LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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\82N072822W.M
Title : SW846 8260

Signal : TIC: VN073737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.081	195	203	216	rVB	260513	611720	3.99%	0.534%
2	4.993	515	528	535	rBV3	45833	173972	1.14%	0.152%
3	5.098	535	546	568	rVB5	83039	437737	2.86%	0.382%
4	5.534	607	620	634	rBV4	51088	181104	1.18%	0.158%
5	7.069	869	881	889	rBV	276751	808848	5.28%	0.706%
6	7.769	991	1000	1012	rVB2	125907	319152	2.08%	0.278%
7	7.951	1020	1031	1036	rBV	274673	673514	4.40%	0.588%
8	8.022	1036	1043	1052	rVV2	772724	1921263	12.54%	1.676%
9	8.375	1094	1103	1114	rBV2	286037	705220	4.60%	0.615%
10	8.516	1116	1127	1133	rBV4	111571	340099	2.22%	0.297%
11	8.904	1183	1193	1205	rBV	731943	1620100	10.57%	1.413%
12	9.392	1260	1276	1286	rBV2	324507	896862	5.85%	0.782%
13	9.739	1328	1335	1337	rBV2	83733	154084	1.01%	0.134%
14	9.910	1357	1364	1369	rBV	264481	532391	3.47%	0.464%
15	9.951	1369	1371	1384	rVB2	94522	179240	1.17%	0.156%
16	10.263	1416	1424	1431	rBV	267494	510065	3.33%	0.445%
17	10.380	1436	1444	1451	rBV	1052643	1911082	12.47%	1.667%
18	10.798	1507	1515	1525	rVB3	119843	265868	1.74%	0.232%
19	11.686	1658	1666	1673	rBV	1015940	1794994	11.71%	1.566%
20	11.780	1678	1682	1692	rVB5	61743	155956	1.02%	0.136%
21	12.521	1802	1808	1815	rVB	289106	456126	2.98%	0.398%
22	12.674	1826	1834	1841	rBV	870495	1462155	9.54%	1.276%
23	12.863	1859	1866	1875	rVB	575700	918597	6.00%	0.801%
24	13.163	1909	1917	1925	rBV	503438	823157	5.37%	0.718%
25	13.439	1955	1964	1970	rBV2	135963	323343	2.11%	0.282%
26	13.616	1986	1994	2005	rBV2	1118309	2114001	13.80%	1.844%
27	13.710	2006	2010	2015	rVB	110151	171449	1.12%	0.150%
28	13.780	2015	2022	2024	rBV	1643302	2719602	17.75%	2.373%
29	13.816	2024	2028	2034	rVV	9526865	15322559	100.00%	13.368%
30	13.857	2034	2035	2044	rVV2	478294	692031	4.52%	0.604%
31	13.945	2044	2050	2056	rVV	460806	726627	4.74%	0.634%
32	14.068	2066	2071	2079	rBV	123445	220875	1.44%	0.193%
33	14.157	2079	2086	2091	rBV	2959275	4463779	29.13%	3.894%
34	14.216	2091	2096	2100	rVV	869259	1471777	9.61%	1.284%
35	14.268	2100	2105	2112	rVV2	4034422	6535594	42.65%	5.702%
36	14.404	2122	2128	2132	rBV	144831	229921	1.50%	0.201%

LSC Area Percent Report

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Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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\82N072822W.M
Title : SW846 8260

37	14.480	2132	2141	2150	rVB	3314734	5125505	33.45%	4.472%
38	14.563	2150	2155	2158	rBV	163677	253547	1.65%	0.221%
39	14.698	2170	2178	2181	rBV2	184132	346917	2.26%	0.303%
40	14.745	2181	2186	2192	rVV	2698316	4484645	29.27%	3.913%
41	14.792	2192	2194	2198	rVV	155105	193864	1.27%	0.169%
42	14.868	2198	2207	2213	rVV2	6116704	12212757	79.70%	10.655%
43	14.927	2213	2217	2223	rVV3	357044	726820	4.74%	0.634%
44	15.021	2226	2233	2240	rVV	1098616	1967802	12.84%	1.717%
45	15.127	2240	2251	2255	rVV2	1182606	2767031	18.06%	2.414%
46	15.168	2255	2258	2264	rVV	543009	1001373	6.54%	0.874%
47	15.245	2264	2271	2281	rVB3	1171524	2703921	17.65%	2.359%
48	15.433	2291	2303	2310	rBV	4312115	7913006	51.64%	6.904%
49	15.492	2310	2313	2317	rVV	188843	304733	1.99%	0.266%
50	15.545	2317	2322	2326	rVV3	322244	716883	4.68%	0.625%
51	15.598	2328	2331	2346	rVB	374318	763161	4.98%	0.666%
52	15.733	2346	2354	2361	rBV	601124	1192271	7.78%	1.040%
53	15.904	2373	2383	2399	rBV4	483468	1667793	10.88%	1.455%
54	16.033	2399	2405	2411	rBV2	253350	539087	3.52%	0.470%
55	16.109	2411	2418	2424	rVB3	334282	778886	5.08%	0.680%
56	16.262	2435	2444	2461	rBV3	360140	986207	6.44%	0.860%
57	16.462	2468	2478	2482	rBV3	288612	667460	4.36%	0.582%
58	16.527	2482	2489	2505	rVB	2798241	6310043	41.18%	5.505%
59	16.733	2515	2524	2533	rBV	3513926	8151098	53.20%	7.111%

