LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 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: VN071122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	37	46	51	rBV3	90946	192109	1.73%	0.226%
2	2.440	71	77	88	rVB	200998	332838	3.01%	0.392%
3	3.128	184	194	214	rVB	633816	1498826	13.53%	1.764%
4	3.511	249	259	276	rBV3	345071	954012	8.61%	1.123%
5	3.716	286	294	305	rVB2	62881	160233	1.45%	0.189%
6	3.993	333	341	356	rVB2	172949	466819	4.21%	0.549%
7	4.958	492	505	515	rBV4	39778	143624	1.30%	0.169%
8	5.081	515	526	527	rBV2	65491	148143	1.34%	0.174%
9	5.163	530	540	541	rBV	162323	411767	3.72%	0.485%
10	5.616	605	617	634	rBV3	176505	631535	5.70%	0.743%
11	5.934	659	671	684	rVB3	38336	124043	1.12%	0.146%
12	6.116	691	702	716	rBV3	106556	327049	2.95%	0.385%
13	6.463	755	761	772	rVB2	106957	315251	2.85%	0.371%
14	6.605	775	785	793	rBV2	73563	226219	2.04%	0.266%
15	6.699	793	801	812	rBV4	36264	133042	1.20%	0.157%
16	6.899	825	835	850	rVB4	83059	250396	2.26%	0.295%
17	7.146	865	877	899	rVB2	684446	2134633	19.27%	2.512%
18	7.846	987	996	1005	rVB2	158403	392807	3.55%	0.462%
19	8.016	1015	1025	1030	rBV	542805	1301389	11.75%	1.532%
20	8.087	1030	1037	1047	rVV2	1618784	4084408	36.88%	4.807%
21	8.175	1047	1052	1063	rVB5	70319	189971	1.72%	0.224%
22	8.293	1064	1072	1078	rBV	64321	141802	1.28%	0.167%
23	8.440	1088	1097	1109	rBV2	805463	2412097	21.78%	2.839%
24	8.581	1111	1121	1126	rVV3	115233	357656	3.23%	0.421%
25	8.640	1127	1131	1136	rVV2	80988	176177	1.59%	0.207%
26	8.704	1137	1142	1152	rVB3	71533	176226	1.59%	0.207%
27	8.822	1152	1162	1175	rVB4	32747	117030	1.06%	0.138%
28	8.963	1175	1186	1200	rBV	1710982	3647706	32.93%	4.293%
29	9.246	1228	1234	1242	rVB2	55582	130129	1.17%	0.153%
30	9.457	1254	1270	1287	rBV	331949	877963	7.93%	1.033%
31	9.969	1350	1357	1362	rBV	159693	316998	2.86%	0.373%
32	10.316	1409	1416	1422	rBV2	106616	203009	1.83%	0.239%
33	10.440	1428	1437	1443	rBV	2460935	4521055	40.82%	5.321%
34	10.504	1443	1448	1461	rVV	366230	742557	6.70%	0.874%
35	10.634	1461	1470	1477	rVV2	124689	276386	2.50%	0.325%
36	10.710	1477	1483	1489	rVB3	103805	186154	1.68%	0.219%

LSC Area Percent Report

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Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 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	10.857	1501	1508	1519	rVB5	53626	126247	1.14%	0.149%
38	11.739	1650	1658	1668	rBV	2160523	3799556	34.30%	4.472%
39	11.839	1668	1675	1685	rVV	3635454	6080525	54.90%	7.157%
40	11.951	1685	1694	1706	rVB	5580248	11075869	100.00%	13.036%
41	12.275	1741	1749	1766	rVB	1803375	3030379	27.36%	3.567%
42	12.575	1792	1800	1809	rVB	263374	426588	3.85%	0.502%
43	12.728	1818	1826	1837	rBV	1753966	3024714	27.31%	3.560%
44	12.916	1849	1858	1863	rBV	623906	1007231	9.09%	1.186%
45	12.981	1863	1869	1872	rVV	1168517	2100874	18.97%	2.473%
46	13.010	1872	1874	1878	rVV	971341	1344947	12.14%	1.583%
47	13.057	1878	1882	1901	rVB	688277	1122026	10.13%	1.321%
48	13.216	1901	1909	1918	rBV	1291276	2126532	19.20%	2.503%
49	13.363	1922	1934	1948	rVV	3980408	6368506	57.50%	7.496%
50	13.669	1979	1986	1989	rBV	1816434	3147896	28.42%	3.705%
51	13.698	1989	1991	2000	rVB	1407021	2034381	18.37%	2.394%
52	13.833	2007	2014	2015	rBV	152407	193912	1.75%	0.228%
53	13.869	2015	2020	2037	rVV	1337438	2845608	25.69%	3.349%
54	14.063	2047	2053	2058	rBV2	130775	234221	2.11%	0.276%
55	14.128	2058	2064	2066	rVV	209510	332732	3.00%	0.392%
56	14.157	2066	2069	2073	rVV	178037	263325	2.38%	0.310%
57	14.210	2073	2078	2084	rVV	366848	587538	5.30%	0.692%
58	14.275	2084	2089	2092	rVV	106720	167675	1.51%	0.197%
59	14.322	2092	2097	2109	rVB2	392926	664845	6.00%	0.783%
60	14.457	2114	2120	2127	rBV	115796	187454	1.69%	0.221%
61	14.533	2127	2133	2136	rBV	235831	373395	3.37%	0.439%
62	14.575	2136	2140	2145	rVB	329954	484931	4.38%	0.571%
63	14.804	2174	2179	2185	rBV2	221805	357690	3.23%	0.421%
64	14.928	2191	2200	2206	rBV2	525811	1079615	9.75%	1.271%
65	15.080	2219	2226	2234	rBV2	130803	237803	2.15%	0.280%
66	15.192	2234	2245	2249	rBV4	70360	189577	1.71%	0.223%
67	15.304	2257	2264	2273	rVB3	72229	182133	1.64%	0.214%
68	15.498	2290	2297	2306	rBV	539750	1059885	9.57%	1.248%

