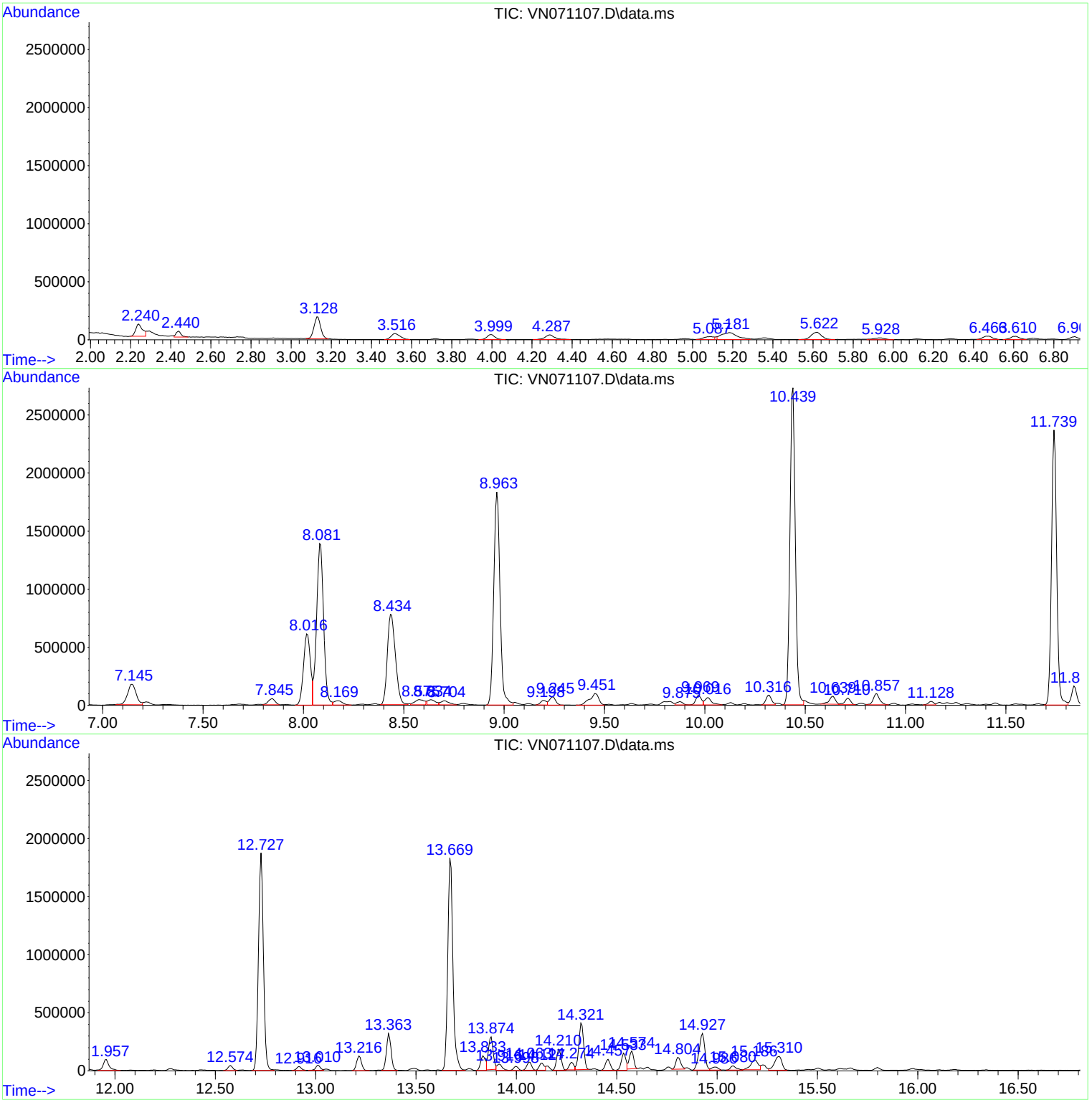
ClientSampleId :
MW-43

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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