Sum of corrected areas: 114619674

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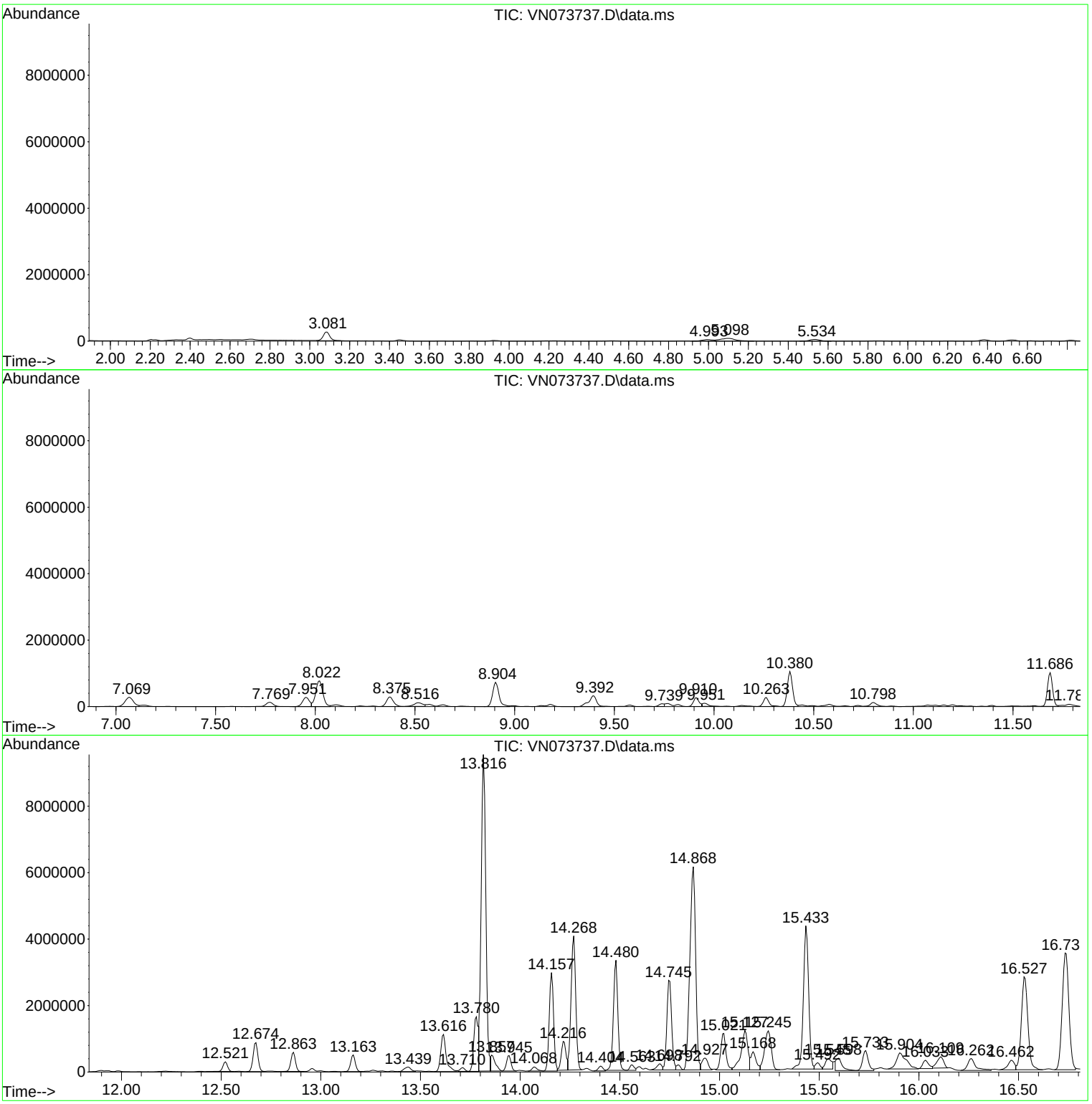
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

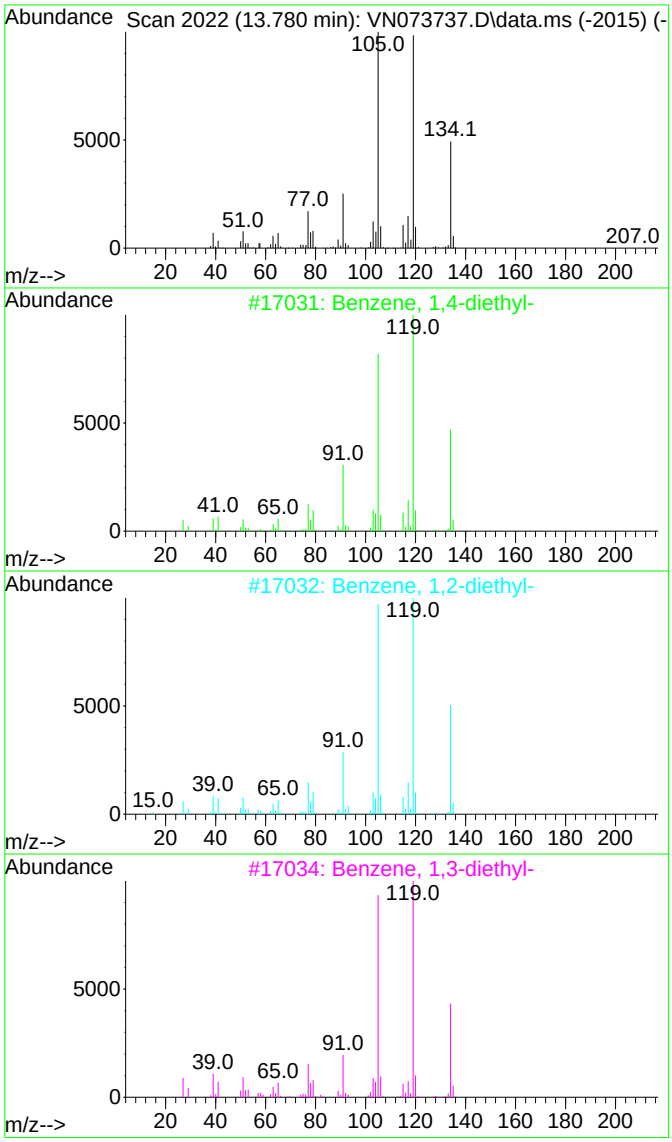
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

