LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071127.D
Acq On : 01 Mar 2022 18:36
Operator : JC\MD
Sample : N1689-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 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: VN071127.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	35	41	50	rBV2	336469	740702	16.00%	2.178%
2	2.440	73	77	87	rVB3	54149	93190	2.01%	0.274%
3	3.128	186	194	212	rVB	183230	445896	9.63%	1.311%
4	3.516	250	260	275	rVB3	45589	123847	2.68%	0.364%
5	4.287	377	391	399	rBV2	25221	87329	1.89%	0.257%
6	5.081	514	526	531	rBV3	25314	85330	1.84%	0.251%
7	5.181	531	543	557	rVB5	49949	259176	5.60%	0.762%
8	5.622	600	618	631	rBV3	60252	217057	4.69%	0.638%
9	7.145	867	877	891	rVB2	168470	509279	11.00%	1.497%
10	8.016	1016	1025	1030	rBV	554349	1328551	28.70%	3.906%
11	8.081	1030	1036	1048	rVV	1272828	3045913	65.80%	8.956%
12	8.169	1049	1051	1063	rVB4	34071	69332	1.50%	0.204%
13	8.439	1087	1097	1111	rBV2	716757	2005236	43.32%	5.896%
14	8.575	1114	1120	1127	rBV8	26601	83411	1.80%	0.245%
15	8.698	1136	1141	1154	rVB7	26636	73781	1.59%	0.217%
16	8.963	1177	1186	1202	rBV	1638946	3348472	72.34%	9.845%
17	9.416	1255	1263	1264	rBV2	45441	66167	1.43%	0.195%
18	9.457	1265	1270	1278	rVB3	87124	194634	4.20%	0.572%
19	10.010	1354	1364	1370	rBV4	39313	84294	1.82%	0.248%
20	10.439	1428	1437	1446	rBV	2514184	4628891	100.00%	13.610%
21	10.639	1460	1471	1478	rVB4	51262	113657	2.46%	0.334%
22	10.710	1478	1483	1490	rVB2	44594	78326	1.69%	0.230%
23	11.739	1650	1658	1669	rBV	2191063	3904311	84.35%	11.480%
24	11.839	1669	1675	1686	rVV	329203	579567	12.52%	1.704%
25	11.957	1688	1695	1706	rVB	97278	198038	4.28%	0.582%
26	12.574	1793	1800	1812	rBV	119661	210052	4.54%	0.618%
27	12.727	1818	1826	1836	rBV	1734021	2941404	63.54%	8.649%
28	12.916	1852	1858	1865	rBV	169850	274357	5.93%	0.807%
29	13.010	1865	1874	1878	rBV	46709	79326	1.71%	0.233%
30	13.216	1903	1909	1916	rVB	129753	215582	4.66%	0.634%
31	13.363	1928	1934	1944	rVB	319594	522387	11.29%	1.536%
32	13.492	1948	1956	1963	rBV2	37104	88927	1.92%	0.261%
33	13.668	1979	1986	1999	rBV	1617586	2923504	63.16%	8.596%
34	13.833	2008	2014	2017	rBV	126301	213818	4.62%	0.629%
35	13.874	2017	2021	2026	rVV	285754	482264	10.42%	1.418%
36	13.916	2026	2028	2037	rVB3	59653	98463	2.13%	0.290%

LSC Area Percent Report

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Sample : N1689-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 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

