LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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: VN071102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	38	46	52	rBV2	154793	267189	2.32%	0.277%
2	2.440	68	77	88	rVB	357011	579488	5.03%	0.601%
3	3.134	183	195	217	rVB	1159822	2724122	23.65%	2.823%
4	3.516	250	260	277	rBV2	610934	1686253	14.64%	1.748%
5	3.722	285	295	306	rVB3	92548	229967	2.00%	0.238%
6	3.899	312	325	332	rBV	54018	144462	1.25%	0.150%
7	3.993	332	341	358	rVB3	225574	615830	5.35%	0.638%
8	4.251	374	385	399	rBV6	33617	138029	1.20%	0.143%
9	4.963	493	506	514	rBV5	48629	173851	1.51%	0.180%
10	5.081	514	526	529	rVV2	123383	369146	3.21%	0.383%
11	5.151	530	538	569	rVB6	398897	2268190	19.69%	2.351%
12	5.622	598	618	634	rBV	311460	1079861	9.38%	1.119%
13	5.934	657	671	688	rVB4	58221	204495	1.78%	0.212%
14	6.122	688	703	718	rBV	195089	600054	5.21%	0.622%
15	6.287	721	731	740	rVV2	46080	135792	1.18%	0.141%
16	6.404	740	751	754	rVV2	48489	143250	1.24%	0.148%
17	6.469	754	762	774	rVV2	148165	448580	3.89%	0.465%
18	6.610	774	786	793	rVV3	97485	303494	2.64%	0.315%
19	6.692	793	800	813	rVV3	57684	275677	2.39%	0.286%
20	6.898	826	835	847	rVB2	113393	326656	2.84%	0.339%
21	7.145	865	877	887	rBV	1015004	2967241	25.76%	3.075%
22	7.839	988	995	1005	rVB2	198530	482227	4.19%	0.500%
23	8.016	1014	1025	1030	rBV	563415	1363395	11.84%	1.413%
24	8.087	1030	1037	1046	rVV2	1823871	4695429	40.77%	4.866%
25	8.175	1047	1052	1063	rVB3	116504	302131	2.62%	0.313%
26	8.292	1063	1072	1079	rBV2	111271	261006	2.27%	0.271%
27	8.439	1088	1097	1110	rBV2	807454	2452375	21.29%	2.542%
28	8.575	1110	1120	1126	rVV5	172034	513683	4.46%	0.532%
29	8.634	1126	1130	1137	rVV3	135689	346488	3.01%	0.359%
30	8.704	1137	1142	1153	rVB2	122790	293686	2.55%	0.304%
31	8.822	1153	1162	1174	rVB3	54002	179733	1.56%	0.186%
32	8.963	1176	1186	1199	rBV	1777851	3856268	33.48%	3.997%
33	9.239	1229	1233	1244	rVB	77288	164192	1.43%	0.170%
34	9.457	1255	1270	1278	rBV	496877	1291518	11.21%	1.339%
35	9.639	1294	1301	1308	rVB2	73052	145227	1.26%	0.151%
36	9.969	1350	1357	1361	rBV	173728	339789	2.95%	0.352%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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	10.016	1361	1365	1371	rVB4	72147	150965	1.31%	0.156%
38	10.316	1410	1416	1422	rBV	117655	213460	1.85%	0.221%
39	10.439	1428	1437	1443	rBV	2521136	4694227	40.76%	4.865%
40	10.498	1443	1447	1455	rVB	340516	632490	5.49%	0.655%
41	10.639	1460	1471	1477	rVV3	134618	317983	2.76%	0.330%
42	10.710	1477	1483	1490	rVB	111172	194892	1.69%	0.202%
43	10.857	1501	1508	1517	rVB5	62252	157710	1.37%	0.163%
44	11.739	1650	1658	1668	rBV	2179488	3939400	34.20%	4.083%
45	11.839	1668	1675	1685	rVV	3825207	6376744	55.37%	6.609%
46	11.945	1685	1693	1706	rVB	5753993	11517143	100.00%	11.936%
47	12.274	1738	1749	1759	rBV	1848160	3107061	26.98%	3.220%
48	12.574	1791	1800	1810	rBV	282700	457898	3.98%	0.475%
49	12.727	1818	1826	1837	rBV	1839149	3121245	27.10%	3.235%
50	12.916	1850	1858	1863	rBV	655220	1055998	9.17%	1.094%
51	12.980	1863	1869	1872	rVV	1175187	2165992	18.81%	2.245%
52	13.010	1872	1874	1878	rVV	1032359	1412985	12.27%	1.464%
53	13.051	1878	1881	1895	rVB	691342	1120593	9.73%	1.161%
54	13.216	1900	1909	1918	rBV	1340879	2170825	18.85%	2.250%
55	13.363	1921	1934	1948	rVV	4014201	6456578	56.06%	6.691%
56	13.669	1979	1986	1989	rBV	1886450	3330475	28.92%	3.452%
57	13.698	1989	1991	2000	rVB	1470143	2051256	17.81%	2.126%
58	13.833	2008	2014	2015	rBV	159706	205278	1.78%	0.213%
59	13.869	2015	2020	2037	rVV2	1380792	2927301	25.42%	3.034%
60	14.063	2047	2053	2058	rVV2	135945	237162	2.06%	0.246%
61	14.121	2058	2063	2066	rVV	216713	349990	3.04%	0.363%
62	14.157	2066	2069	2073	rVV	183011	264874	2.30%	0.275%
63	14.210	2073	2078	2084	rVV	394870	602768	5.23%	0.625%
64	14.274	2084	2089	2092	rVV	103649	169489	1.47%	0.176%
65	14.321	2092	2097	2107	rVB	399987	668727	5.81%	0.693%
66	14.457	2114	2120	2125	rBV	116055	189472	1.65%	0.196%
67	14.533	2125	2133	2136	rBV	233459	376462	3.27%	0.390%
68	14.574	2136	2140	2145	rVB	327040	489232	4.25%	0.507%
69	14.804	2174	2179	2184	rBV2	223398	356692	3.10%	0.370%
70	14.927	2191	2200	2206	rBV2	540387	1093964	9.50%	1.134%
71	15.080	2218	2226	2234	rBV2	125825	236781	2.06%	0.245%
72	15.192	2234	2245	2248	rBV6	71158	170347	1.48%	0.177%
73	15.310	2258	2265	2272	rVB3	74447	179315	1.56%	0.186%
74	15.498	2289	2297	2305	rBV	497739	957355	8.31%	0.992%

