LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071120.D
Acq On : 01 Mar 2022 15:48
Operator : JC\MD
Sample : N1689-01 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

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: VN071120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	34	42	51	rBV5	41834	148149	1.60%	0.230%
2	2.440	69	77	86	rVB2	56825	123372	1.33%	0.191%
3	3.087	178	187	199	rVB	81298	204135	2.20%	0.317%
4	3.504	246	258	269	rBV3	52485	191523	2.06%	0.297%
5	3.698	282	291	306	rBV2	58101	144645	1.56%	0.224%
6	3.875	310	321	329	rBV2	34963	95944	1.03%	0.149%
7	3.981	329	339	357	rVB2	106483	290718	3.13%	0.451%
8	4.945	491	503	515	rBV	53948	178191	1.92%	0.276%
9	5.181	531	543	558	rVB5	44552	187888	2.02%	0.291%
10	5.381	563	577	596	rVB2	56268	237086	2.55%	0.368%
11	5.610	604	616	628	rBV3	52492	173851	1.87%	0.270%
12	6.463	753	761	774	rVB4	40490	135635	1.46%	0.210%
13	6.898	825	835	846	rVB4	35253	101765	1.10%	0.158%
14	7.139	861	876	884	rBV3	101468	323631	3.49%	0.502%
15	7.833	986	994	1004	rVB2	53184	133638	1.44%	0.207%
16	8.016	1015	1025	1030	rBV	583938	1395850	15.04%	2.165%
17	8.080	1030	1036	1046	rVB	1219677	2794891	30.11%	4.335%
18	8.451	1086	1099	1110	rBV2	3652671	9282873	100.00%	14.398%
19	8.580	1116	1121	1127	rVB2	43396	94227	1.02%	0.146%
20	8.963	1176	1186	1199	rBV	1707260	3574510	38.51%	5.544%
21	9.451	1257	1269	1279	rBV3	48202	141536	1.52%	0.220%
22	9.969	1350	1357	1361	rBV2	50601	96634	1.04%	0.150%
23	10.439	1428	1437	1443	rBV	2543628	4819567	51.92%	7.475%
24	10.498	1443	1447	1460	rVB	481230	903718	9.74%	1.402%
25	10.639	1465	1471	1477	rVV2	51921	95307	1.03%	0.148%
26	11.127	1538	1554	1559	rBV	42191	94844	1.02%	0.147%
27	11.739	1648	1658	1668	rBV	2434184	4251870	45.80%	6.595%
28	11.839	1668	1675	1685	rVV	2857627	4777456	51.47%	7.410%
29	11.951	1685	1694	1708	rVB	3258112	6263802	67.48%	9.715%
30	12.274	1736	1749	1764	rBV	2598049	4319528	46.53%	6.700%
31	12.574	1792	1800	1807	rVB	169251	272803	2.94%	0.423%
32	12.727	1818	1826	1836	rBV	1906144	3223245	34.72%	4.999%
33	12.915	1852	1858	1863	rBV	332628	549537	5.92%	0.852%
34	12.980	1863	1869	1872	rVV	664771	1155299	12.45%	1.792%
35	13.010	1872	1874	1878	rVV	491073	694091	7.48%	1.077%
36	13.057	1878	1882	1893	rVB	488205	785707	8.46%	1.219%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071120.D
Acq On : 01 Mar 2022 15:48
Operator : JC\MD
Sample : N1689-01 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

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

37	13.215	1902	1909	1918	rBV	594541	986994	10.63%	1.531%
38	13.362	1925	1934	1949	rVB	2009517	3228248	34.78%	5.007%
39	13.668	1979	1986	2000	rBV2	1761737	4191794	45.16%	6.502%
40	13.874	2015	2021	2036	rVB2	685182	1465522	15.79%	2.273%
41	14.062	2047	2053	2058	rBV2	75142	129781	1.40%	0.201%
42	14.127	2058	2064	2066	rVV	89945	140832	1.52%	0.218%
43	14.215	2073	2079	2084	rVV	151170	235721	2.54%	0.366%
44	14.321	2092	2097	2106	rVB2	146960	250565	2.70%	0.389%
45	14.533	2125	2133	2136	rBV	94849	151175	1.63%	0.234%
46	14.574	2136	2140	2145	rVB	126207	189436	2.04%	0.294%
47	14.804	2174	2179	2185	rBV2	85451	141864	1.53%	0.220%
48	14.921	2191	2199	2206	rBV3	222131	493396	5.32%	0.765%
49	15.080	2220	2226	2234	rBV3	63110	109299	1.18%	0.170%
50	15.504	2291	2298	2306	rBV	267985	501526	5.40%	0.778%