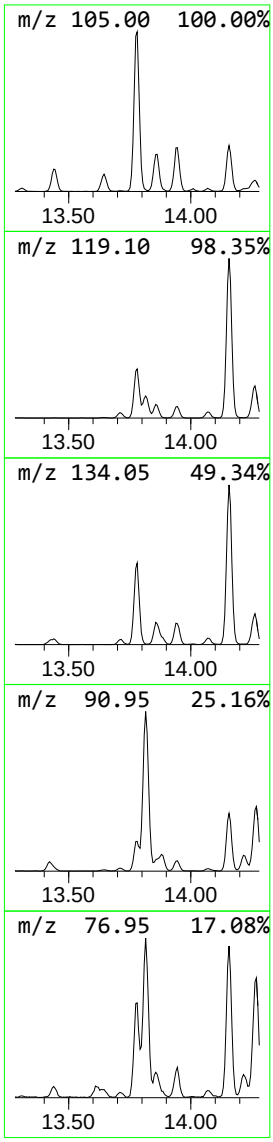
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1,4-diethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	64.32 ug/l	2719600	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

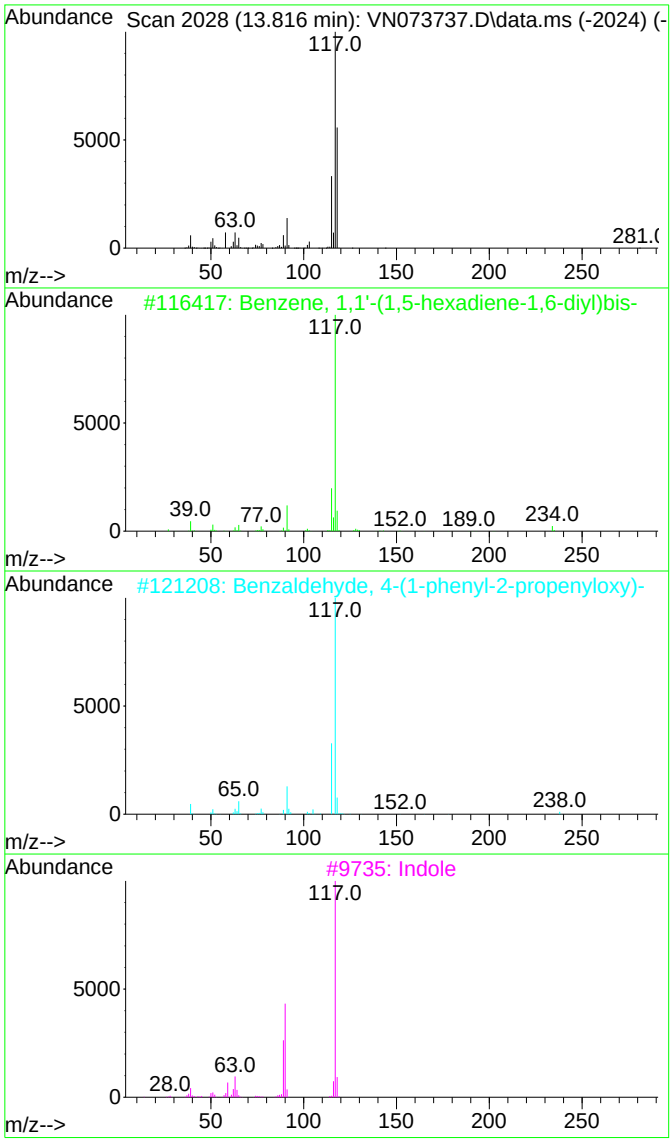
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

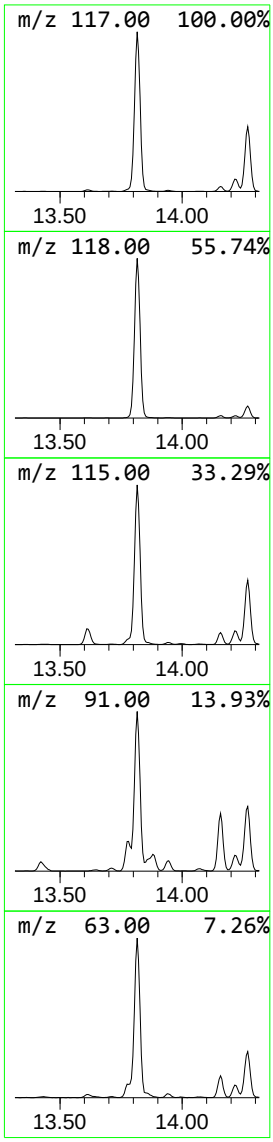
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	362.41 ug/l	15322600	1,4-Dichlorobenzene-d4	13.616

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	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
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	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