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Peak separation: 5

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

37	13.998	2037	2042	2048	rVB2	32454	51558	1.11%	0.152%
38	14.063	2048	2053	2058	rBV	70377	112063	2.42%	0.329%
39	14.127	2058	2064	2067	rBV	65238	111249	2.40%	0.327%
40	14.210	2073	2078	2084	rBV	180294	279555	6.04%	0.822%
41	14.274	2084	2089	2092	rBV	66674	108872	2.35%	0.320%
42	14.321	2092	2097	2104	rVB	389259	653831	14.13%	1.922%
43	14.457	2114	2120	2126	rBV2	89197	150518	3.25%	0.443%
44	14.533	2126	2133	2136	rBV	148192	231605	5.00%	0.681%
45	14.574	2136	2140	2145	rVB	136302	212962	4.60%	0.626%
46	14.757	2166	2171	2174	rBV2	28788	46509	1.00%	0.137%
47	14.804	2174	2179	2185	rVV3	106978	210337	4.54%	0.618%
48	14.927	2192	2200	2206	rVV3	308096	614505	13.28%	1.807%
49	14.986	2206	2210	2217	rVV5	22722	51751	1.12%	0.152%
50	15.080	2220	2226	2234	rVV3	39457	77915	1.68%	0.229%
51	15.192	2234	2245	2249	rVV4	83369	231038	4.99%	0.679%
52	15.227	2249	2251	2256	rVV2	49005	76142	1.64%	0.224%
53	15.310	2256	2265	2272	rVB2	118912	300965	6.50%	0.885%
54	15.504	2292	2298	2304	rVB2	37103	74343	1.61%	0.219%