Sum of corrected areas: 64473619

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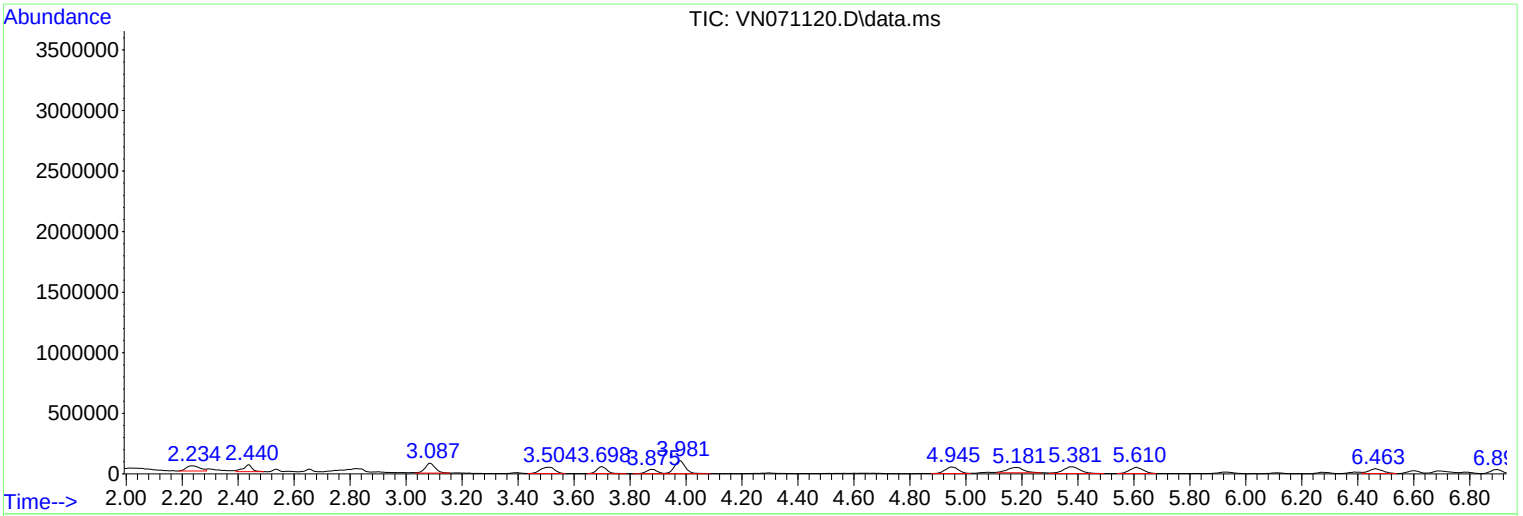
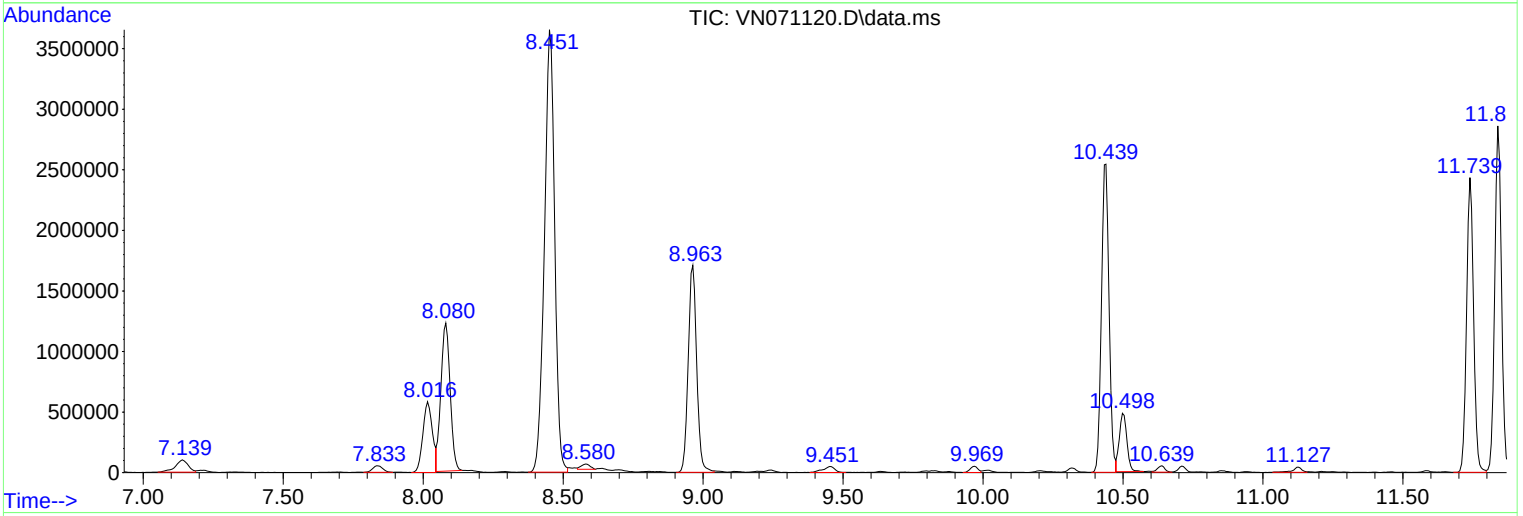
ALS Vial : 9 Sample Multiplier: 1