Sum of corrected areas: 84960669

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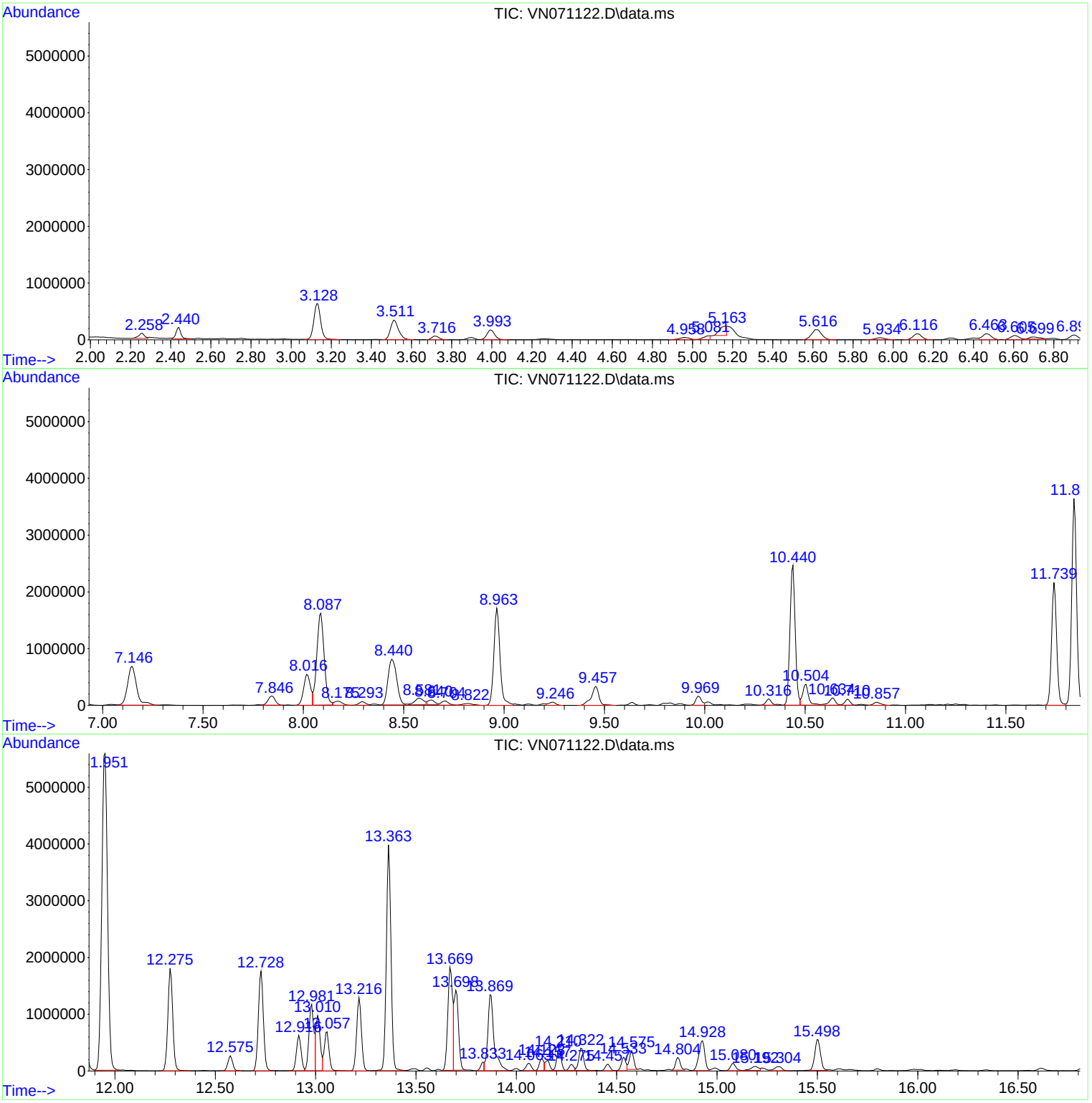
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
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Operator : JC\MD
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Quant Title : SW846 8260

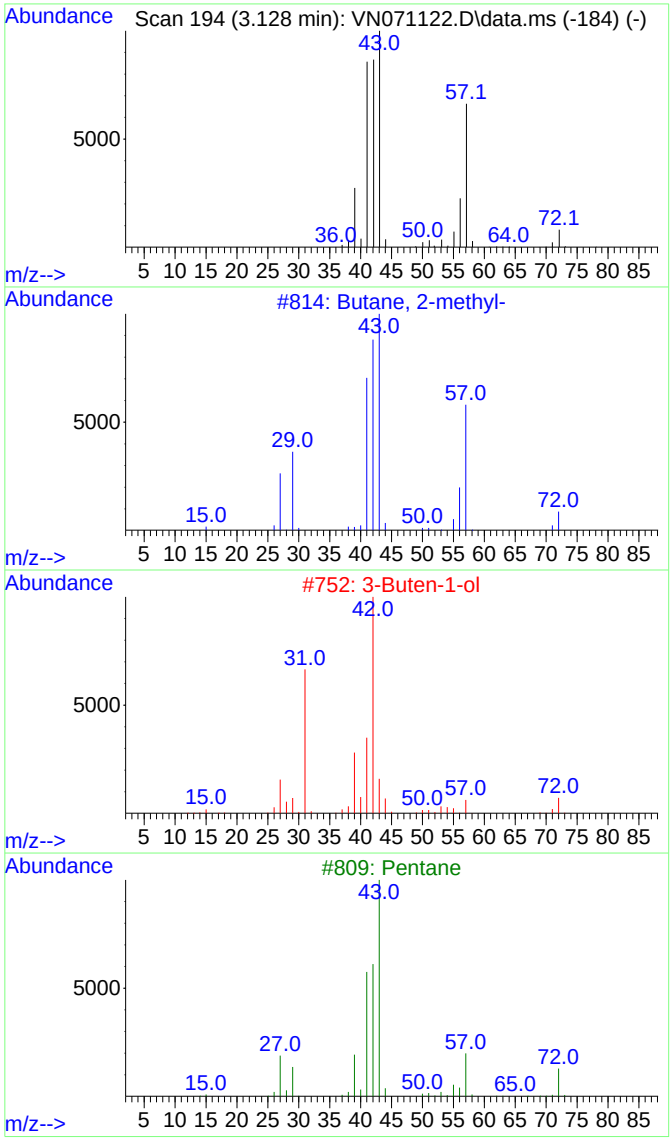
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