Sum of corrected areas: 34010189

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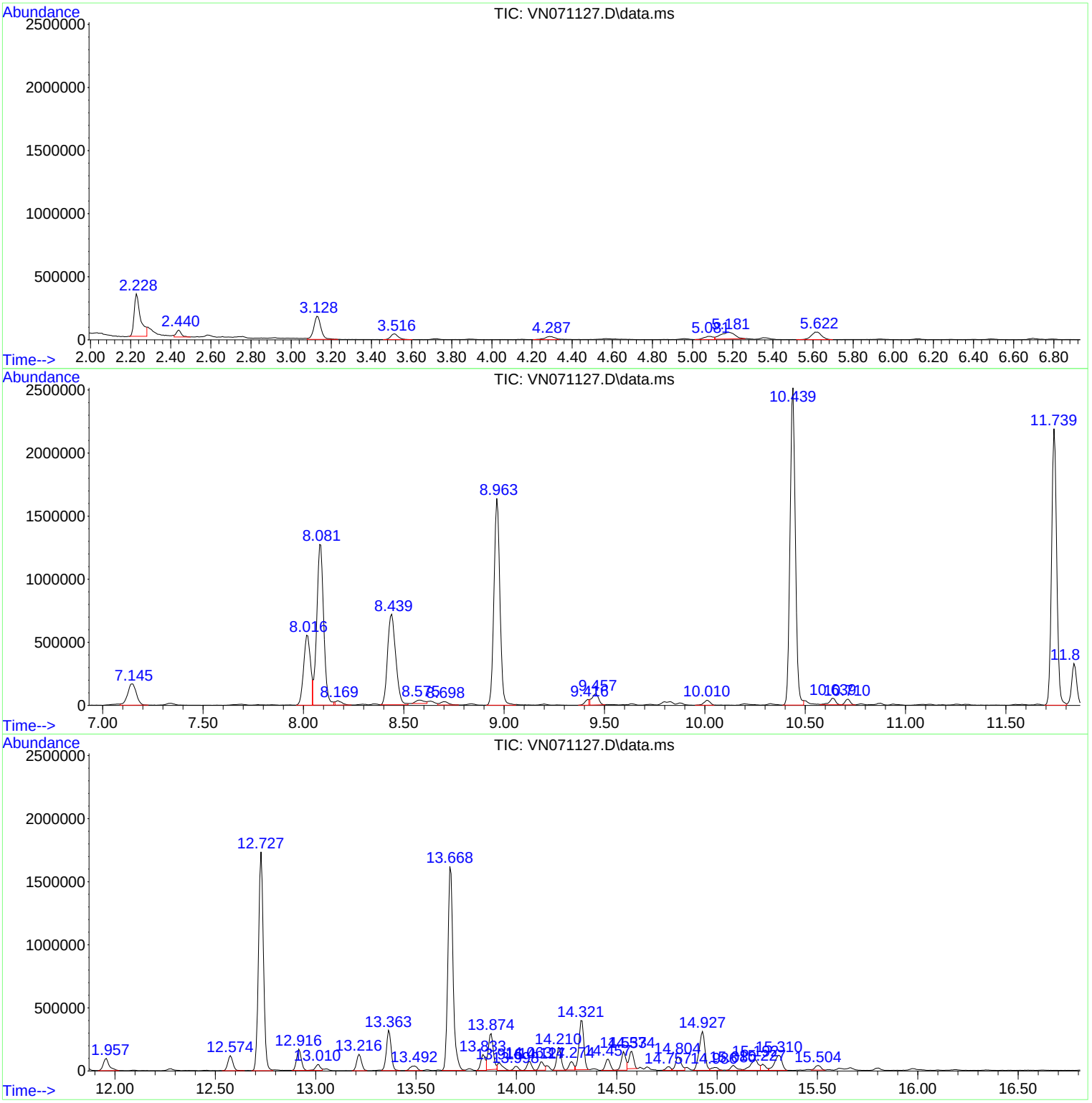
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071127.D
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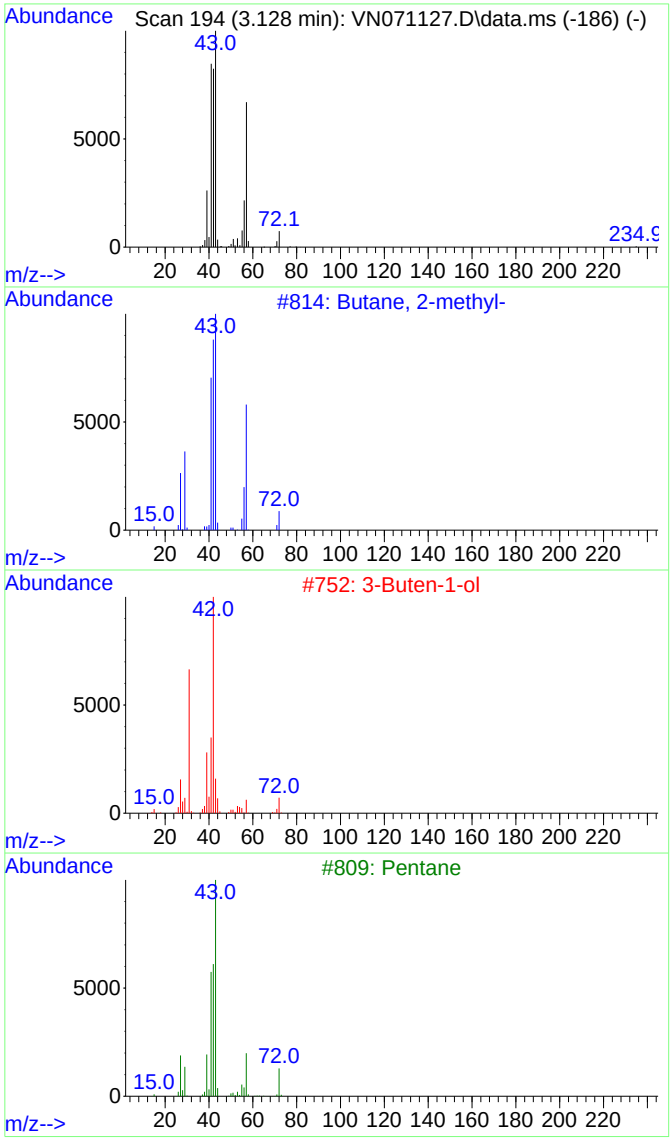
Quant Title : SW846 8260