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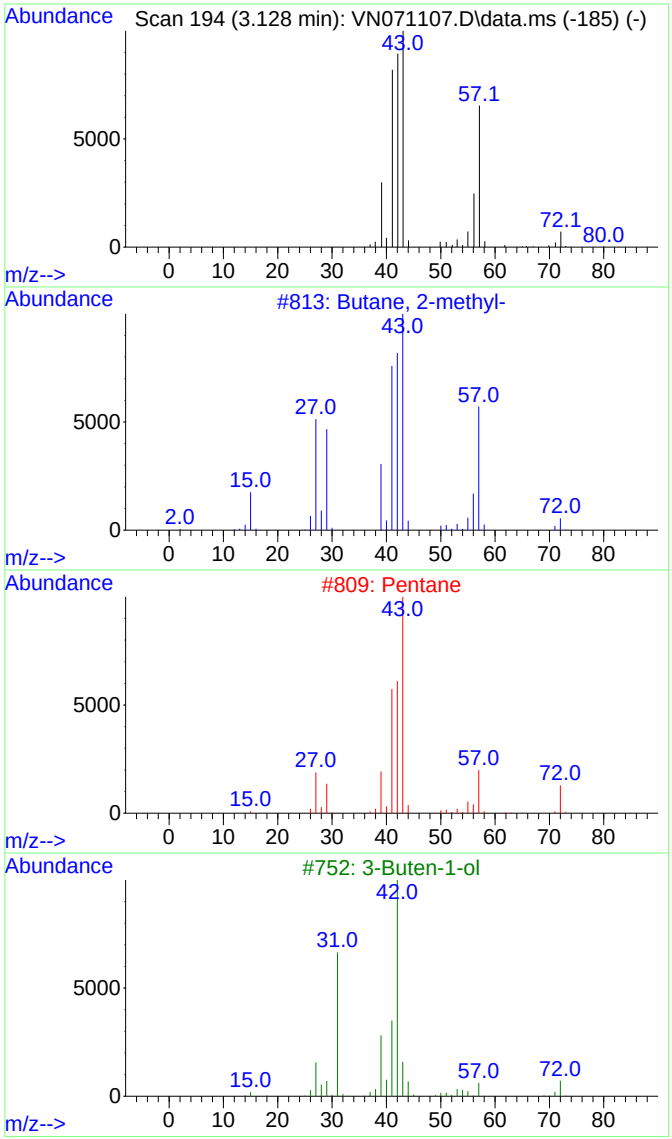
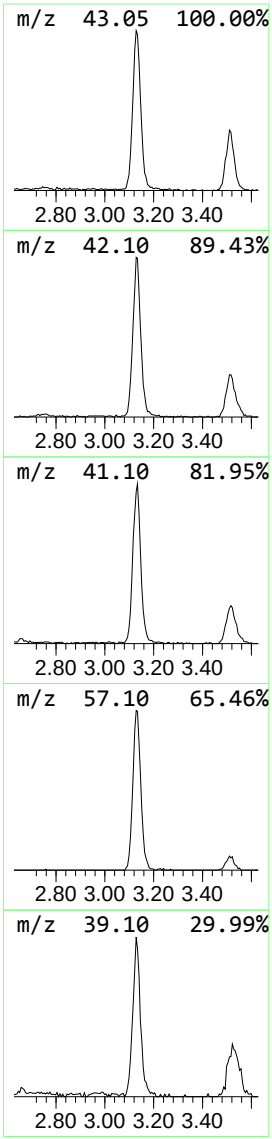
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	6.51 ug/l	434566	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	14
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10





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MSVOA_N
ClientSampleId :
MW-43

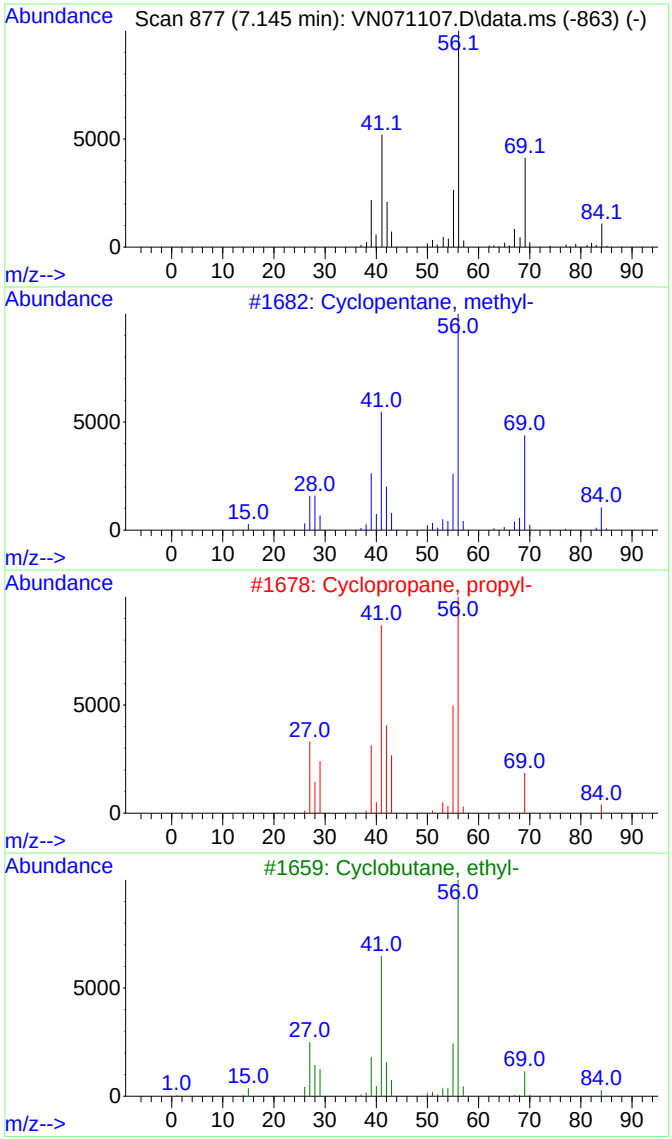
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