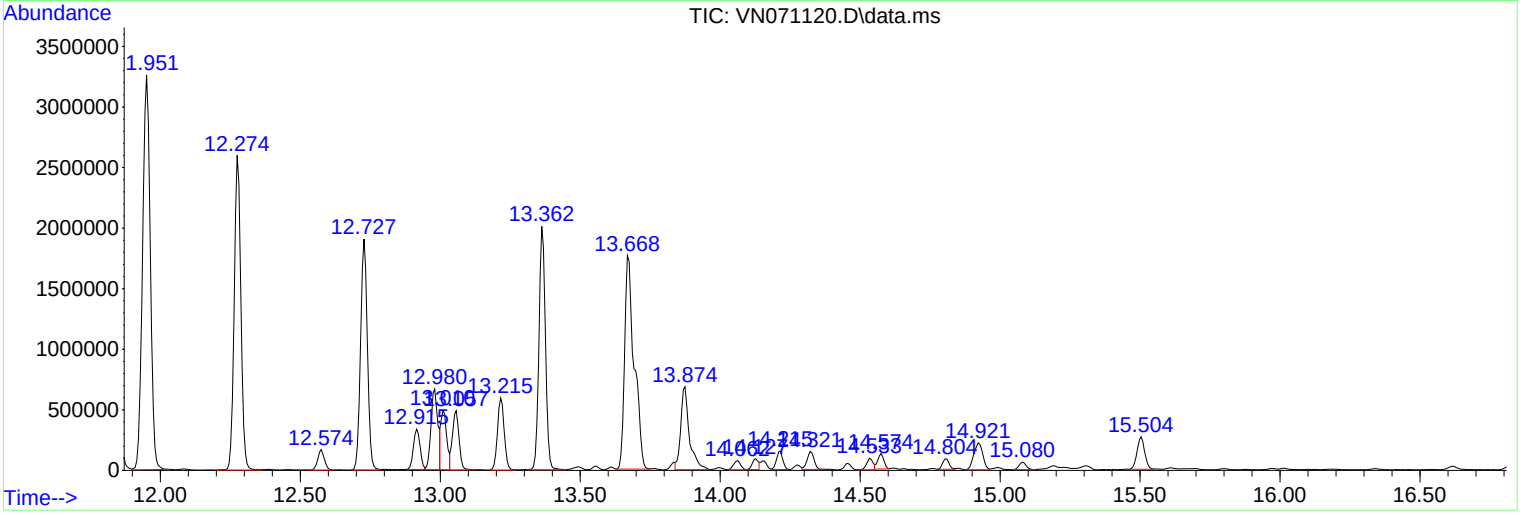
Instrument :
MSVOA_N
ClientSampleId :
MW-38

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 : VN071120.D
Acq On : 01 Mar 2022 15:48
Operator : JC\MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