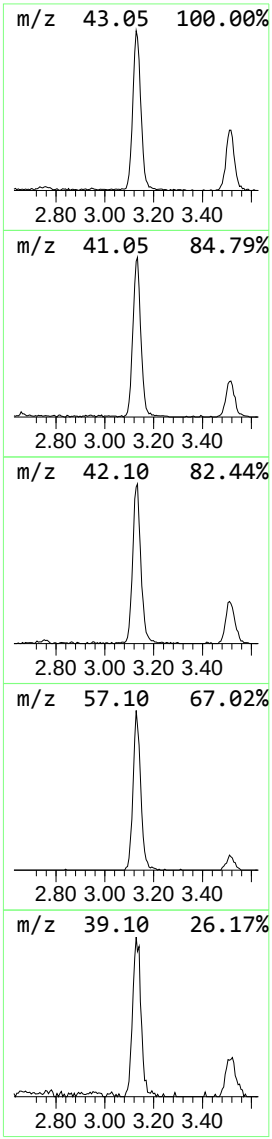
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	7.32 ug/l	445896	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	38
4	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	12
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-43

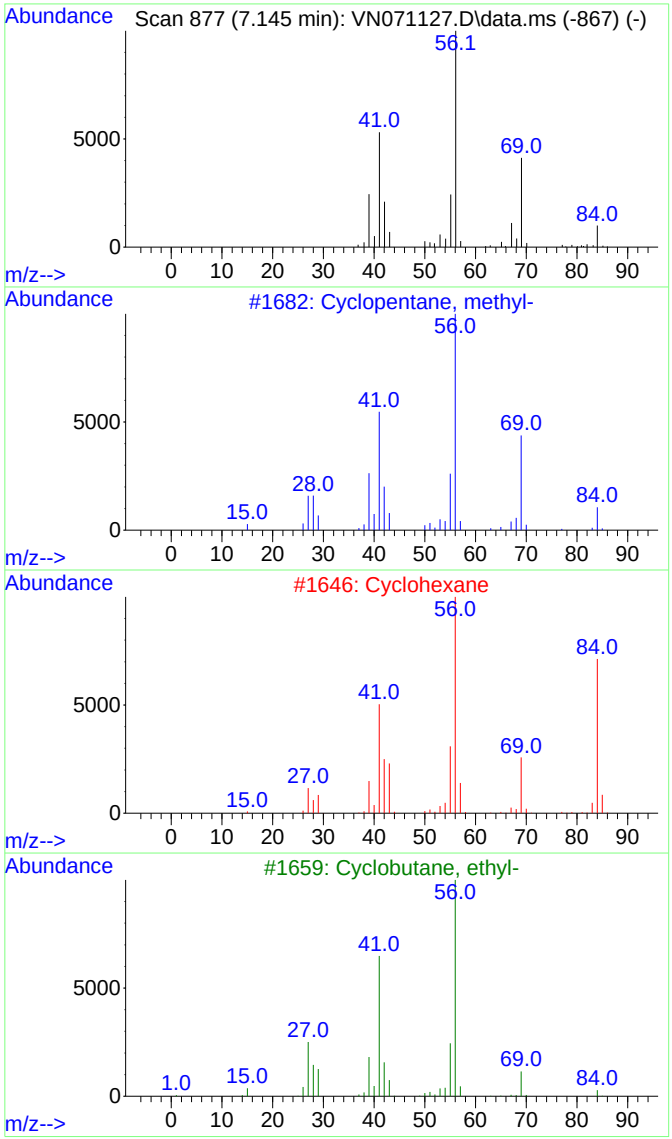
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

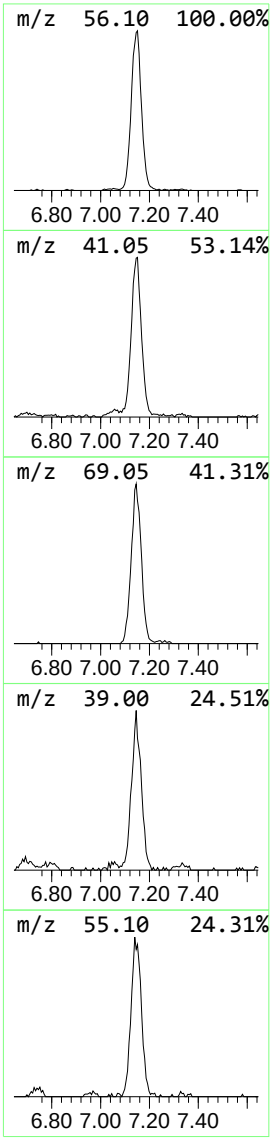
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	8.36 ug/l	509279	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2	Cyclohexane	84	C6H12	000110-82-7	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	47