Sum of corrected areas: 96489903

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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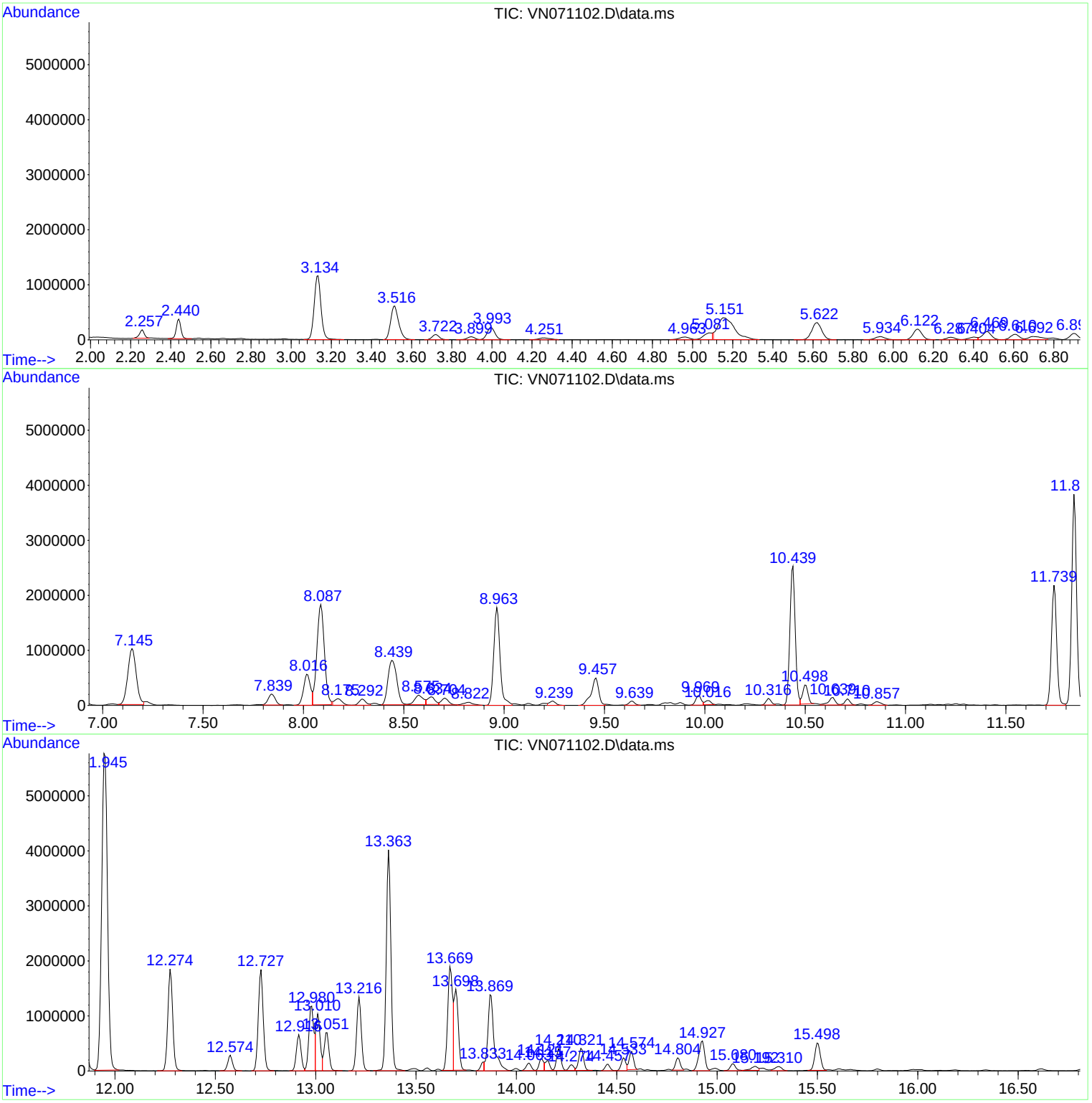
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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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Data File : VN071102.D
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MSVOA_N
ClientSampleId :
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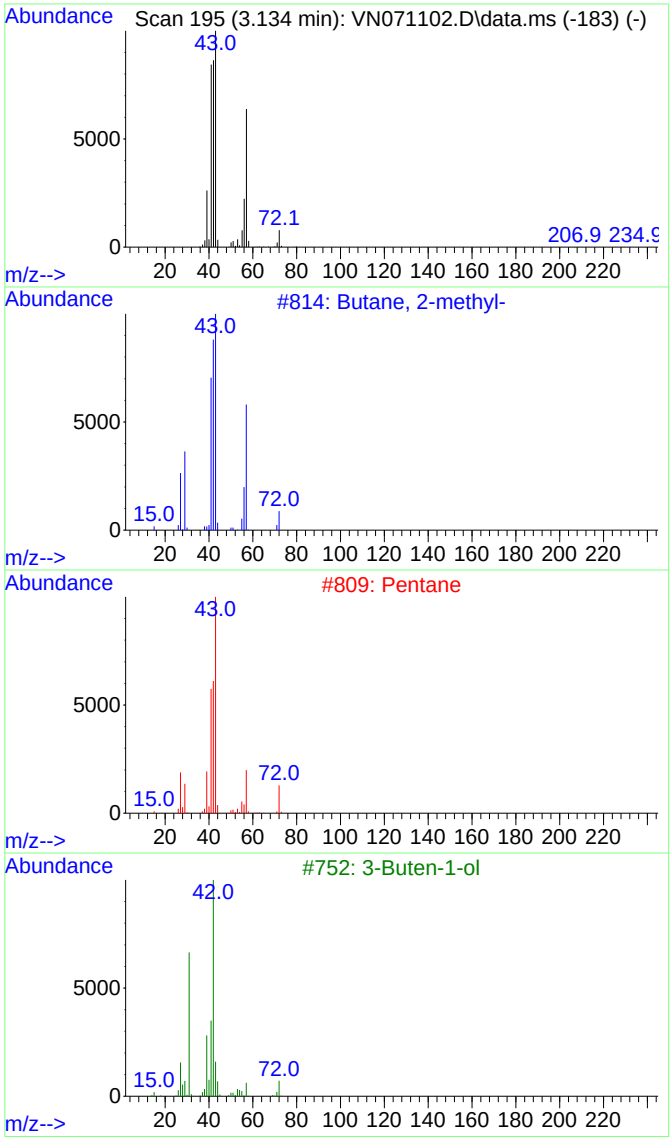
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