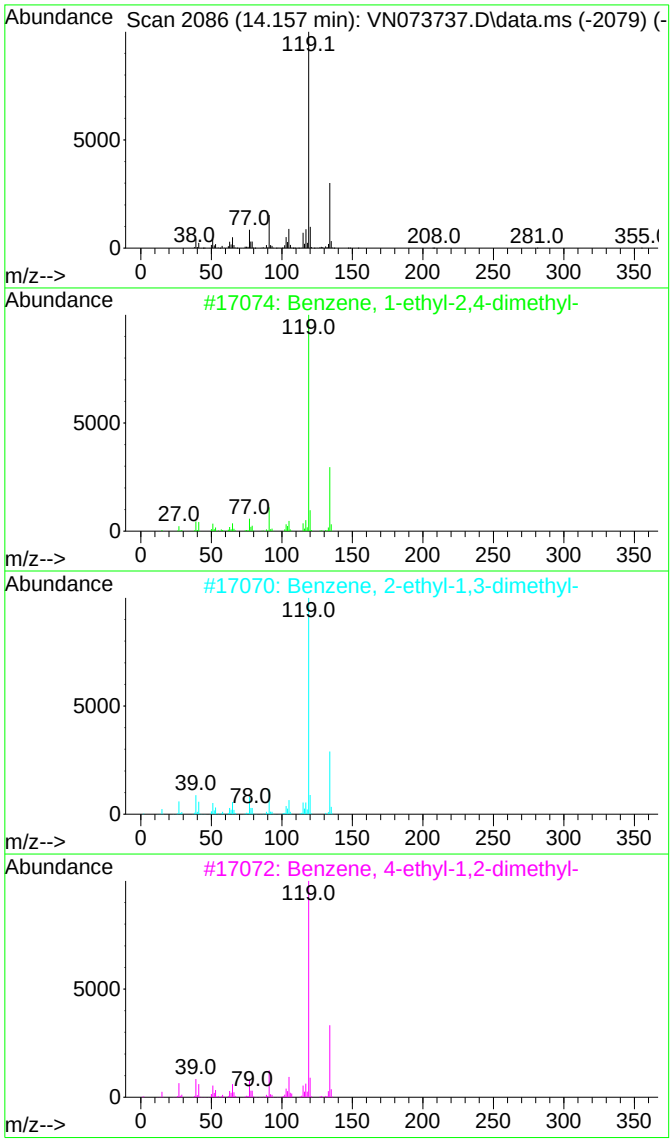
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

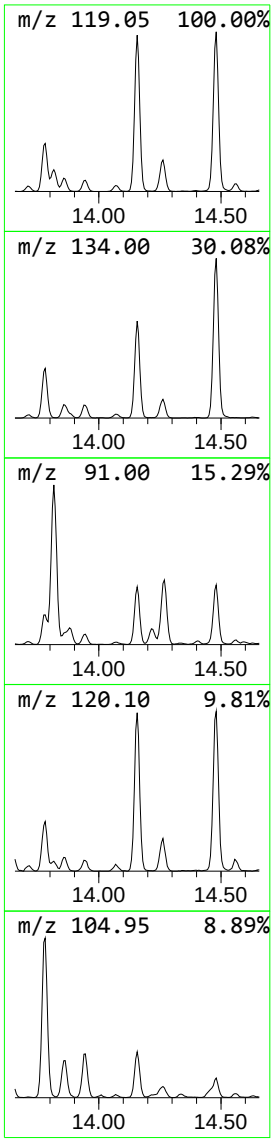
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	105.58 ug/l	4463780	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

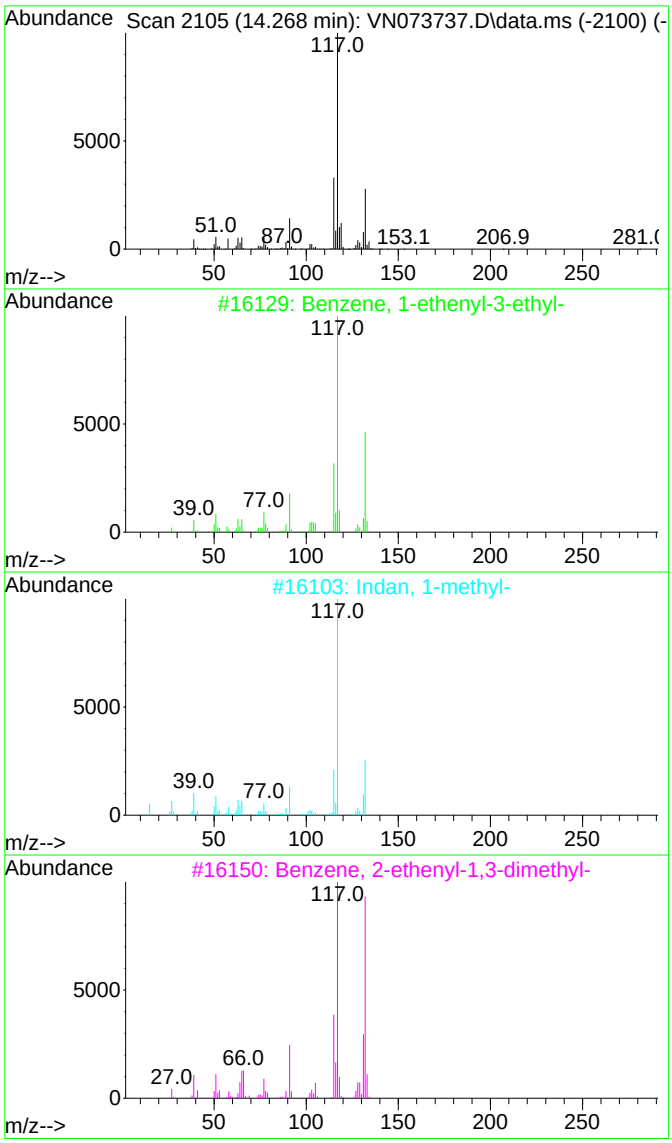
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

