LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073135.D
Acq On : 26 Jun 2022 03:19
Operator : JC\MD
Sample : N3494-21
Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

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\82N061722W.M
Title : SW846 8260

Signal : TIC: VN073135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.769	479	490	512	rBV	366610	1146943	1.10%	0.542%
2	8.375	1093	1103	1113	rBV3	731339	1910366	1.83%	0.902%
3	8.898	1183	1192	1201	rBV	604964	1282104	1.23%	0.606%
4	10.375	1437	1443	1458	rVB2	1127417	2441525	2.33%	1.153%
5	11.280	1591	1597	1603	rBV	1058101	1893124	1.81%	0.894%
6	11.710	1660	1670	1678	rBV	9403411	17864075	17.08%	8.437%
7	11.921	1702	1706	1711	rBV	600808	1132243	1.08%	0.535%
8	12.192	1744	1752	1758	rBV3	999577	2345974	2.24%	1.108%
9	12.304	1764	1771	1776	rVB	968461	1619408	1.55%	0.765%
10	12.392	1776	1786	1787	rBV5	772587	1586255	1.52%	0.749%
11	12.421	1788	1791	1797	rVB2	907125	1758629	1.68%	0.831%
12	12.669	1828	1833	1840	rBV2	1041253	1833921	1.75%	0.866%
13	12.833	1857	1861	1868	rVB3	1001185	1783054	1.70%	0.842%
14	12.992	1881	1888	1894	rBV7	842561	2270141	2.17%	1.072%
15	13.221	1923	1927	1934	rVB	1203170	1845585	1.76%	0.872%
16	13.504	1967	1975	1979	rBV6	1007205	2423644	2.32%	1.145%
17	13.610	1989	1993	2003	rVB2	1181690	2516215	2.41%	1.188%
18	13.933	2042	2048	2053	rBV3	1701867	3063217	2.93%	1.447%
19	14.151	2081	2085	2090	rVB	2529052	3690713	3.53%	1.743%
20	14.263	2098	2104	2109	rVB4	973556	1970481	1.88%	0.931%
21	14.445	2130	2135	2137	rBV2	1344592	2147207	2.05%	1.014%
22	14.474	2137	2140	2144	rVB	1661981	2341392	2.24%	1.106%
23	14.557	2150	2154	2158	rBV2	840268	1109613	1.06%	0.524%
24	14.604	2158	2162	2169	rBV3	694075	1747347	1.67%	0.825%
25	14.792	2190	2194	2198	rBV2	803389	1089420	1.04%	0.515%
26	14.851	2198	2204	2210	rVV3	3550553	7381906	7.06%	3.487%
27	14.915	2210	2215	2221	rVB3	1830651	3425284	3.27%	1.618%
28	15.015	2228	2232	2237	rBV	863621	1436835	1.37%	0.679%
29	15.133	2247	2252	2256	rBV2	1837161	3221733	3.08%	1.522%
30	15.239	2265	2270	2276	rVB5	1789601	3686135	3.52%	1.741%
31	15.321	2281	2284	2291	rVB6	780664	1683381	1.61%	0.795%
32	15.439	2291	2304	2315	rBV2	44074525	104609652	100.00%	49.408%
33	15.733	2347	2354	2361	rBV7	723339	2237593	2.14%	1.057%
34	15.809	2363	2367	2371	rVB4	651348	1131116	1.08%	0.534%
35	15.939	2386	2389	2394	rVB2	789272	1196480	1.14%	0.565%
36	16.251	2435	2442	2452	rBV4	1673830	4451170	4.26%	2.102%

LSC Area Percent Report

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ClientSampleId :
SP-EXC-1-3

Integration Parameters: RTEINT.P
Integrator: RTE
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Title : SW846 8260

37	16.451	2472	2476	2482	rVB2	584173	1188238	1.14%	0.561%
38	16.527	2483	2489	2494	rBV	1677564	3512474	3.36%	1.659%
39	16.733	2516	2524	2533	rBV2	2935375	7752430	7.41%	3.662%