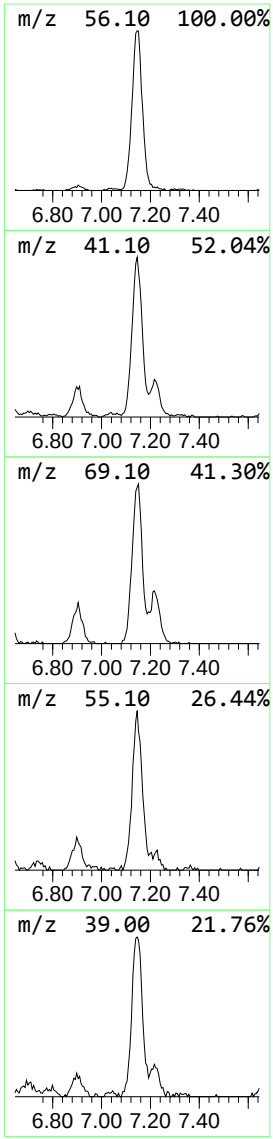
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	7.95 ug/l	530498	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46





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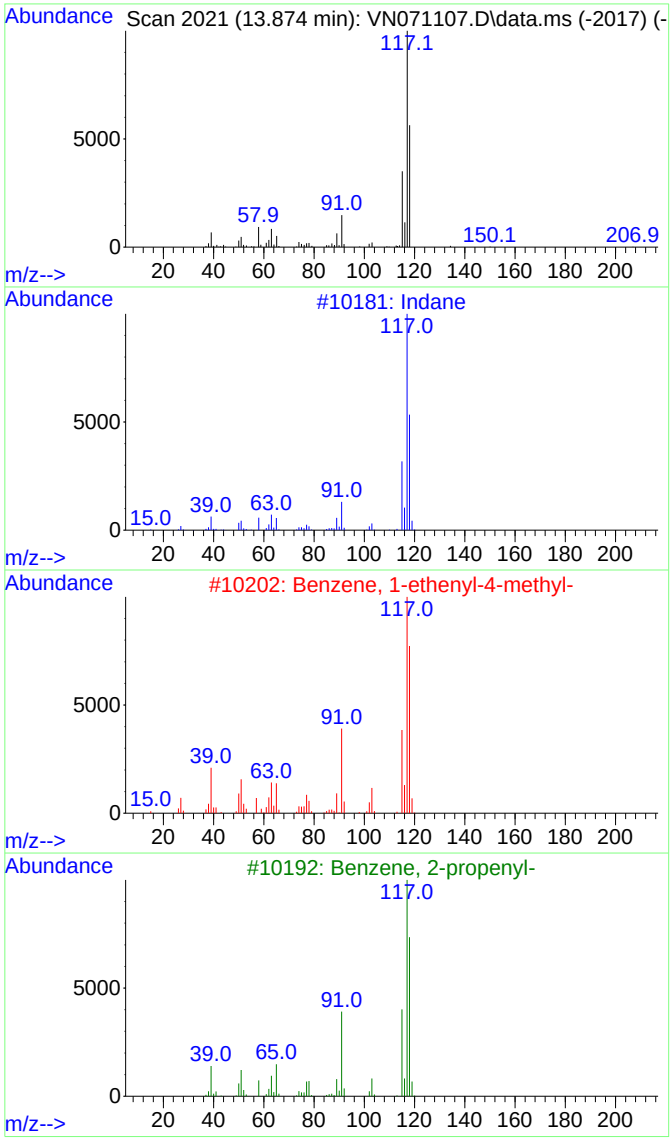
Quant Title : SW846 8260