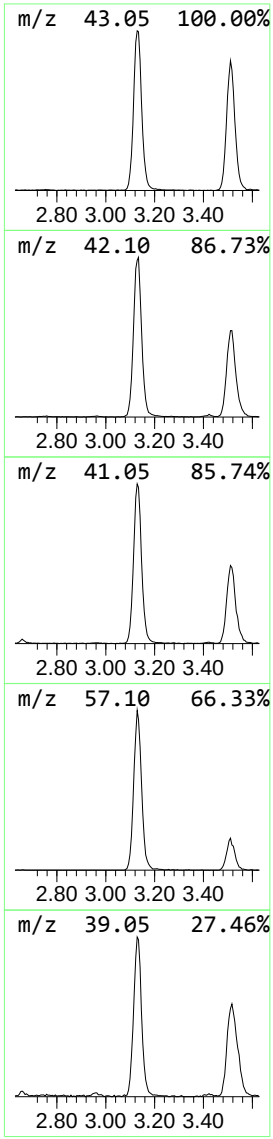
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	18.35 ug/l	1498830	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	38
4	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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

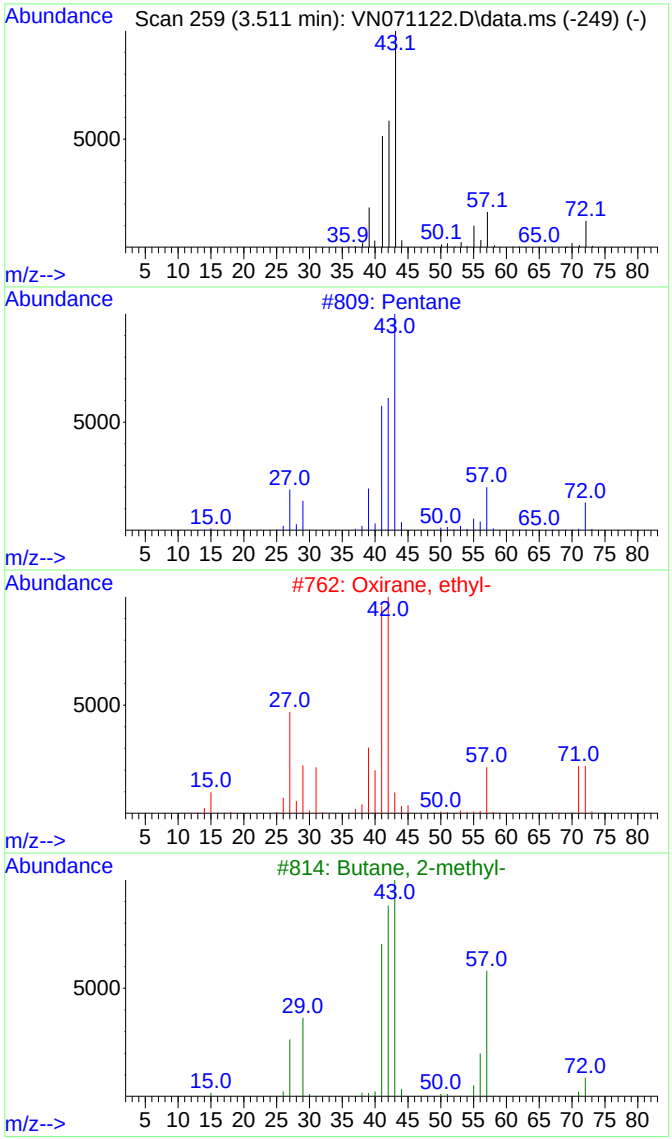
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

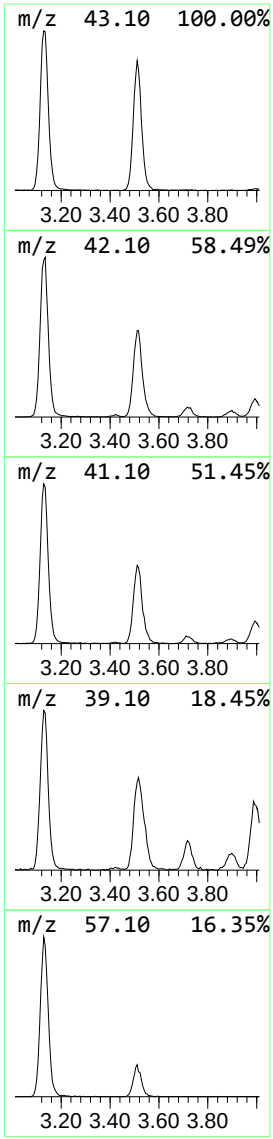
****

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.511	11.68 ug/l	954012	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	Butane, 2-methyl-	72	C5H12	000078-78-4	40
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12





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Data File : VN071122.D
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Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