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-43

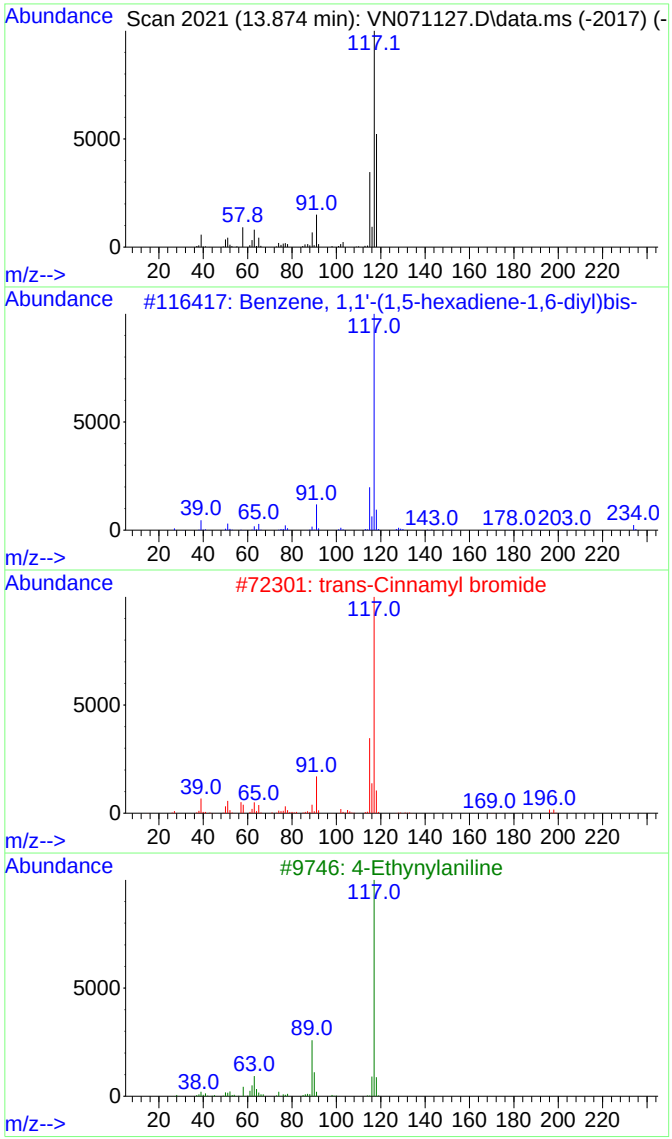
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

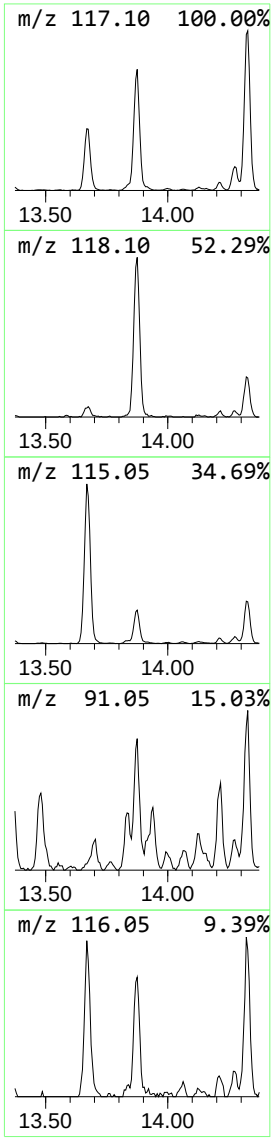
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	8.25 ug/l	482264	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3	4-Ethynylaniline	117	C8H7N	014235-81-5	47
4	Indole	117	C8H7N	000120-72-9	43
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	33