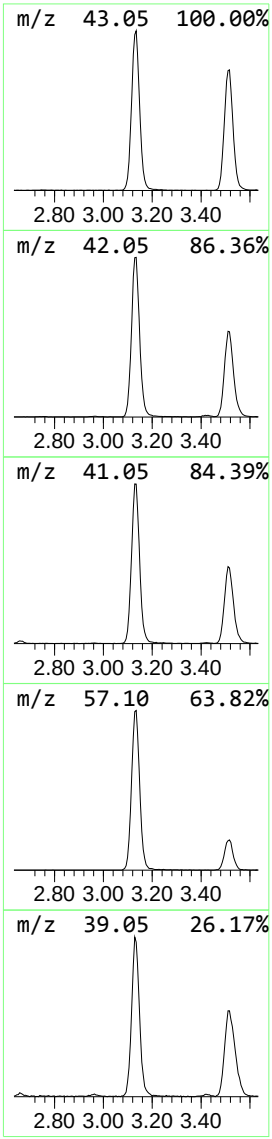
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	29.01 ug/l	2724120	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	42
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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

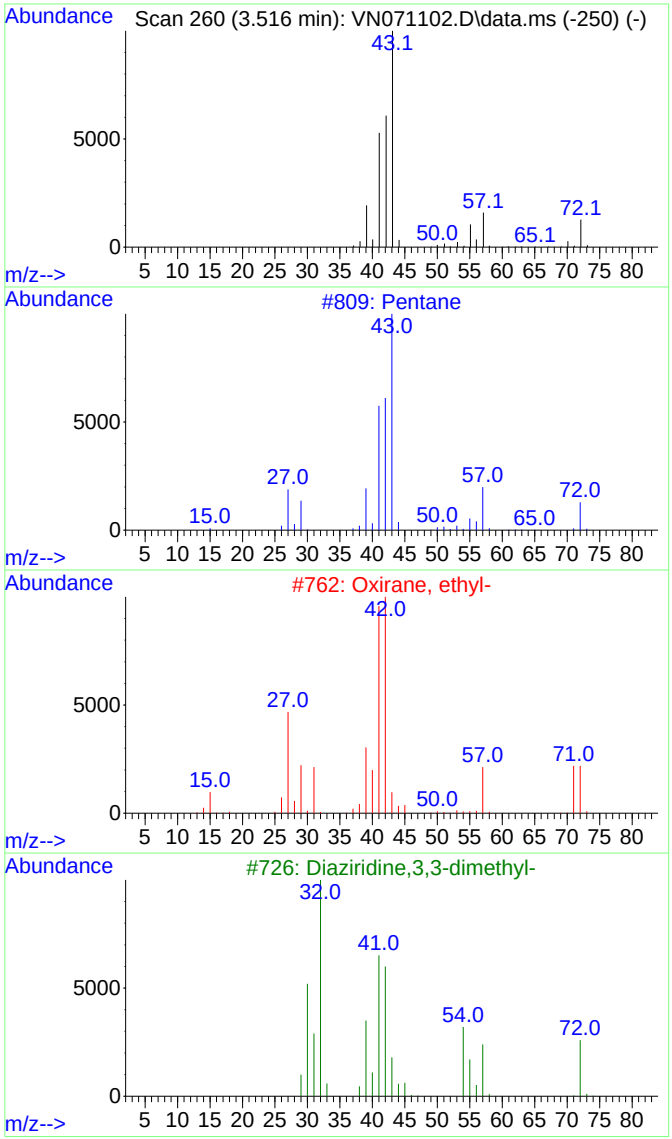
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

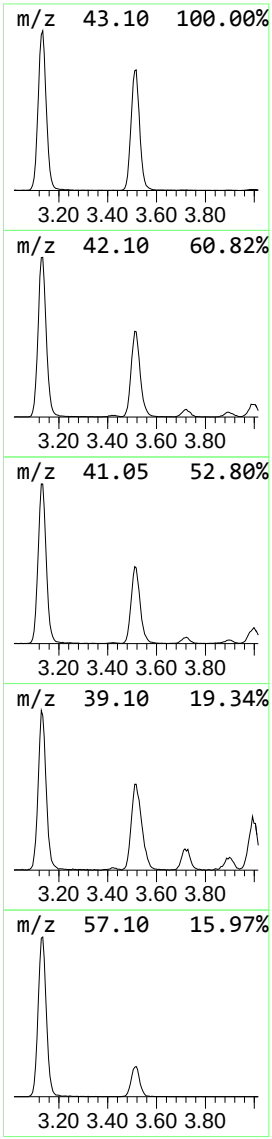
****

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	17.96 ug/l	1686250	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	38
5	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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