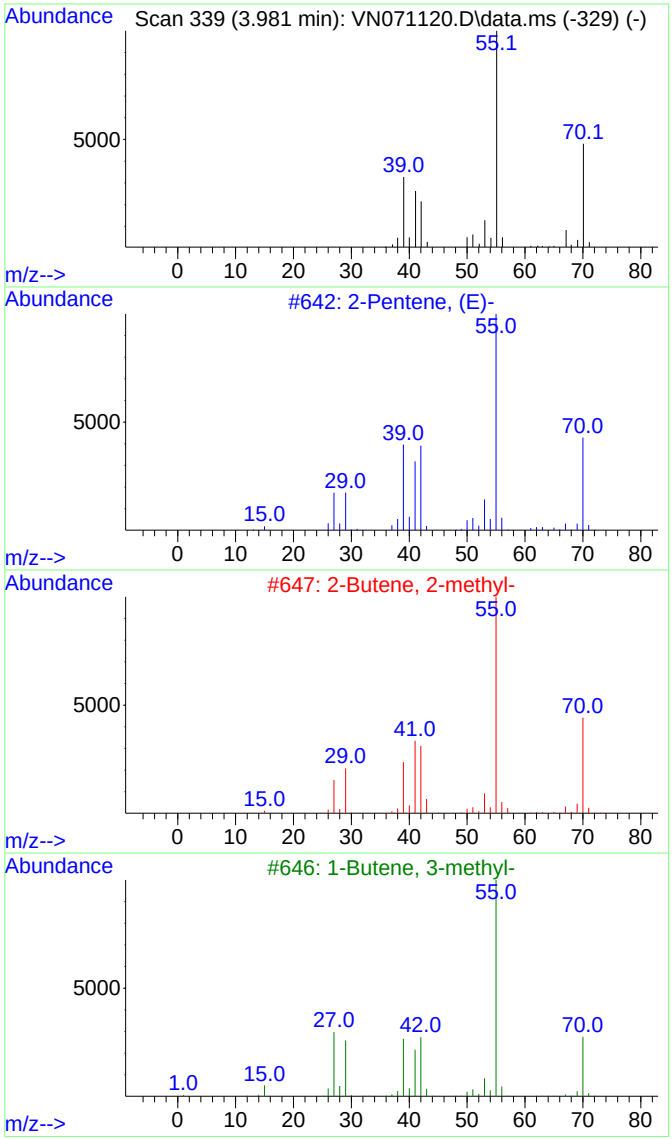
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

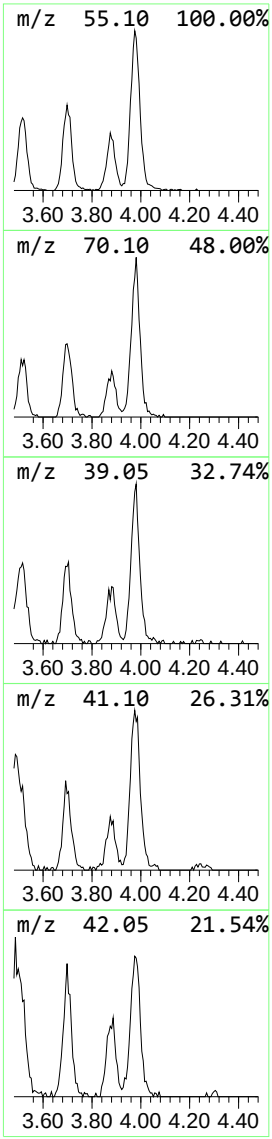
****

Peak Number 1 2-Pentene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	5.20 ug/l	290718	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	87
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	83
5	2-Methyl-1-butene	70	C5H10	000563-46-2	78





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Data File : VN071120.D
Acq On : 01 Mar 2022 15:48
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