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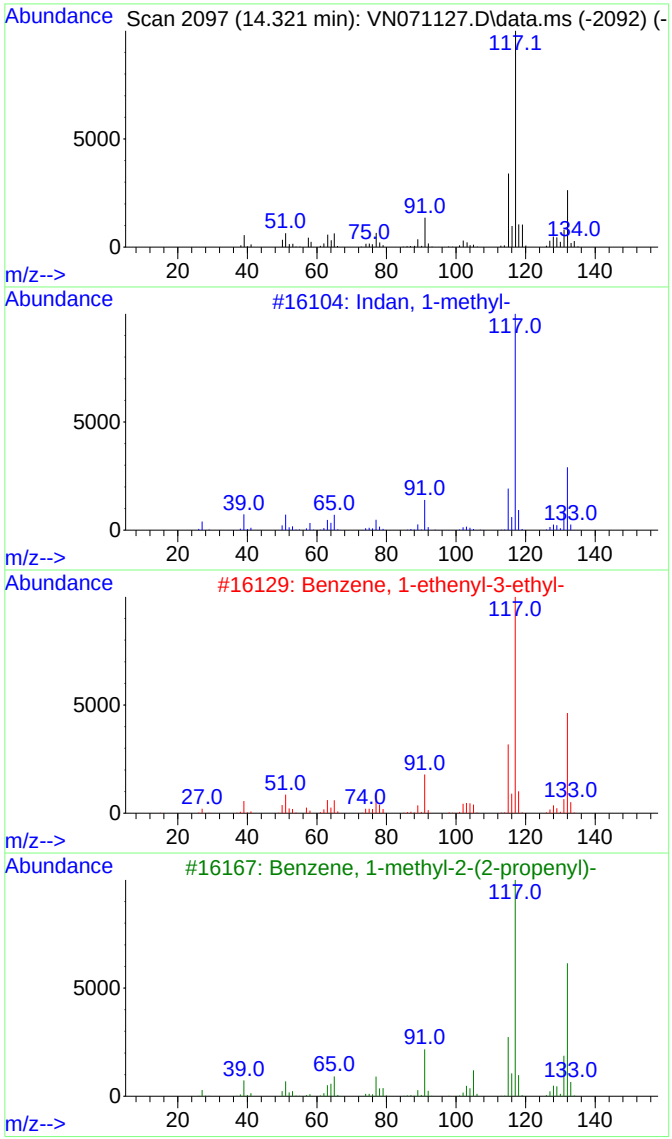
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

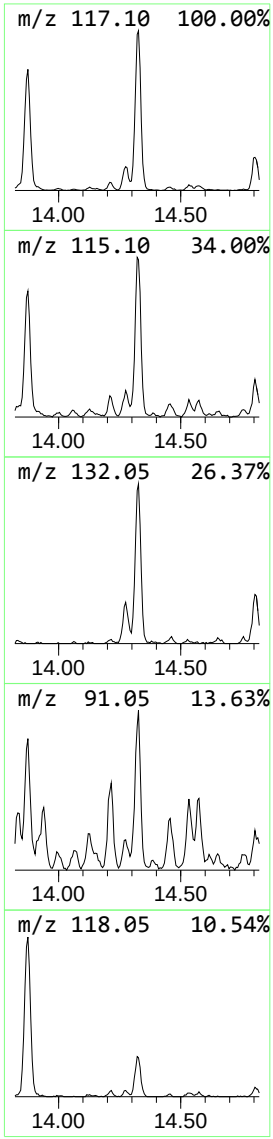
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	11.18 ug/l	653831	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	80
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	74