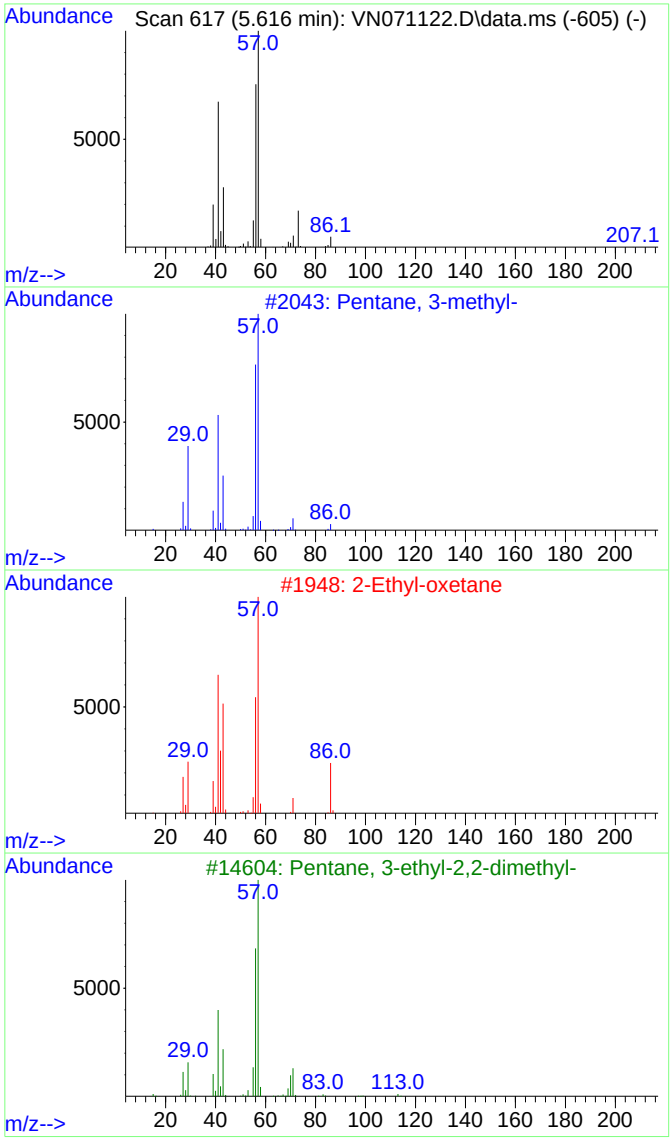
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

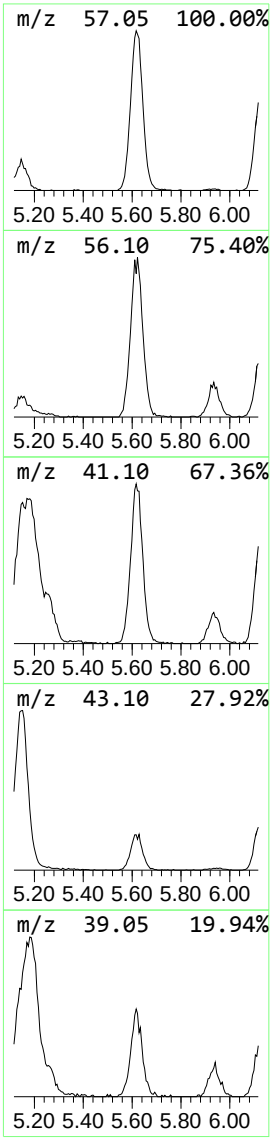
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	7.73 ug/l	631535	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	64
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
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Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 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
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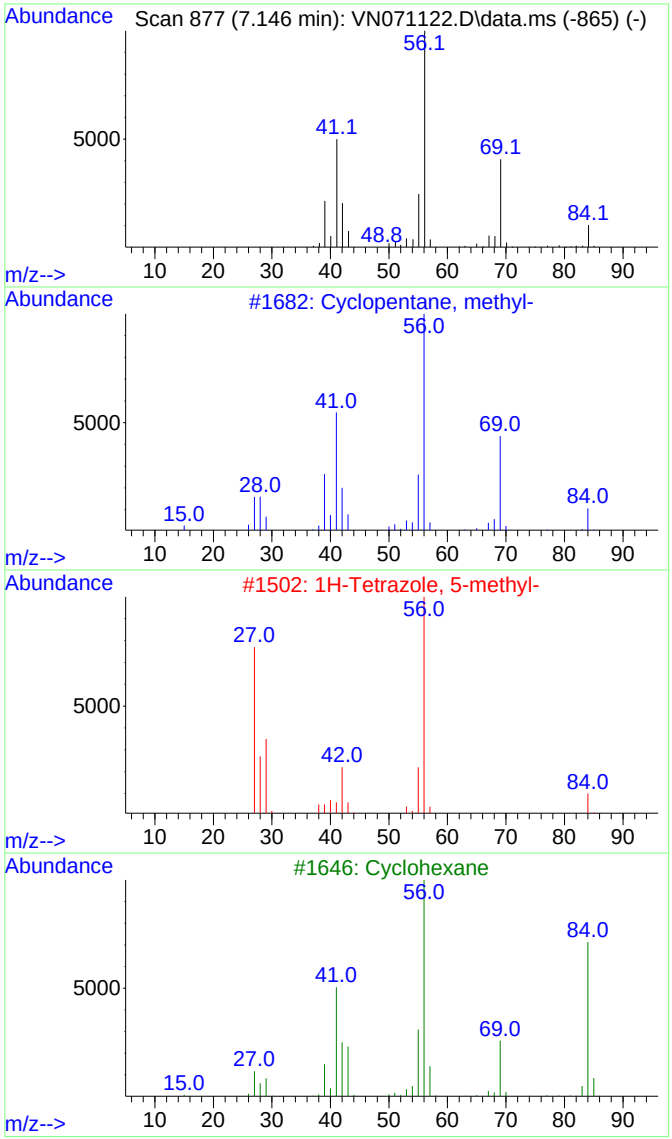
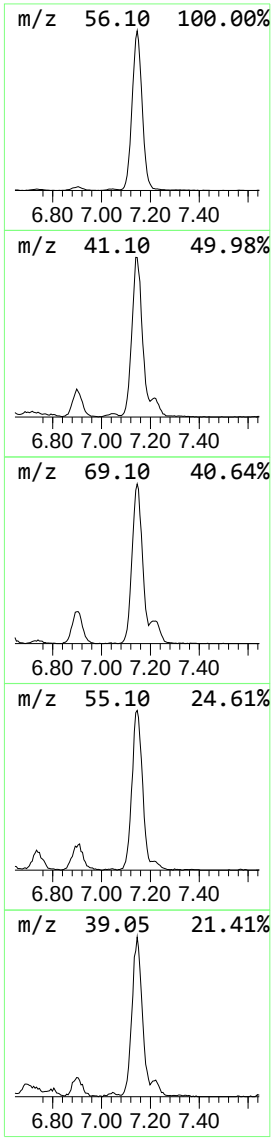
****