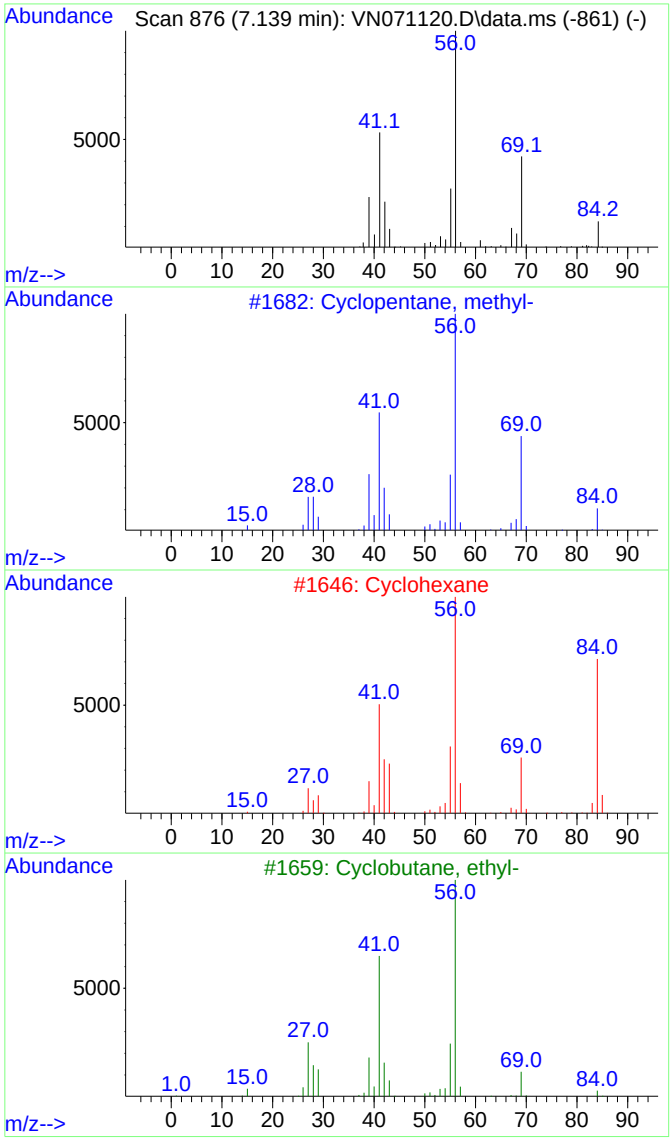
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

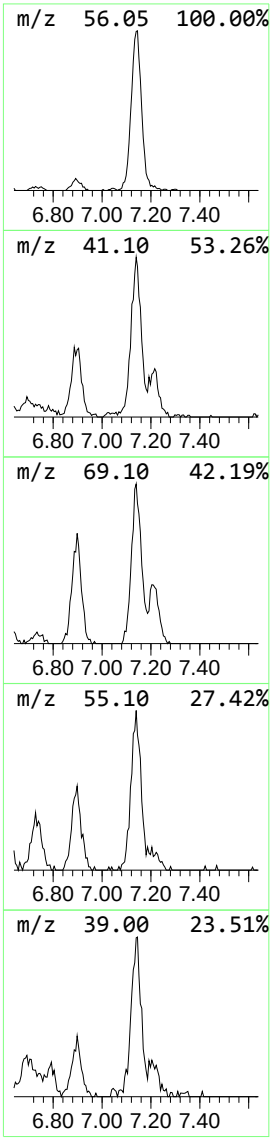
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.139	5.79 ug/l	323631	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclohexane	84	C6H12	000110-82-7	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	50
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
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Operator : JC\MD
Sample : N1689-01 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

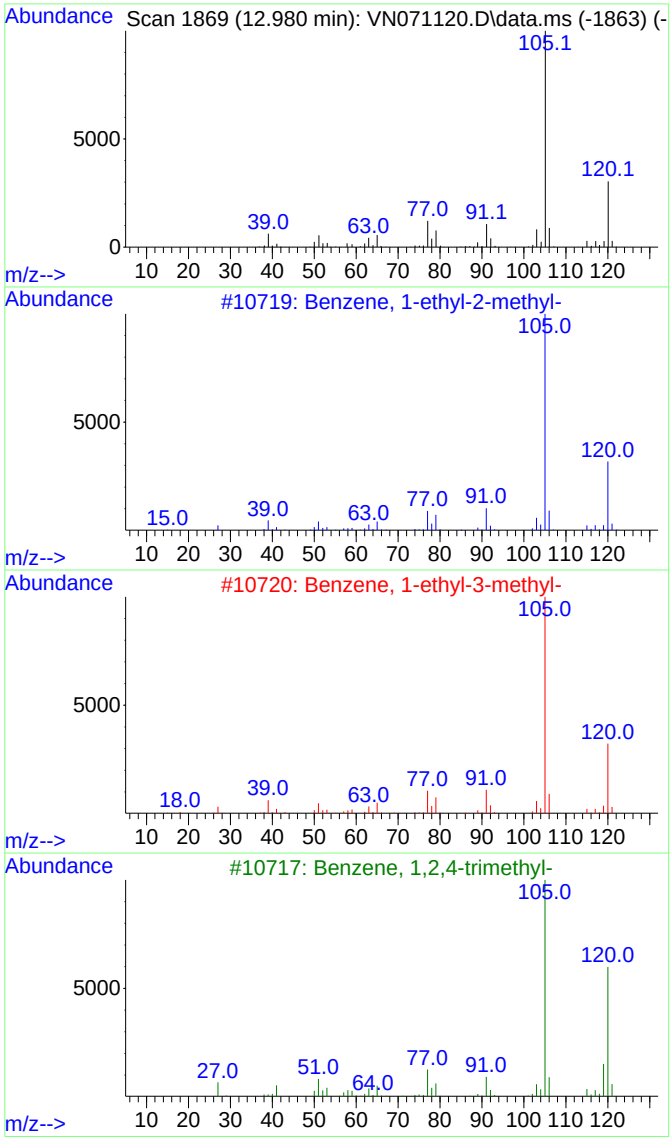
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