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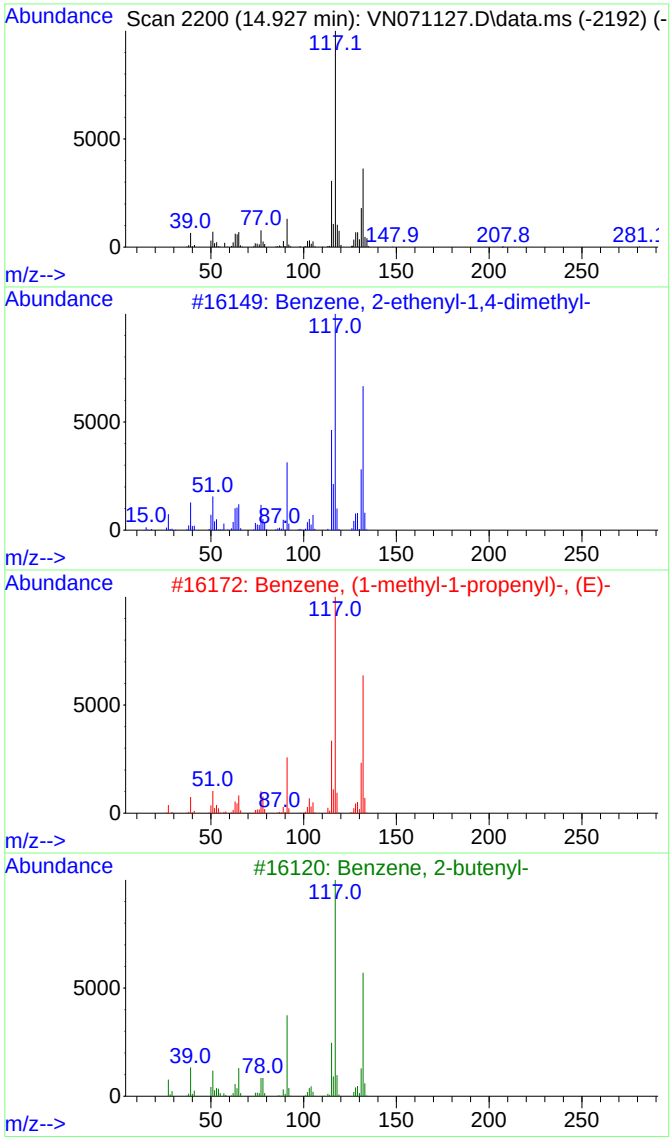
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

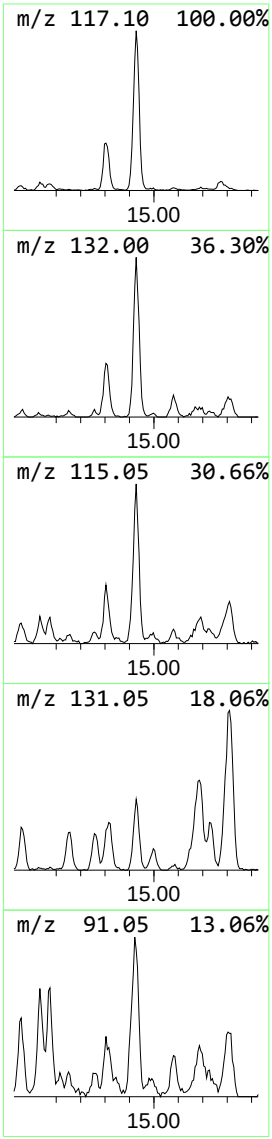
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	10.51 ug/l	614505	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90