Peak Number 4 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.146	26.13 ug/l	2134630	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
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Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

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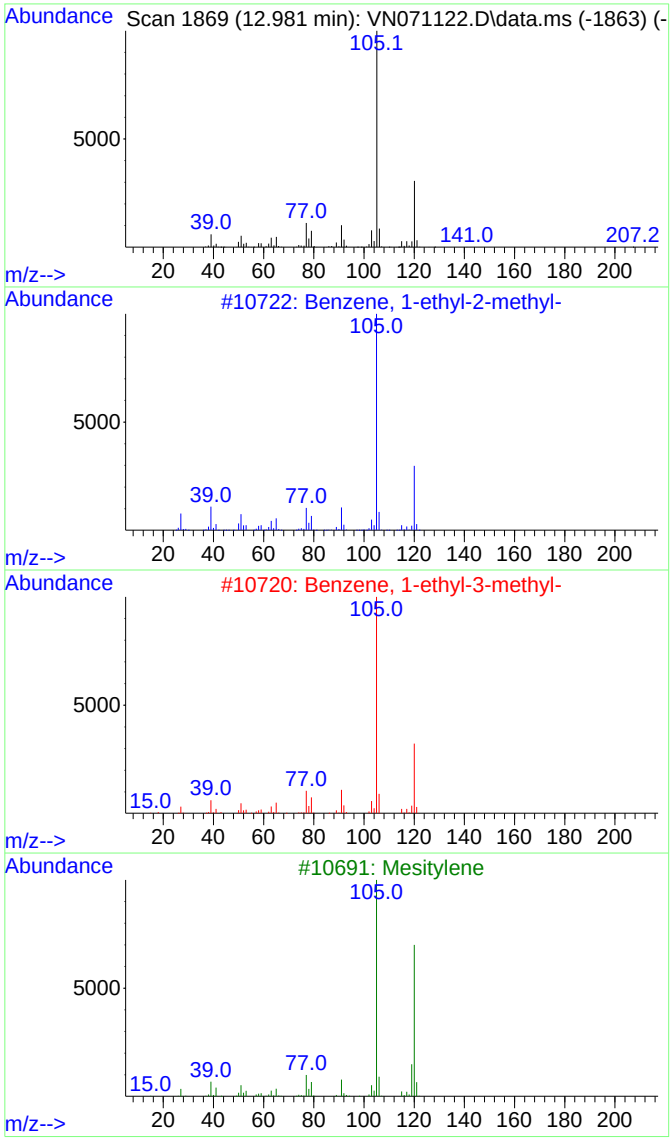
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

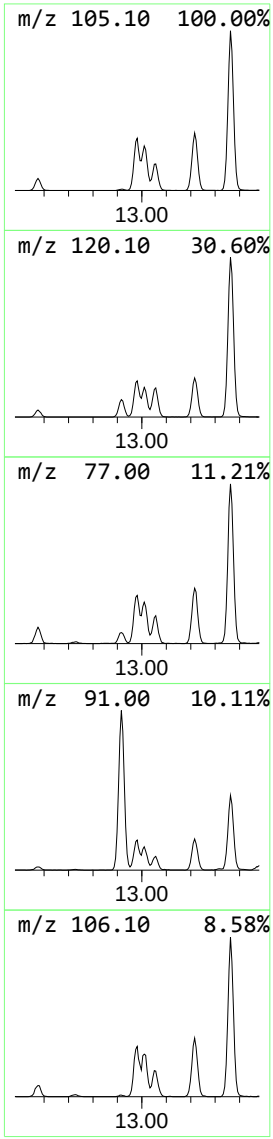
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.981	33.37 ug/l	2100870	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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

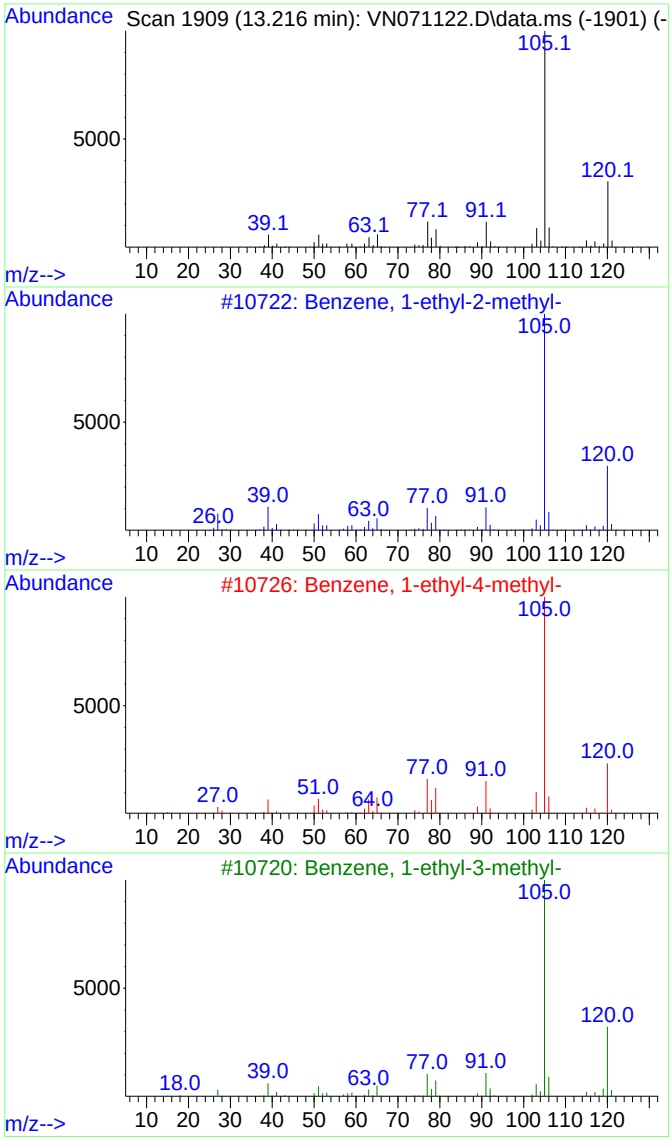
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