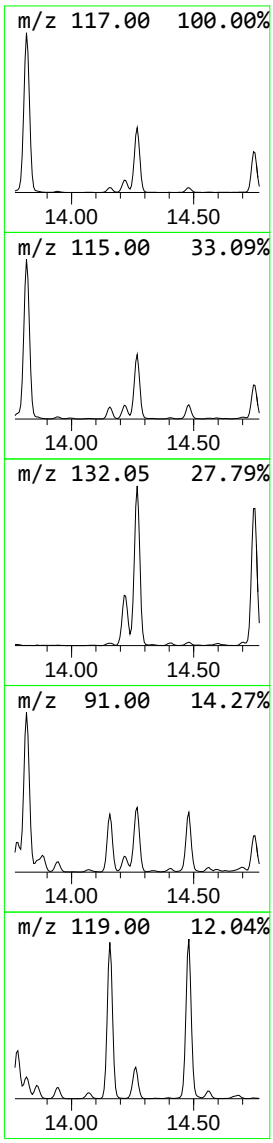
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	154.58 ug/l	6535590	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
2	Indan, 1-methyl-	132	C10H12	000767-58-8	76
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	74
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	74
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

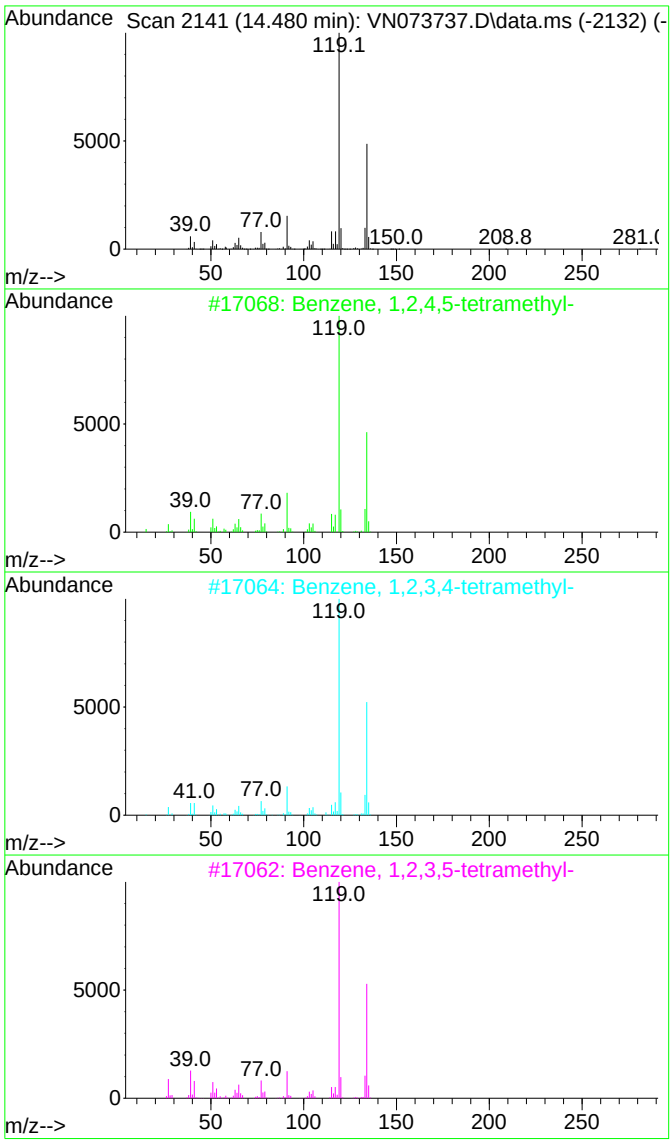
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

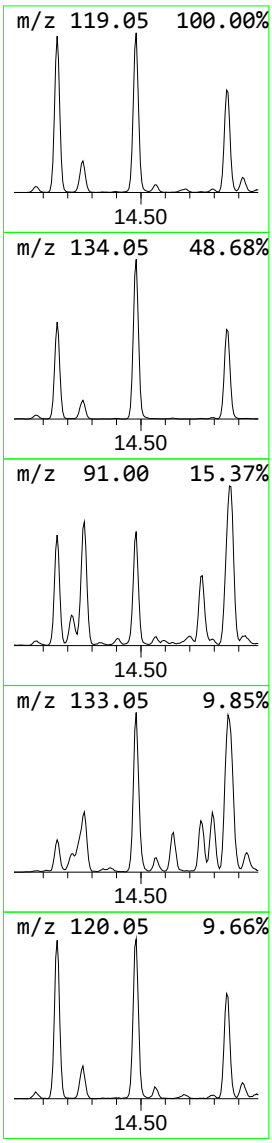
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	121.23 ug/l	5125510	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

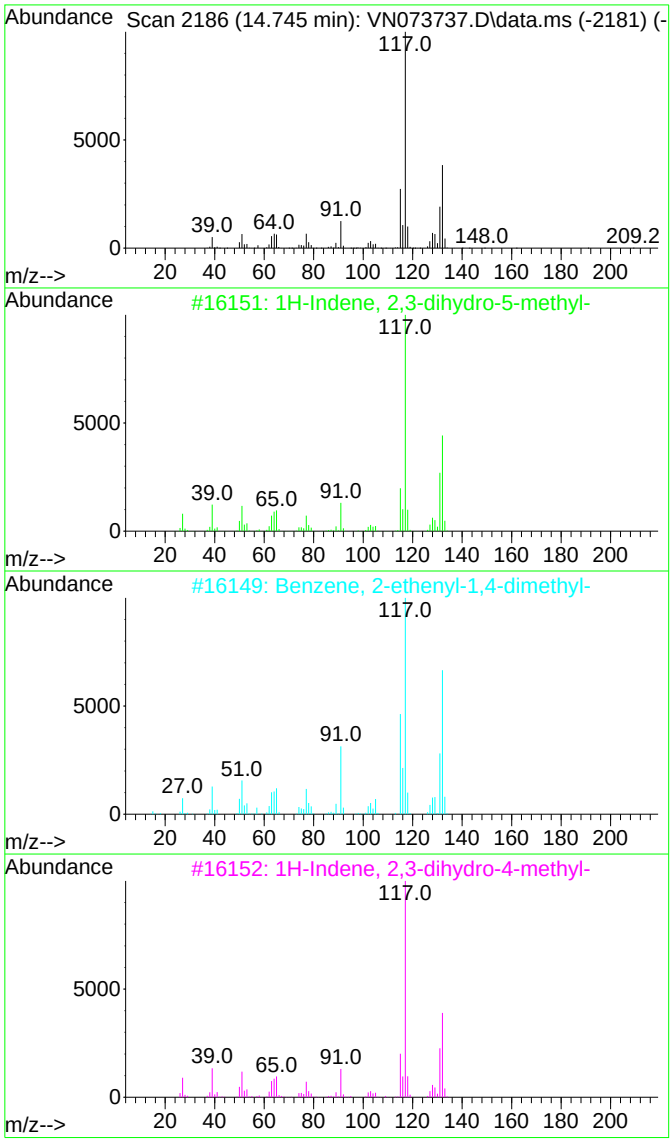
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