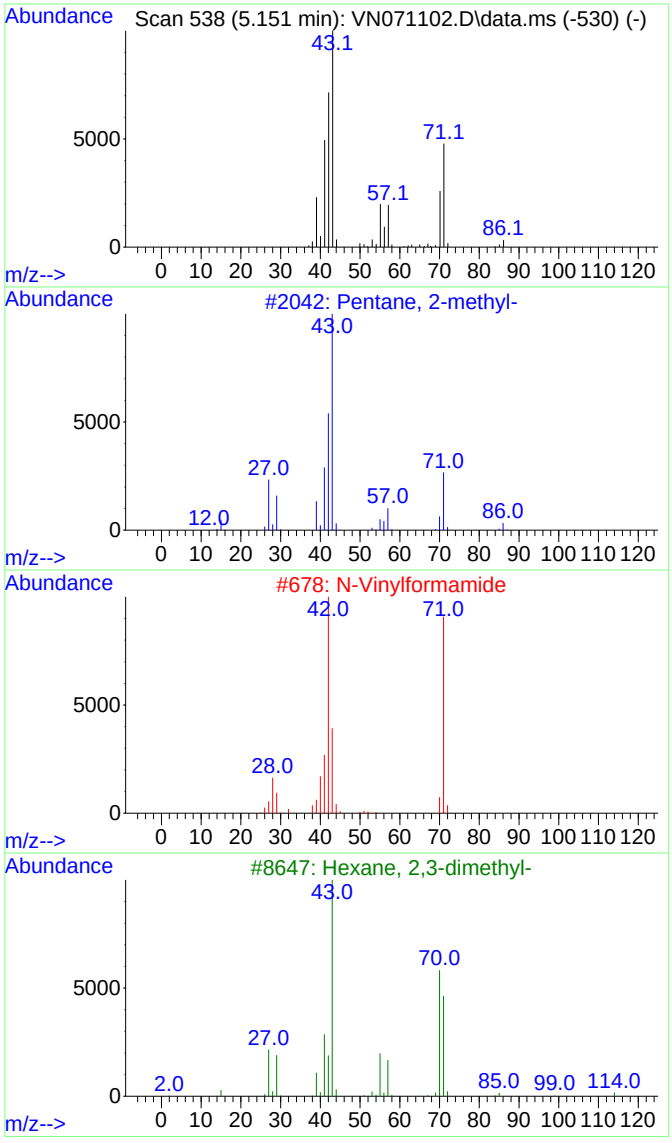
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

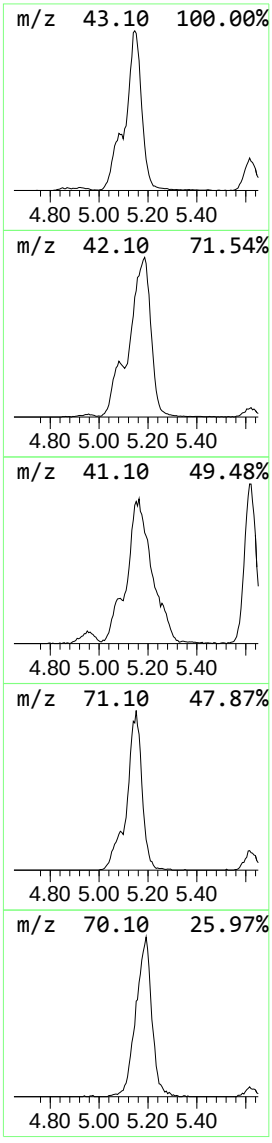
****

Peak Number 3 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	24.15 ug/l	2268190	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	80
2	N-Vinylformamide	71	C3H5NO	013162-05-5	38
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
4	Pentane	72	C5H12	000109-66-0	38
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38





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Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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

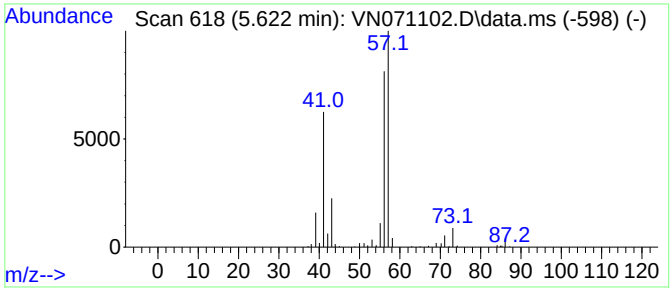
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

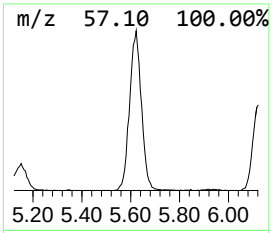
****

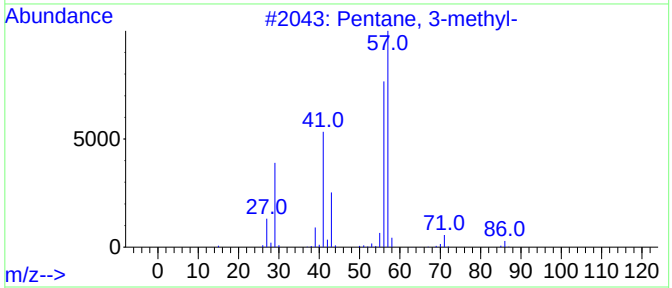
Peak Number 4 Pentane, 3-methyl- Concentration Rank 9

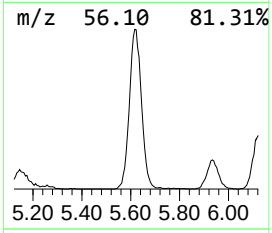
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	11.50 ug/l	1079860	Pentafluorobenzene	8.081

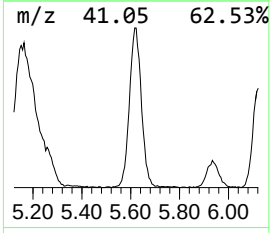
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50