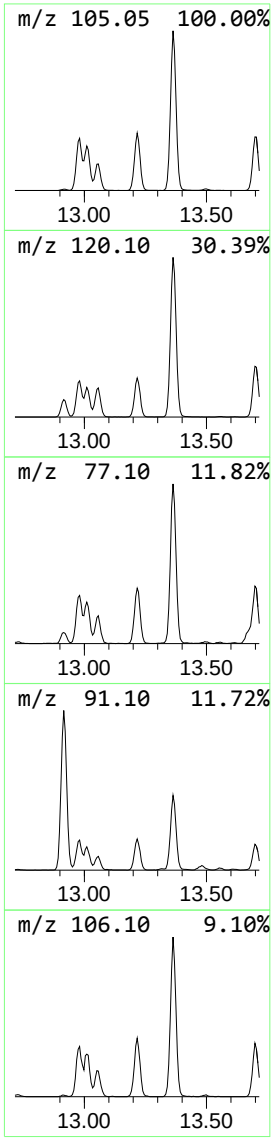
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	33.78 ug/l	2126530	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-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

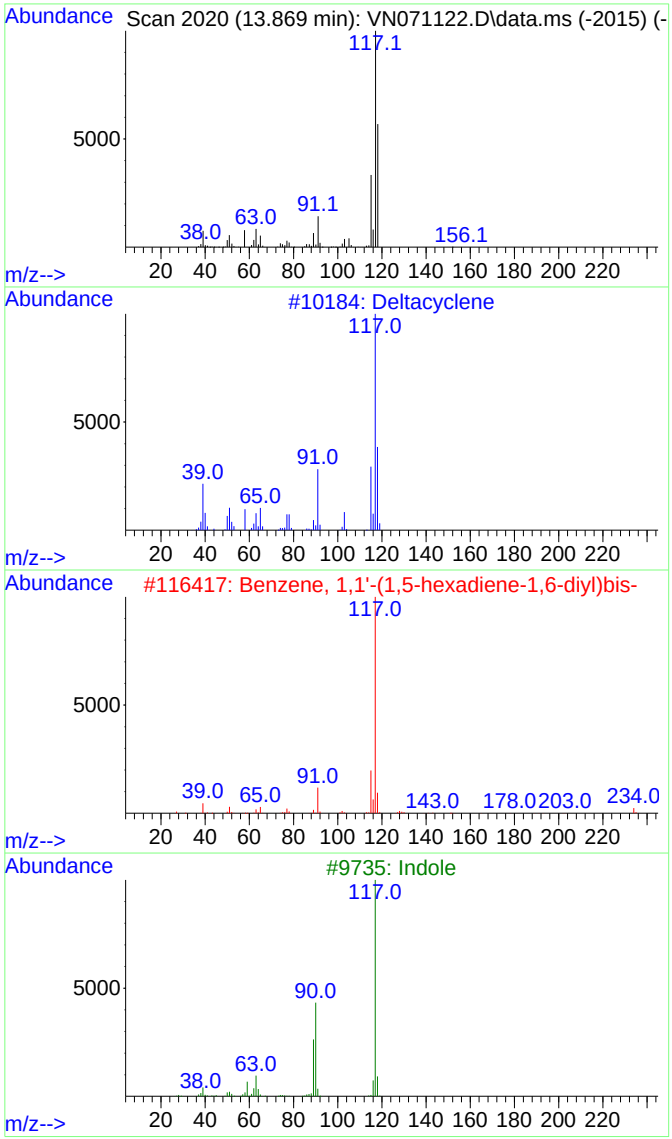
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

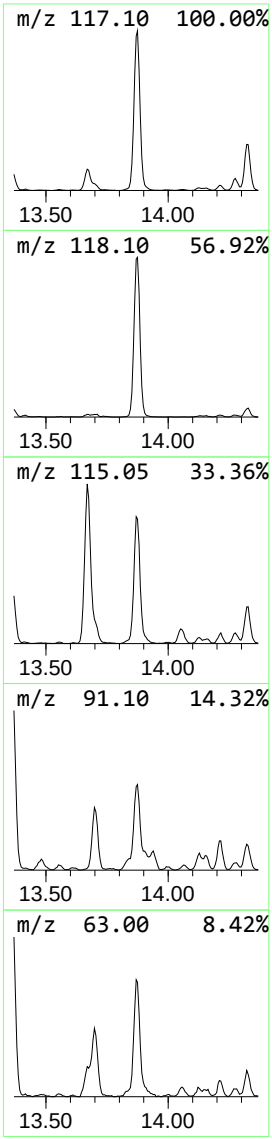
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	45.20 ug/l	2845610	1,4-Dichlorobenzene-d4	13.669

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	43
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	42





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Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