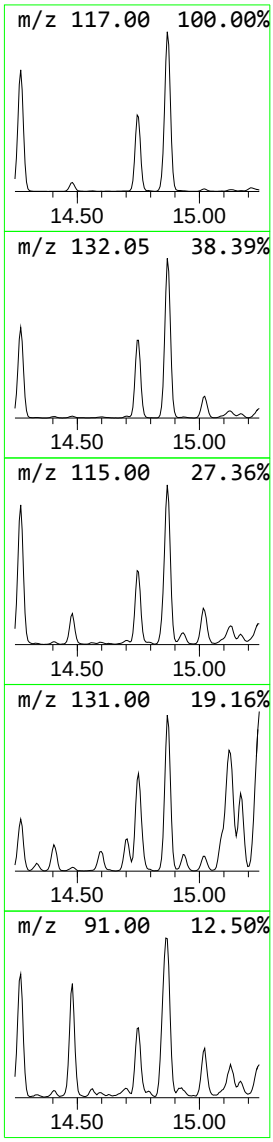
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	106.07 ug/l	4484650	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

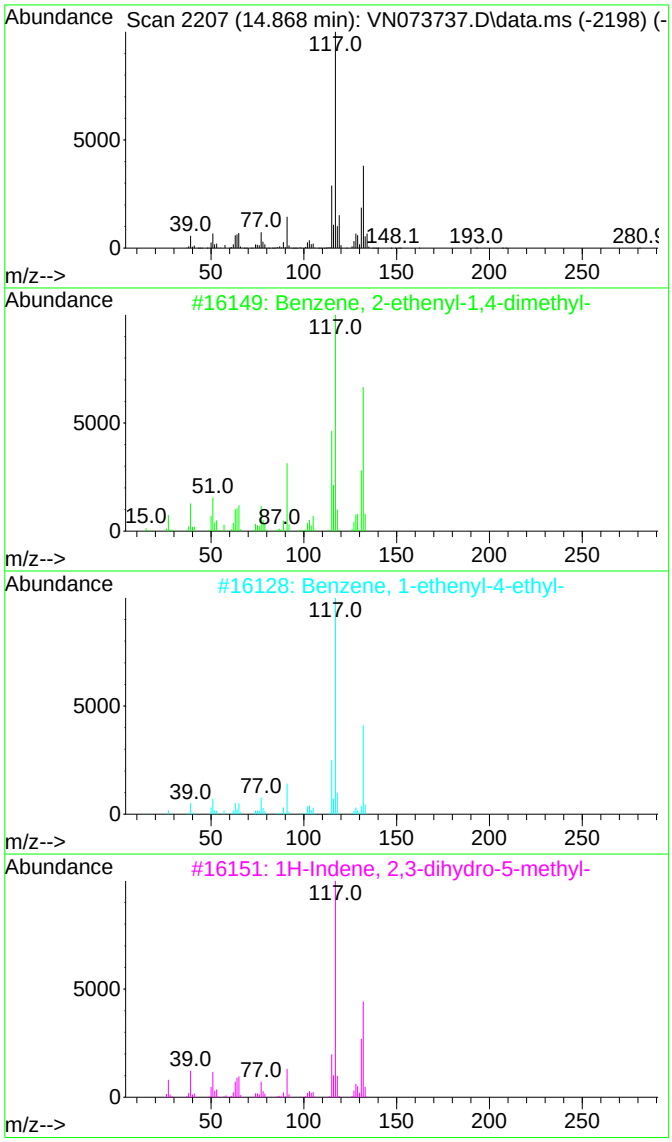
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

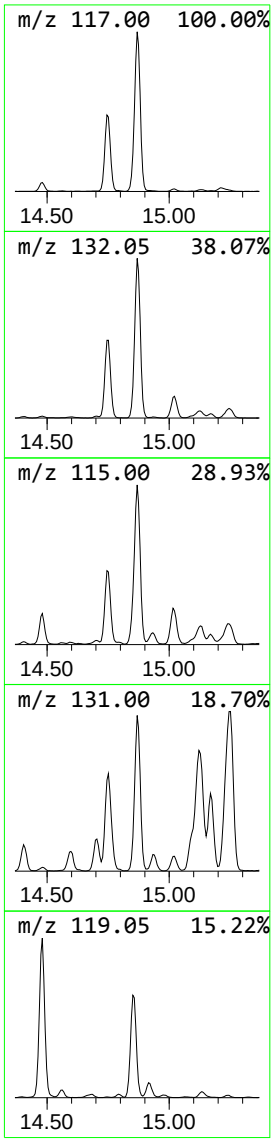
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	288.85 ug/l	12212800	1,4-Dichlorobenzene-d4	13.616

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-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