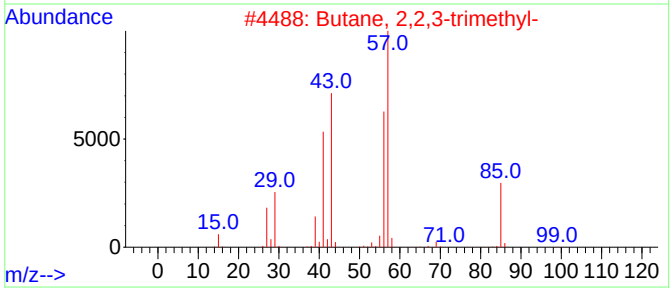


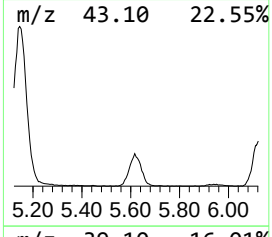


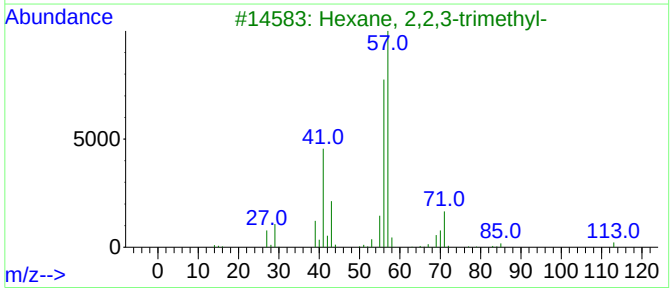


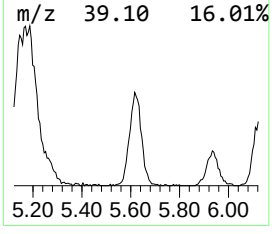












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ClientSampleId :
DUP022522

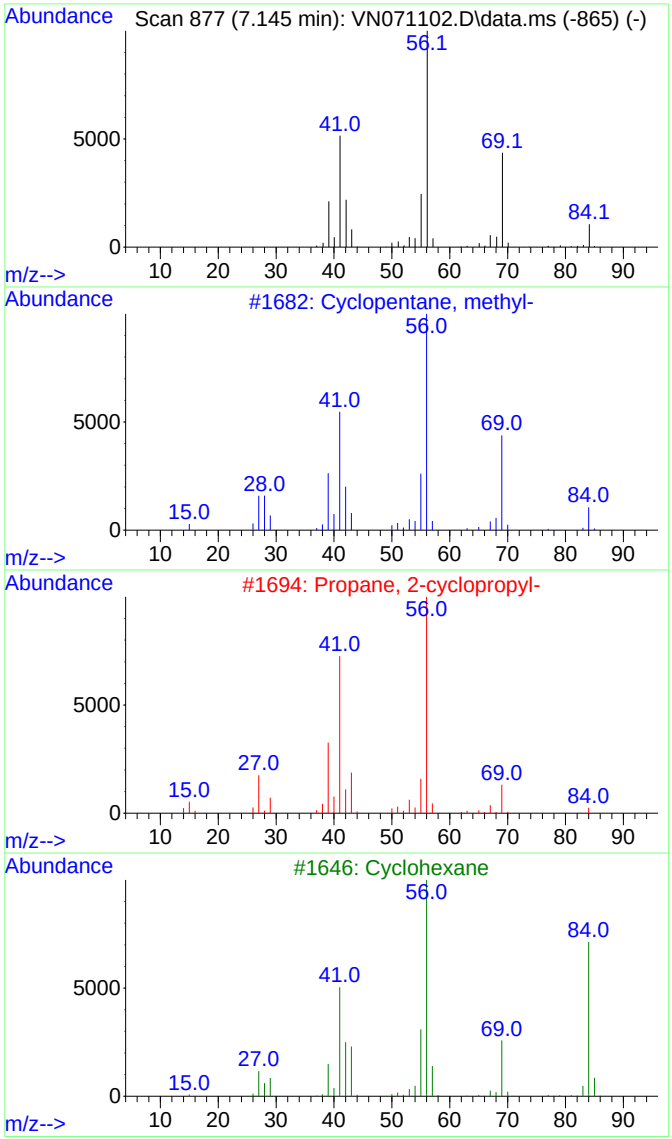
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

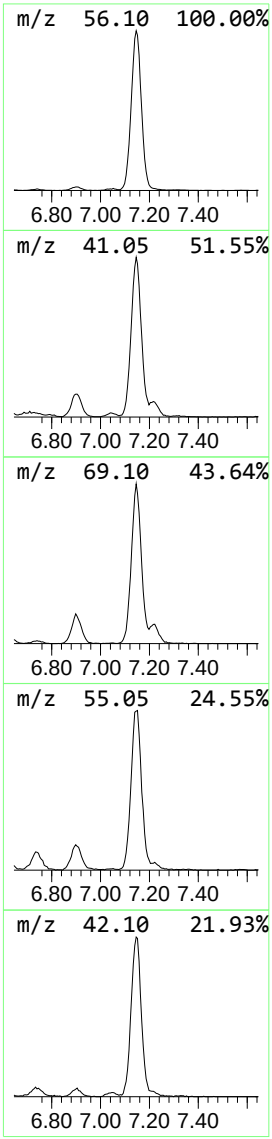
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	31.60 ug/l	2967240	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