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

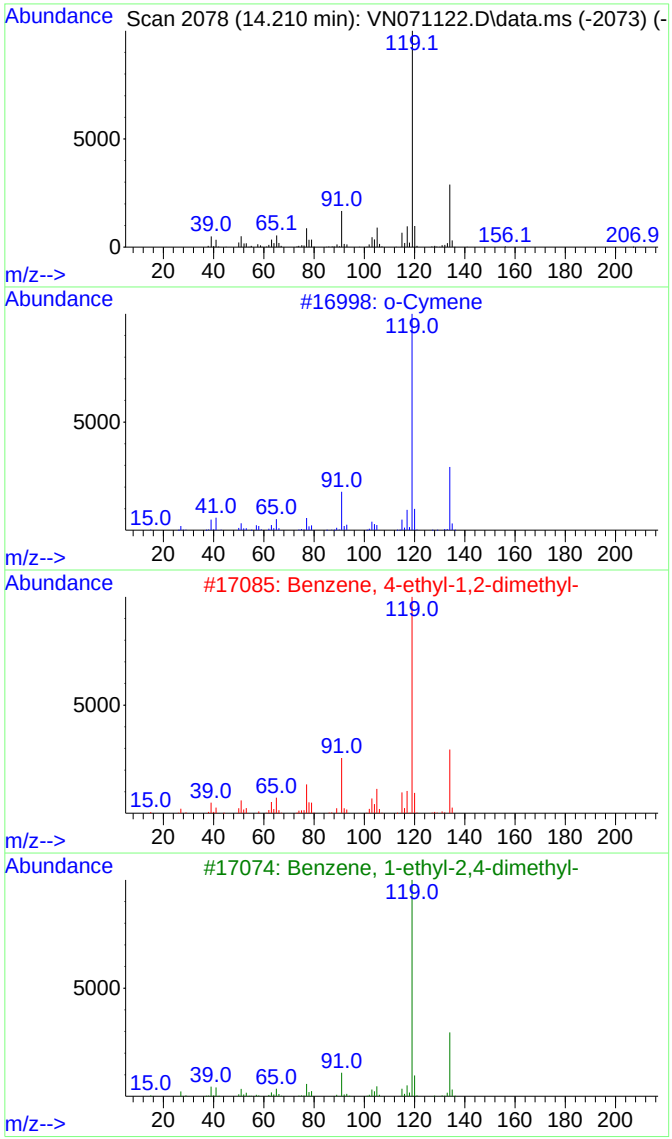
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

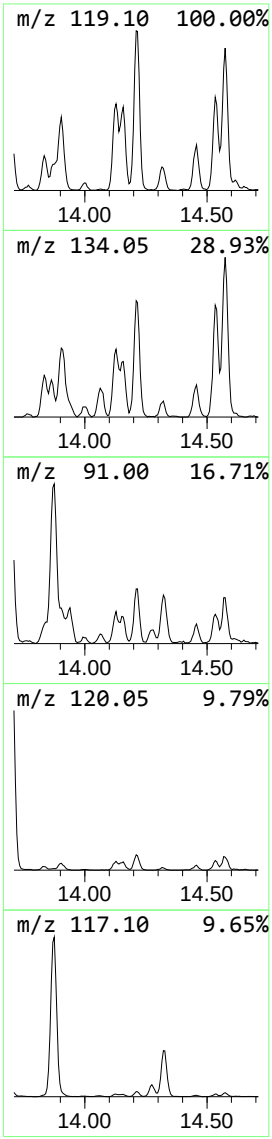
****

Peak Number 8 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	9.33 ug/l	587538	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

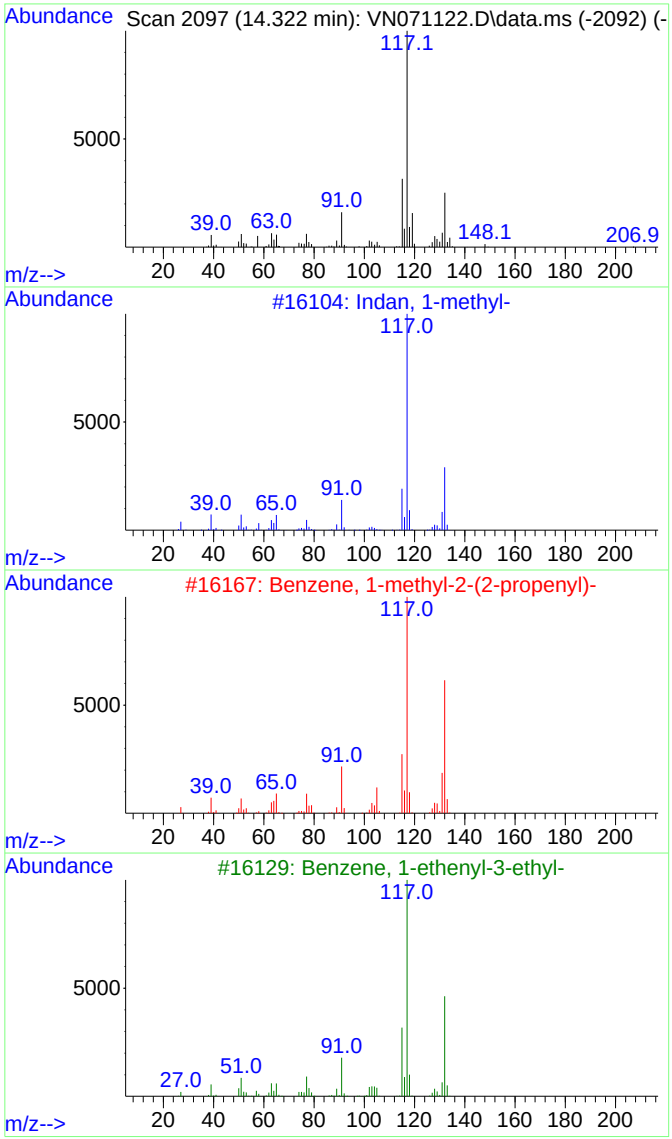
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