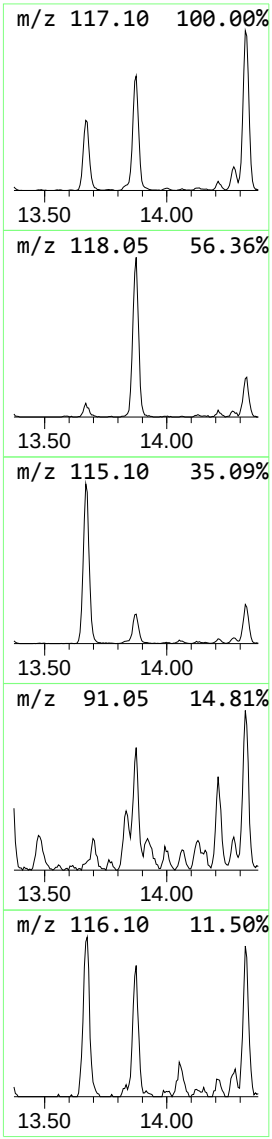
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.99 ug/l	455882	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	59
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53





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Instrument :
MSVOA_N
ClientSampleId :
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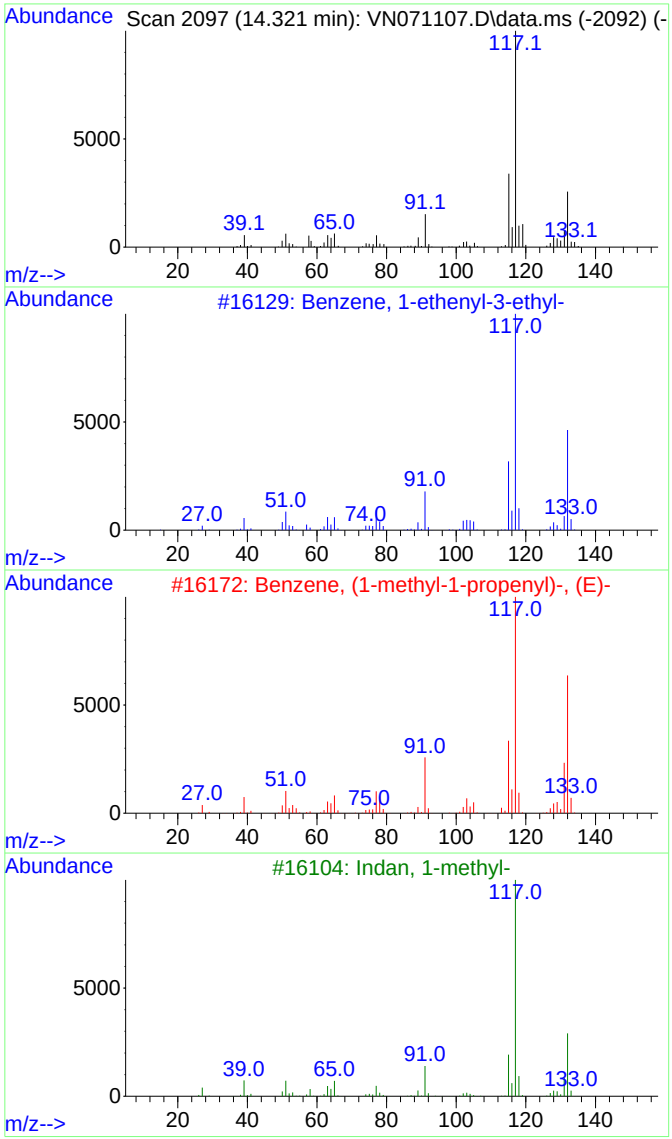
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

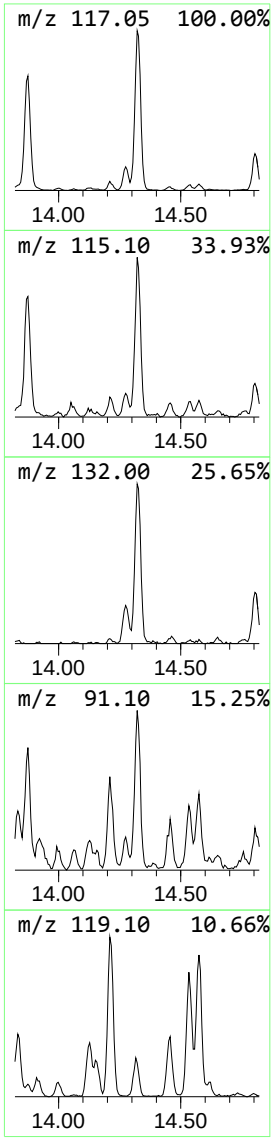
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	10.12 ug/l	659505	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	80