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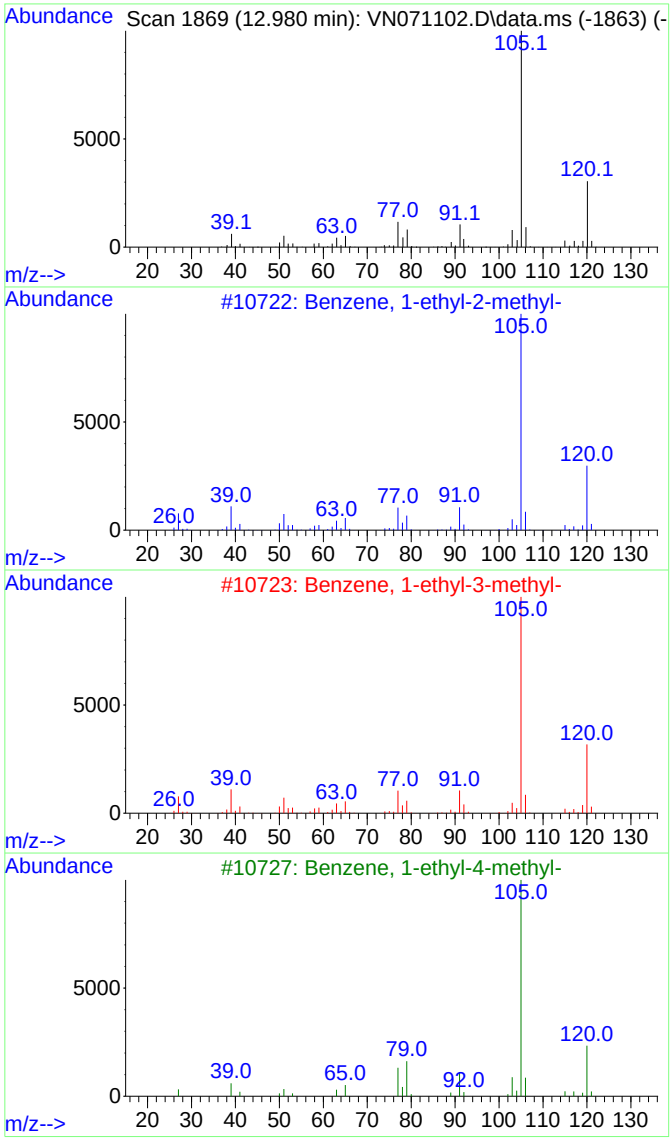
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

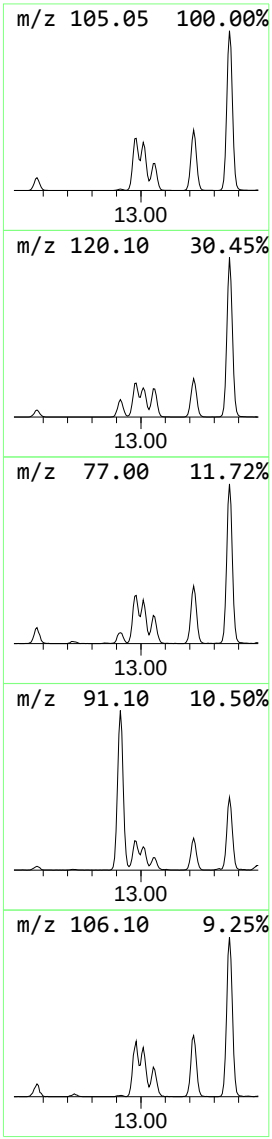
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	32.52 ug/l	2165990	1,4-Dichlorobenzene-d4	13.669

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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

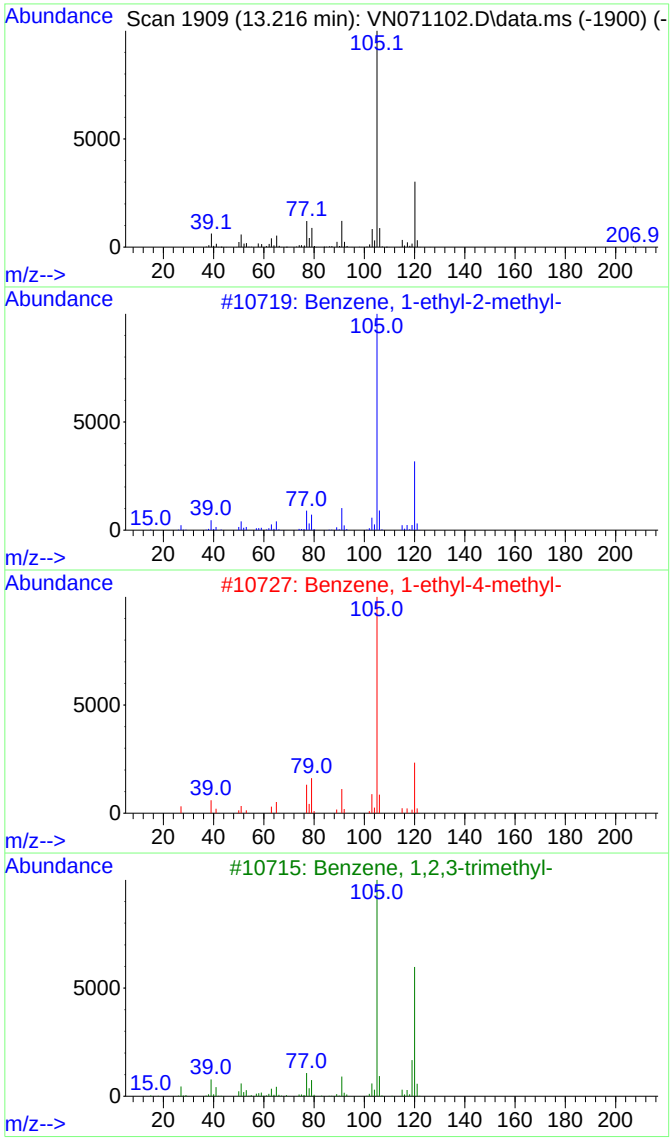
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

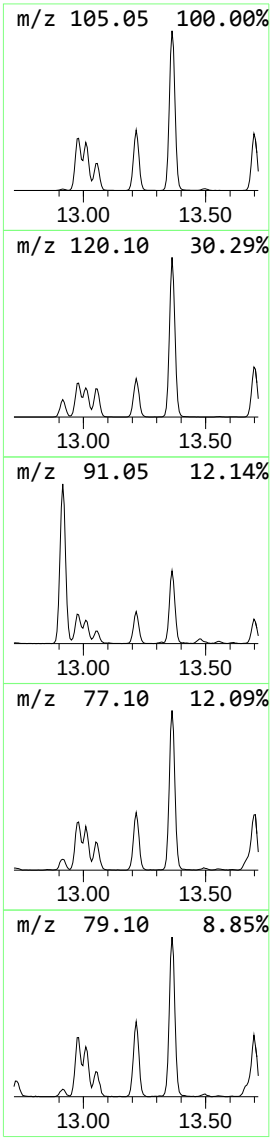
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	32.59 ug/l	2170830	1,4-Dichlorobenzene-d4	13.669

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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