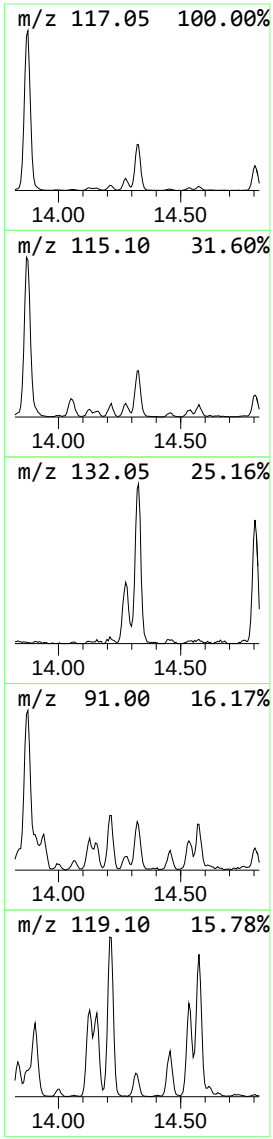
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	10.56 ug/l	664845	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP022522

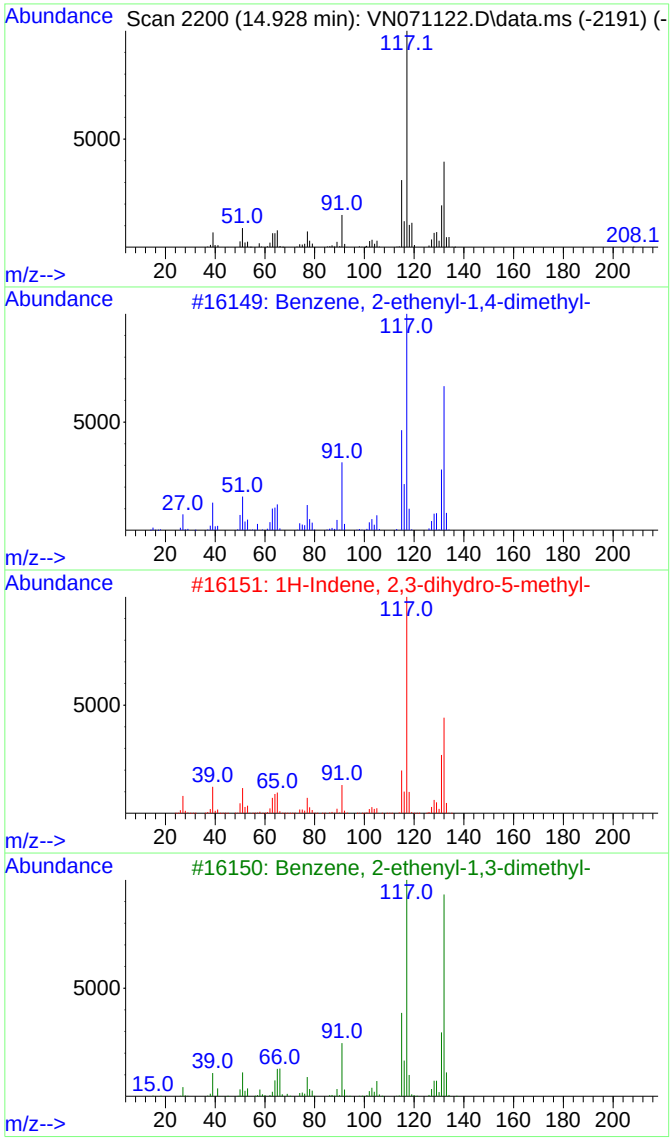
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

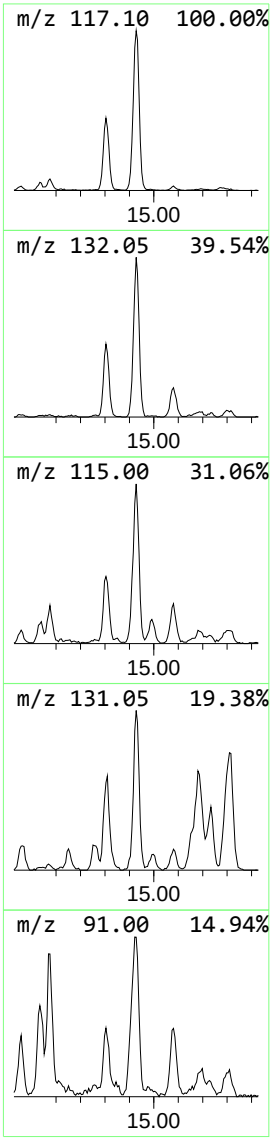
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.928	17.15 ug/l	1079620	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	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	93
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030122\
Data File : VN071122.D
Acq On : 01 Mar 2022 16:36
Operator : JC\MD
Sample : N1689-11 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	3.128	18.4	ug/l	1498830	1	8.081	4084410	50.0
Pentane	3.511	11.7	ug/l	954012	1	8.081	4084410	50.0
Pentane, 3-methyl-	5.616	7.7	ug/l	631535	1	8.081	4084410	50.0
Cyclopentane, m...	7.146	26.1	ug/l	2134630	1	8.081	4084410	50.0
Benzene, 1-ethy...	12.981	33.4	ug/l	2100870	4	13.669	3147900	50.0
Benzene, 1-ethy...	13.216	33.8	ug/l	2126530	4	13.669	3147900	50.0
Benzene, 1,1'-(...	13.869	45.2	ug/l	2845610	4	13.669	3147900	50.0
o-Cymene	14.210	9.3	ug/l	587538	4	13.669	3147900	50.0
Indan, 1-methyl-	14.322	10.6	ug/l	664845	4	13.669	3147900	50.0
Benzene, 2-ethe...	14.928	17.1	ug/l	1079620	4	13.669	3147900	50.0