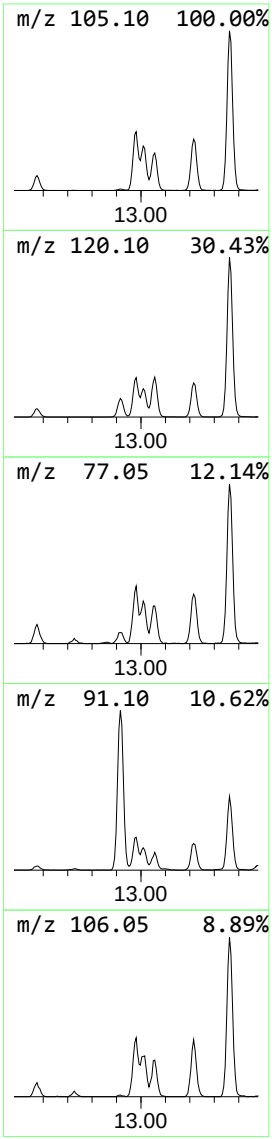
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	13.78 ug/l	1155300	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071120.D
Acq On : 01 Mar 2022 15:48
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

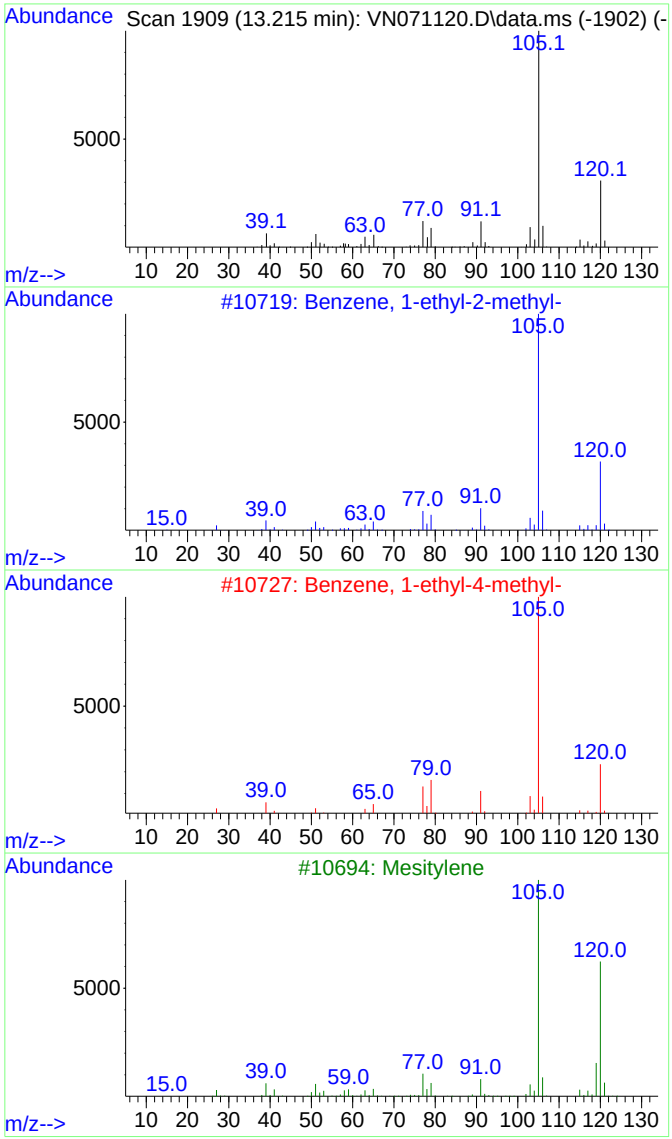
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