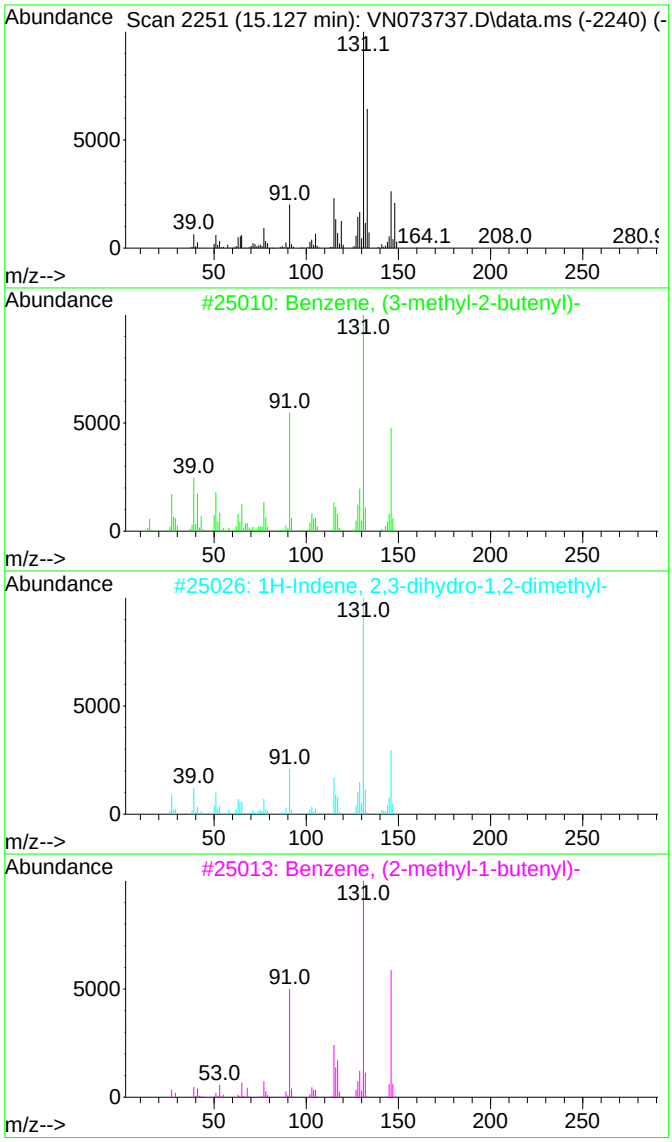
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

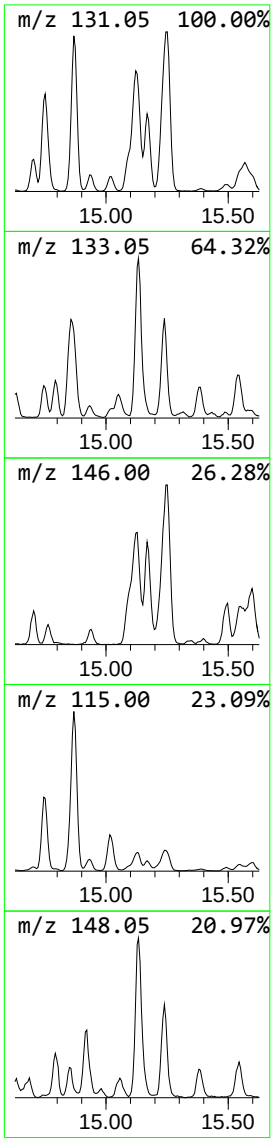
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	65.45 ug/l	2767030	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	91
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91
3	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	86
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	83
5	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

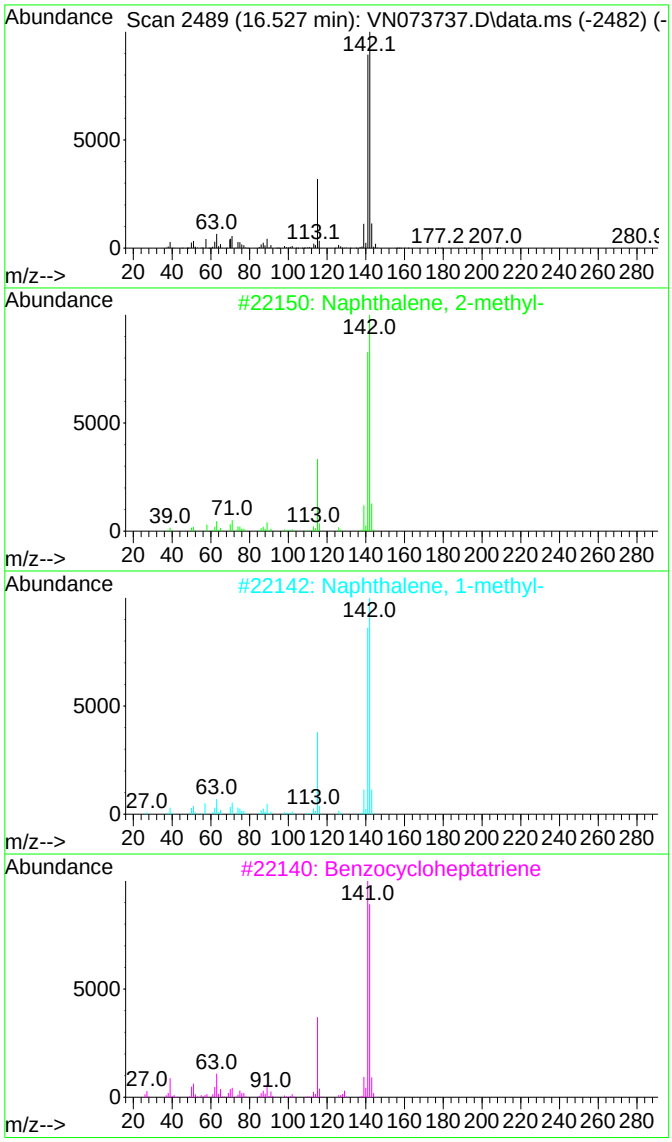
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