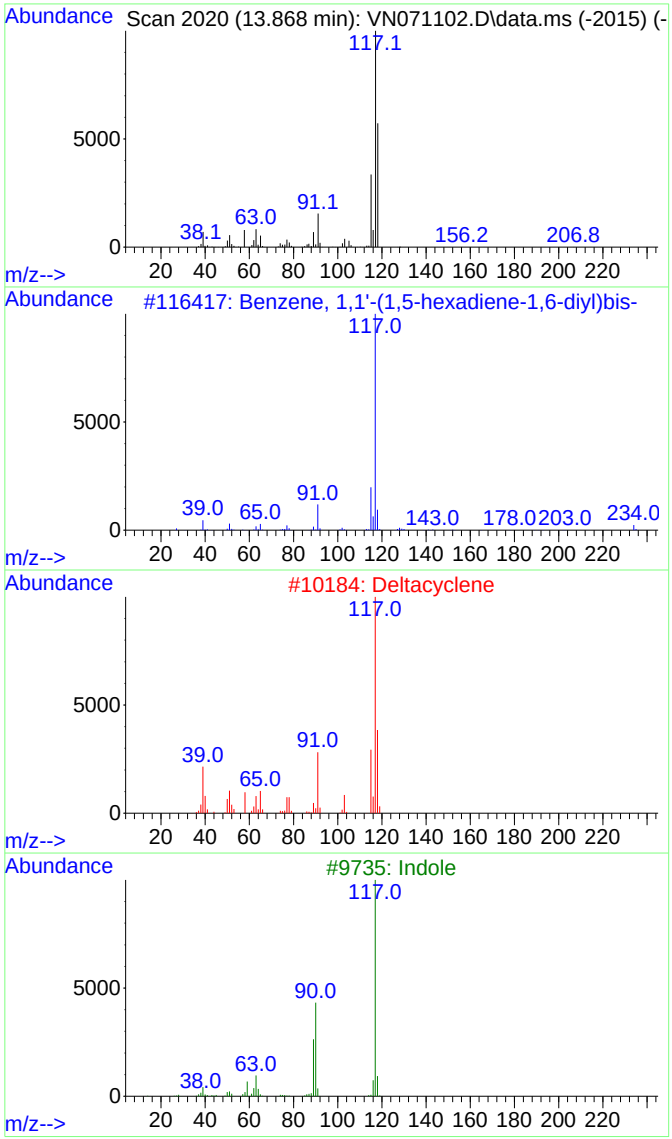
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

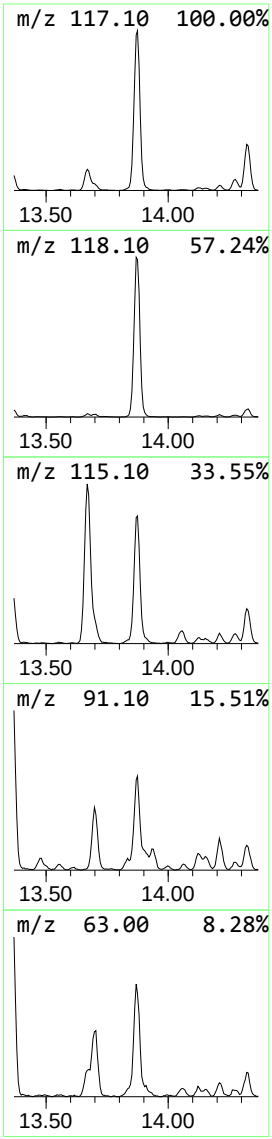
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	43.95 ug/l	2927300	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	Deltacyclene	118	C9H10	007785-10-6	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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

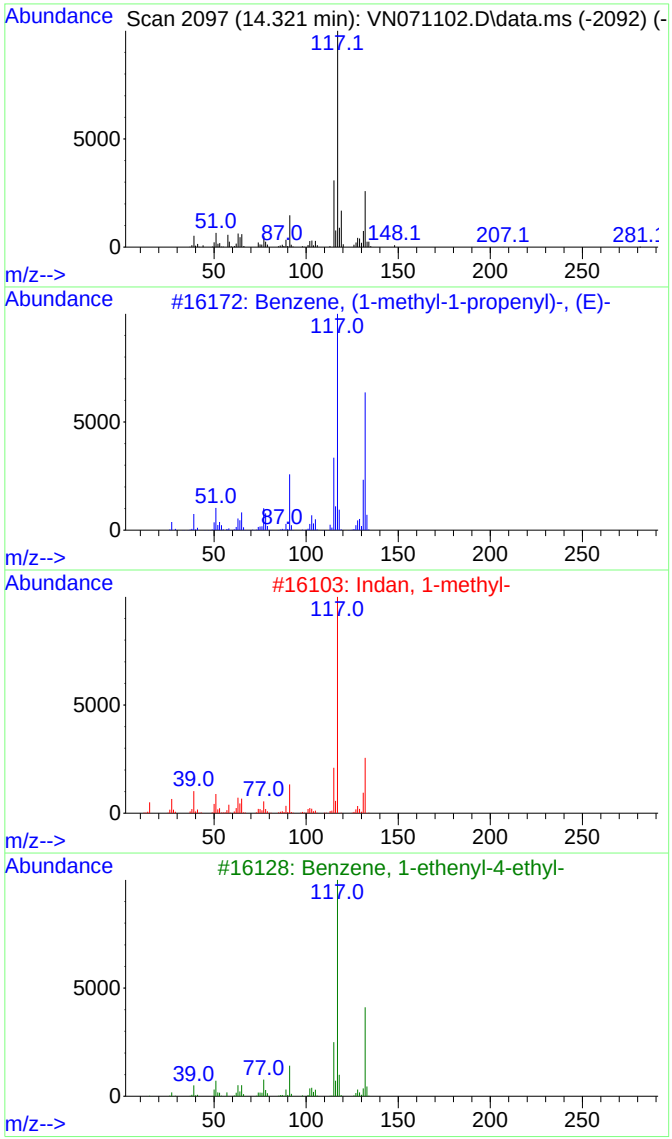
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