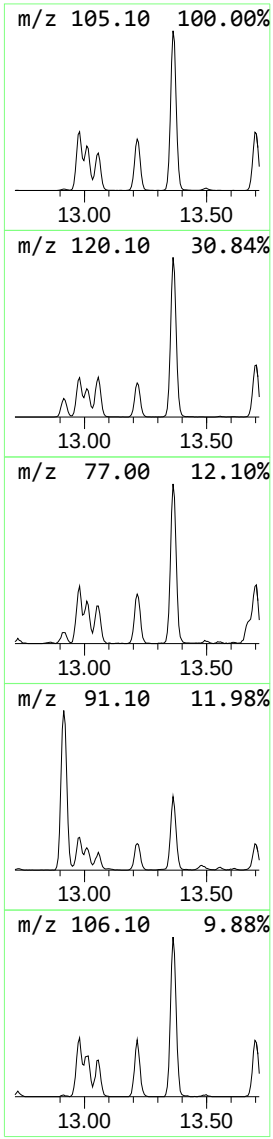
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	11.77 ug/l	986994	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

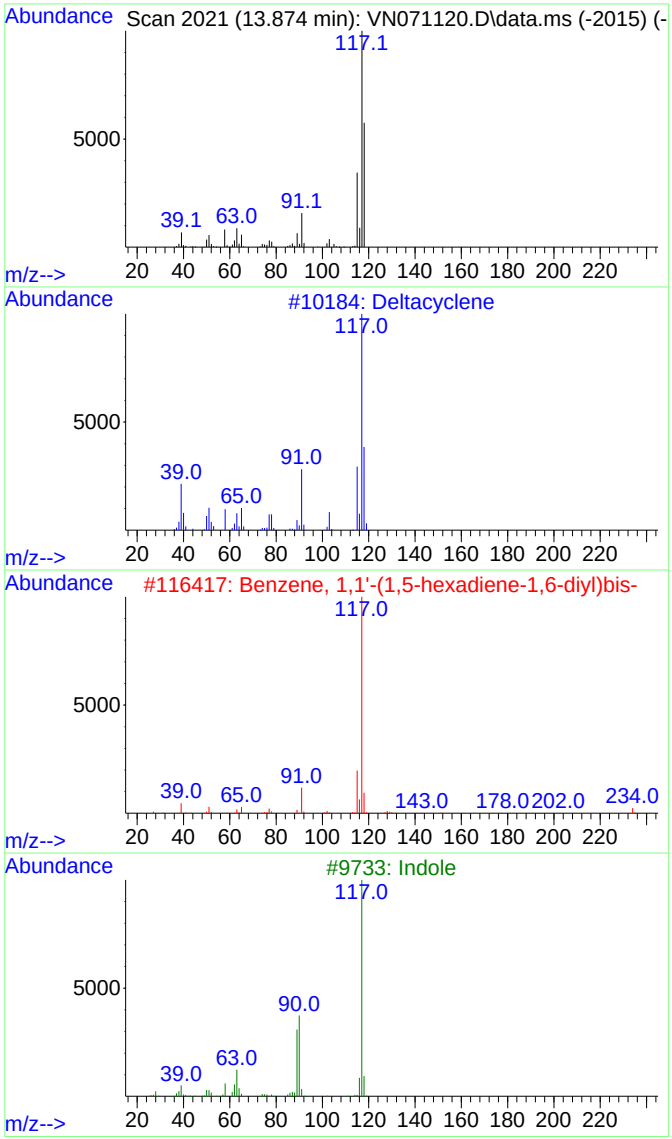
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

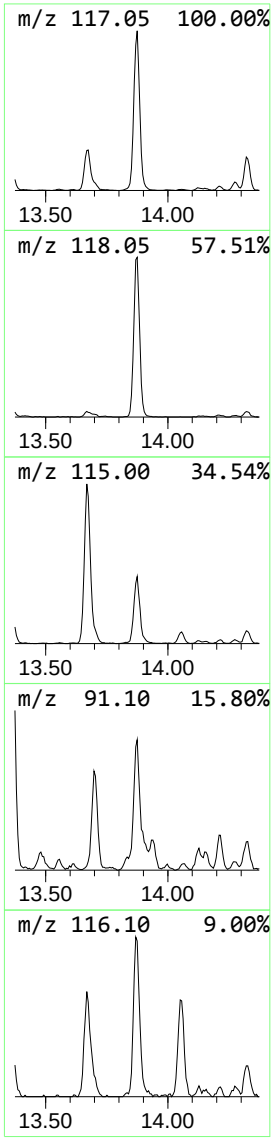
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	17.48 ug/l	1465520	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3	Indole	117	C8H7N	000120-72-9	46
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45