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TIC Library : C:\Database\NIST20.L
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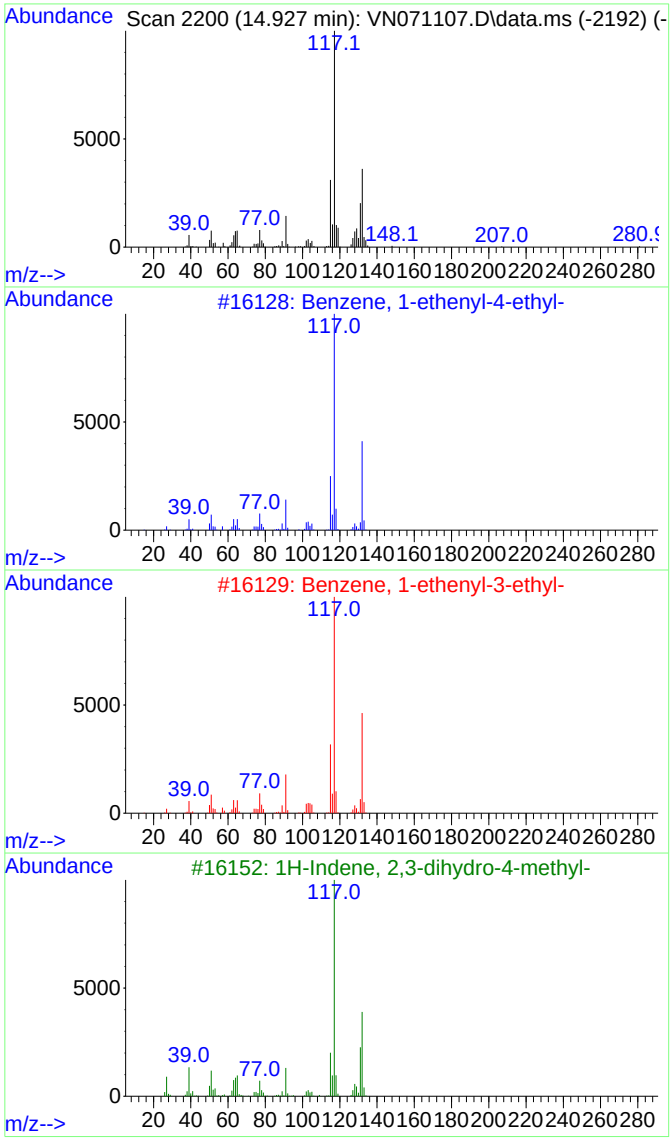
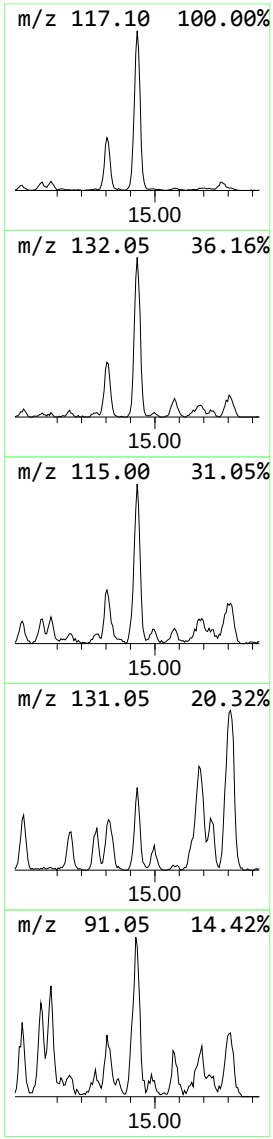
****
Peak Number 5 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	9.67 ug/l	630149	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methyl-	3.128	6.5	ug/l	434566	1	8.081	3336860	50.0
Cyclopentane, m...	7.145	8.0	ug/l	530498	1	8.081	3336860	50.0
Indane	13.874	7.0	ug/l	455882	4	13.669	3258760	50.0
Benzene, 1-ethe...	14.321	10.1	ug/l	659505	4	13.669	3258760	50.0
Benzene, 1-ethe...	14.927	9.7	ug/l	630149	4	13.669	3258760	50.0