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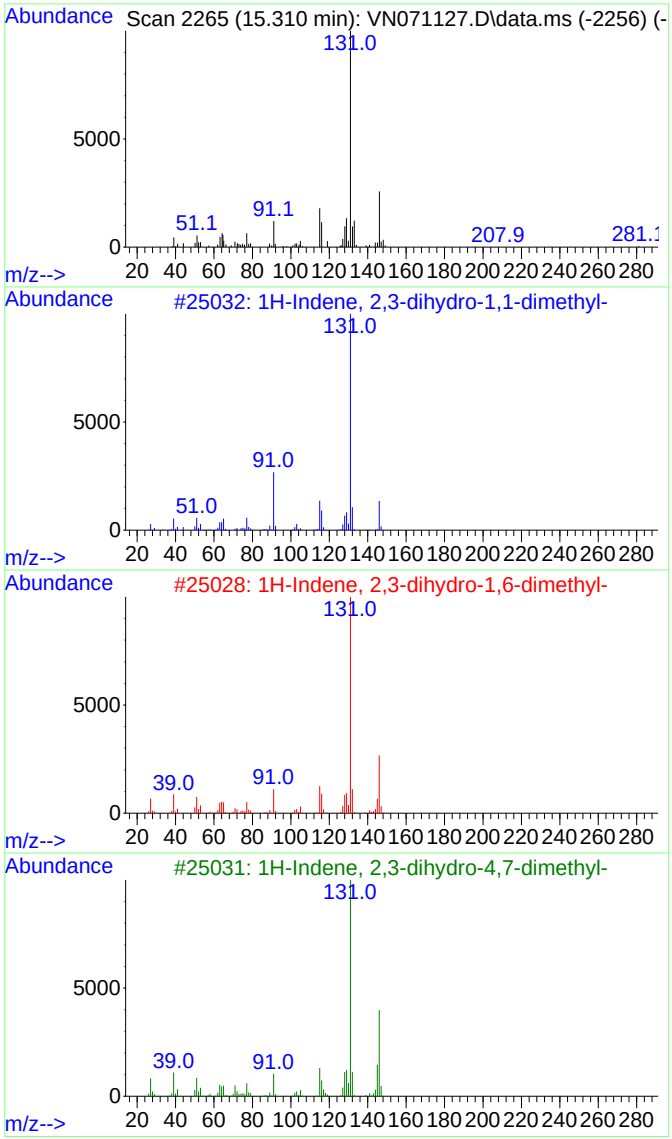
Quant Title : SW846 8260

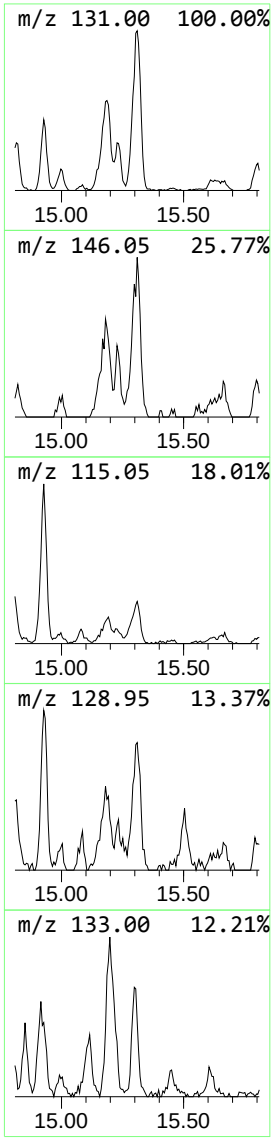
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	5.15 ug/l	300965	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	91
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	90
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
4	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	87
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	83





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	3.128	7.3	ug/l	445896	1	8.081	3045910	50.0
Cyclopentane, m...	7.145	8.4	ug/l	509279	1	8.081	3045910	50.0
Benzene, 1,1'-(...	13.874	8.3	ug/l	482264	4	13.669	2923500	50.0
Indan, 1-methyl-	14.321	11.2	ug/l	653831	4	13.669	2923500	50.0
Benzene, 2-ethe...	14.927	10.5	ug/l	614505	4	13.669	2923500	50.0
1H-Indene, 2,3-...	15.310	5.2	ug/l	300965	4	13.669	2923500	50.0