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ClientSampleId :
MW-38

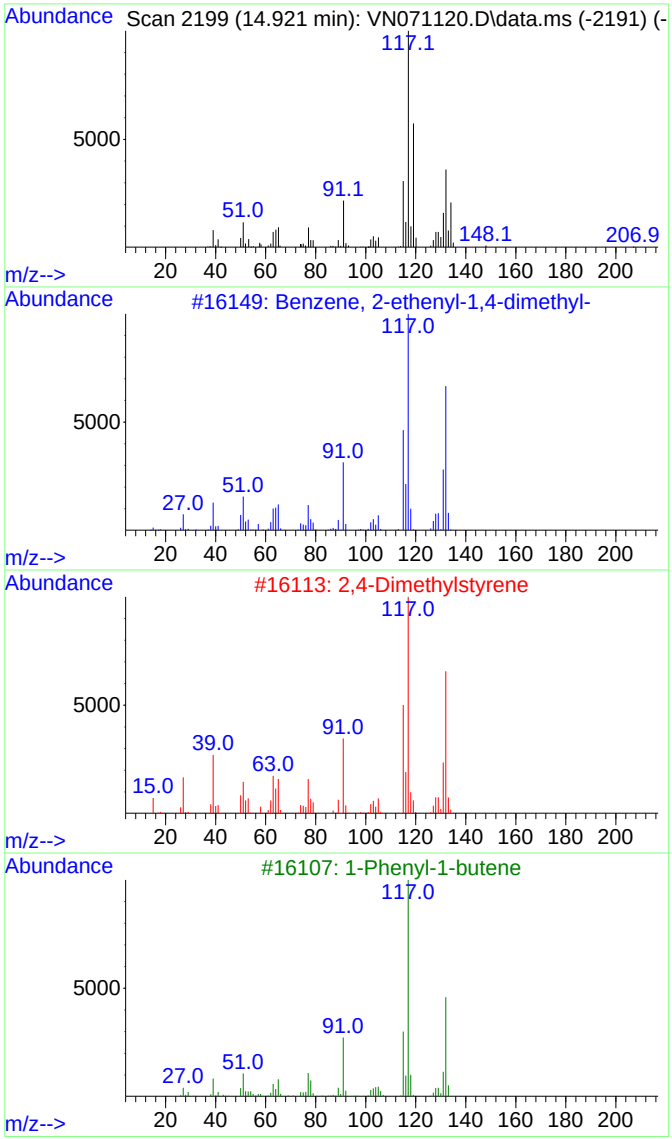
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

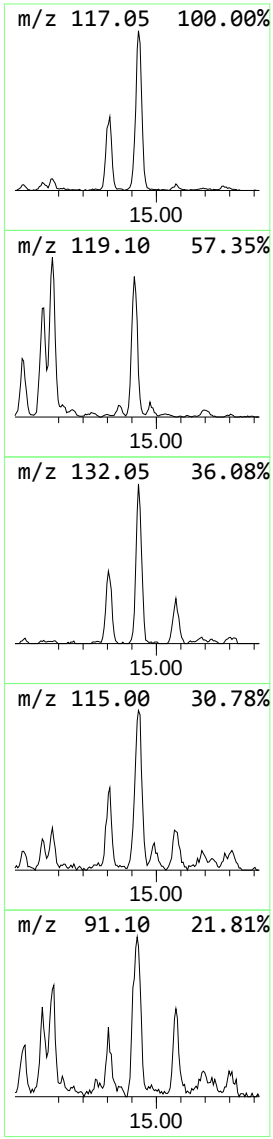
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	5.89 ug/l	493396	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071120.D
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Operator : JC\MD
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

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
2-Pentene, (E)-	3.981	5.2	ug/l	290718	1	8.080	2794890	50.0
Cyclopentane, m...	7.139	5.8	ug/l	323631	1	8.080	2794890	50.0
Benzene, 1-ethy...	12.980	13.8	ug/l	1155300	4	13.668	4191790	50.0
Benzene, 1-ethy...	13.215	11.8	ug/l	986994	4	13.668	4191790	50.0
Benzene, 1,1'-(...	13.874	17.5	ug/l	1465520	4	13.668	4191790	50.0
Benzene, 2-ethe...	14.921	5.9	ug/l	493396	4	13.668	4191790	50.0