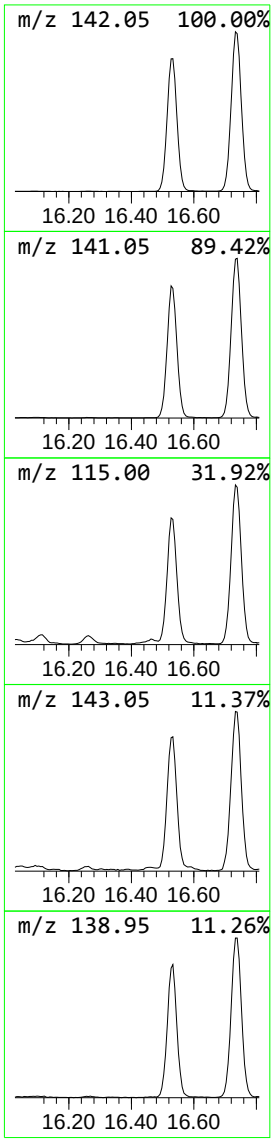
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	149.24 ug/l	6310040	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

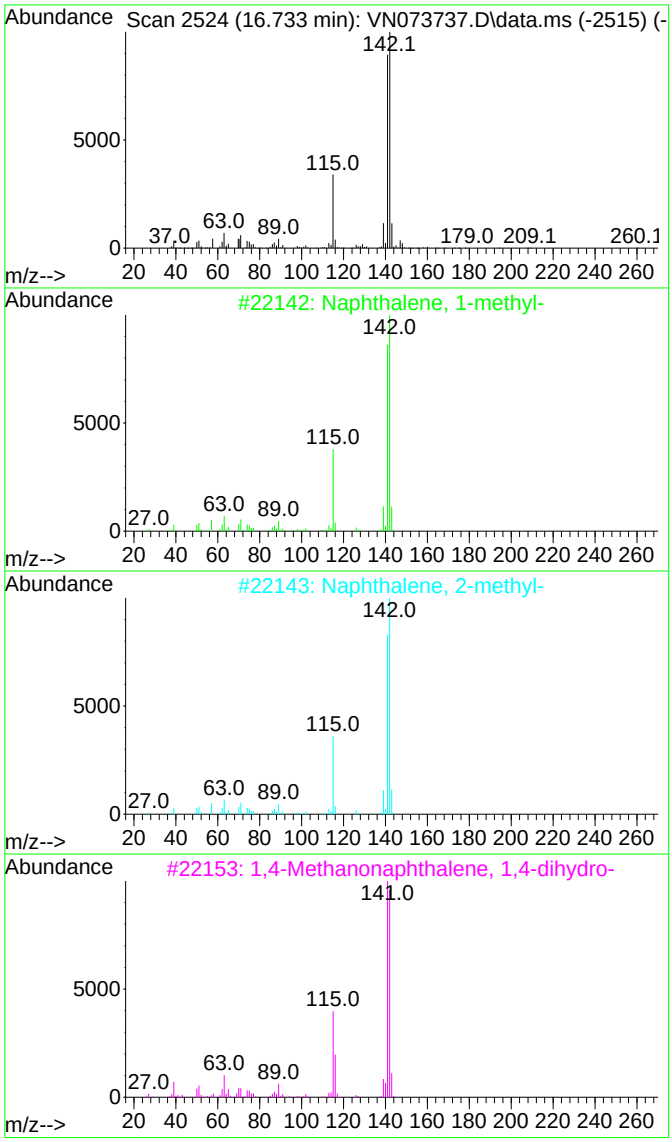
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

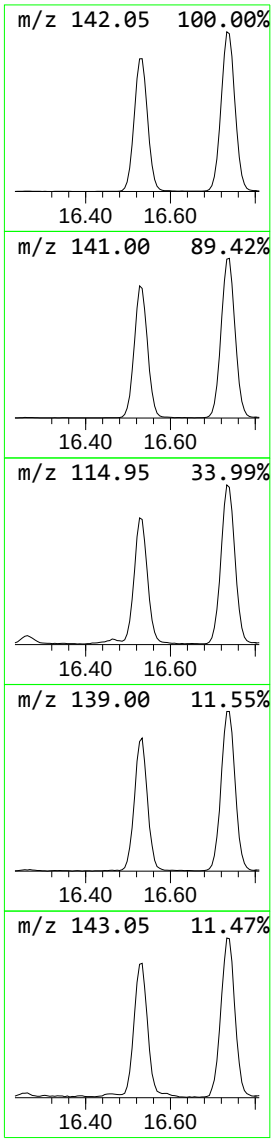
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	192.79 ug/l	8151100	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073737.D
Acq On : 04 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Benzene, 1,4-di...	13.780	64.3	ug/l	2719600	4	13.616	2114000	50.0
Benzene, 1,1'-(...	13.816	362.4	ug/l	15322600	4	13.616	2114000	50.0
Benzene, 1-ethy...	14.157	105.6	ug/l	4463780	4	13.616	2114000	50.0
Benzene, 1-ethe...	14.268	154.6	ug/l	6535590	4	13.616	2114000	50.0
Benzene, 1,2,4,...	14.480	121.2	ug/l	5125510	4	13.616	2114000	50.0
1H-Indene, 2,3-...	14.745	106.1	ug/l	4484650	4	13.616	2114000	50.0
Benzene, 2-ethe...	14.868	288.9	ug/l	12212800	4	13.616	2114000	50.0
Benzene, (3-met...	15.127	65.5	ug/l	2767030	4	13.616	2114000	50.0
Naphthalene, 1-...	16.527	149.2	ug/l	6310040	4	13.616	2114000	50.0
1,4-Methanonaph...	16.733	192.8	ug/l	8151100	4	13.616	2114000	50.0