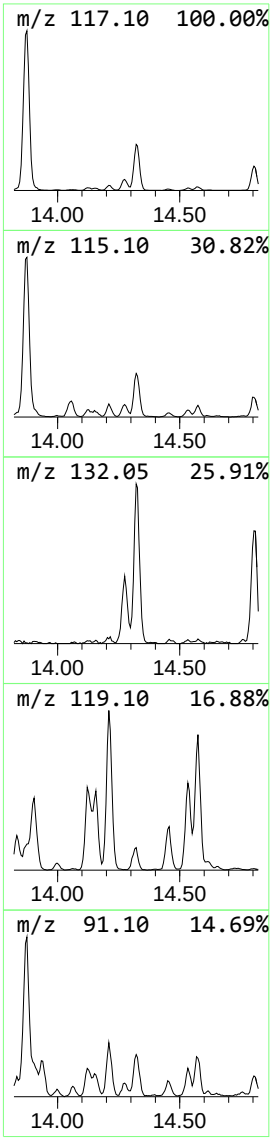
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-propen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	10.04 ug/l	668727	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
2	Indan, 1-methyl-	132	C10H12	000767-58-8	81
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	74
4	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	72
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	72





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Data File : VN071102.D
Acq On : 28 Feb 2022 18:20
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

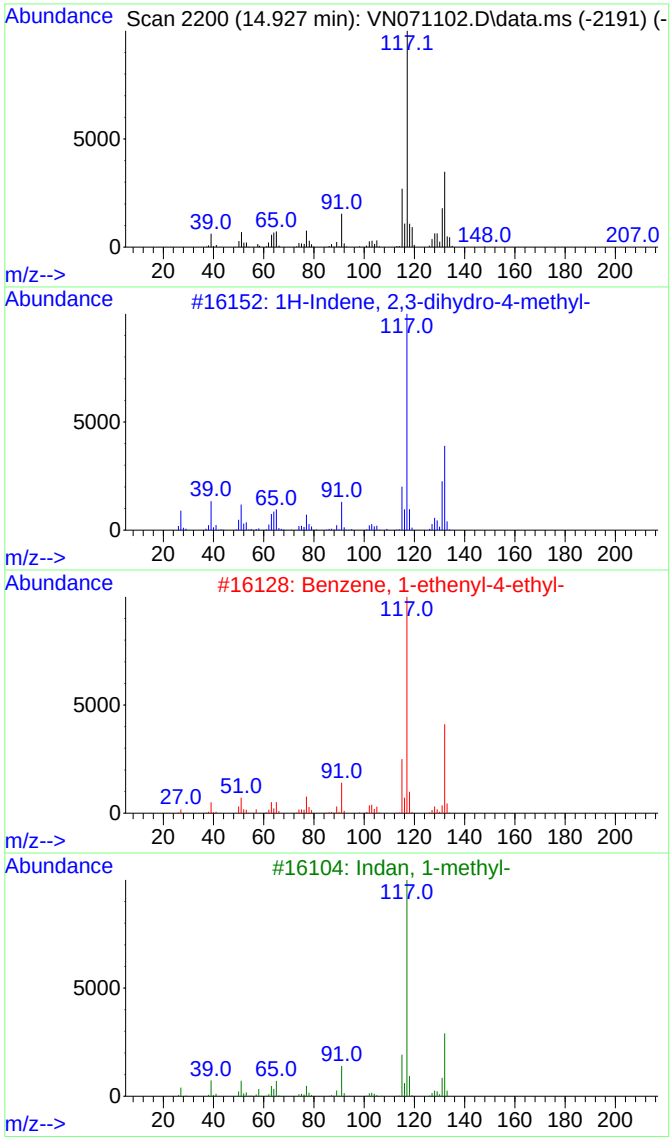
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

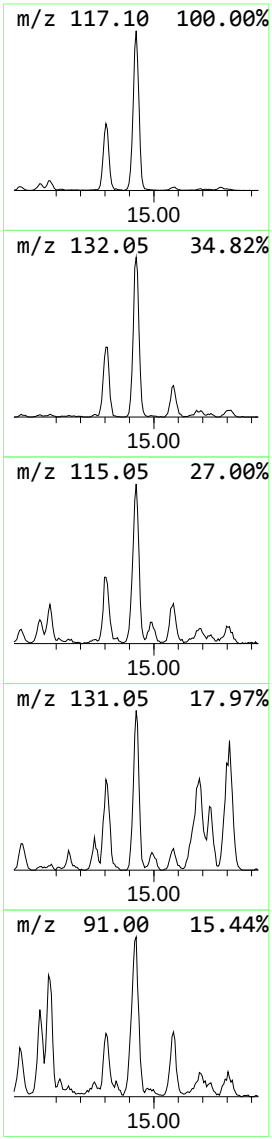
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	16.42 ug/l	1093960	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	Indan, 1-methyl-	132	C10H12	000767-58-8	90
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022822\
Data File : VN071102.D
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Operator : JC\MD
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ALS Vial : 17 Sample Multiplier: 1

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MSVOA_N
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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-	3.134	29.0	ug/l	2724120	1	8.081	4695430	50.0
Pentane	3.516	18.0	ug/l	1686250	1	8.081	4695430	50.0
Pentane, 2-methyl-	5.151	24.1	ug/l	2268190	1	8.081	4695430	50.0
Pentane, 3-methyl-	5.622	11.5	ug/l	1079860	1	8.081	4695430	50.0
Cyclopentane, m...	7.145	31.6	ug/l	2967240	1	8.081	4695430	50.0
Benzene, 1-ethy...	12.980	32.5	ug/l	2165990	4	13.669	3330480	50.0
Benzene, 1-ethy...	13.216	32.6	ug/l	2170830	4	13.669	3330480	50.0
Benzene, 1,1'-(...	13.868	44.0	ug/l	2927300	4	13.669	3330480	50.0
Benzene, (1-met...	14.321	10.0	ug/l	668727	4	13.669	3330480	50.0
1H-Indene, 2,3-...	14.927	16.4	ug/l	1093960	4	13.669	3330480	50.0