Sum of corrected areas: 211727023

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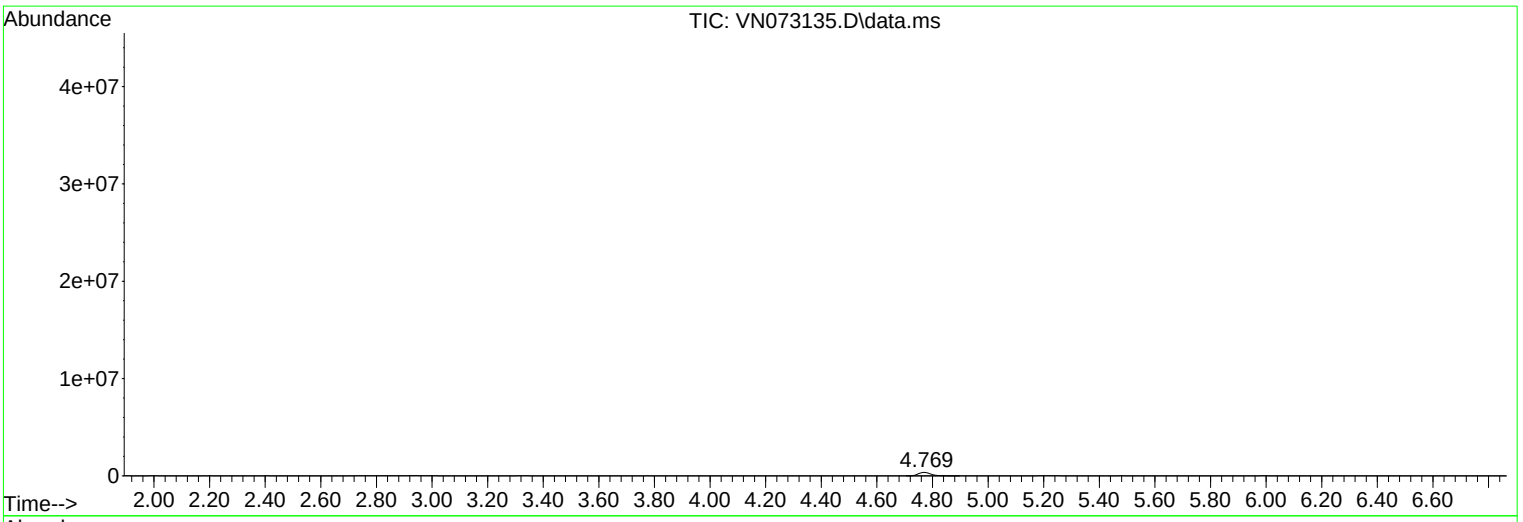
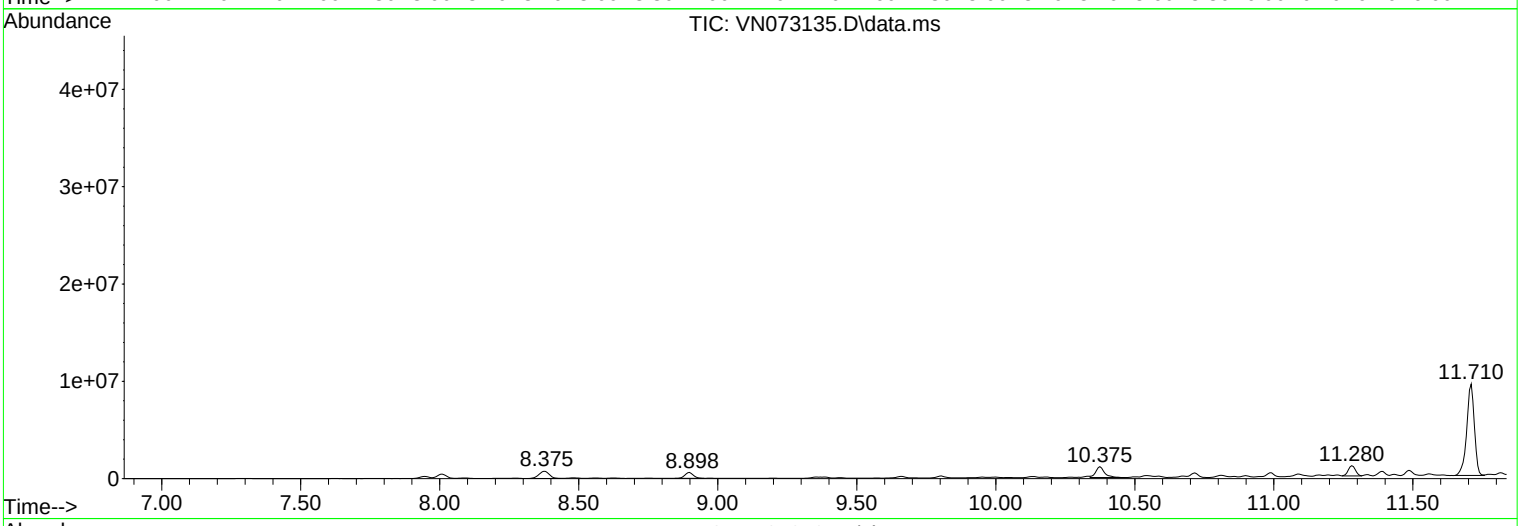
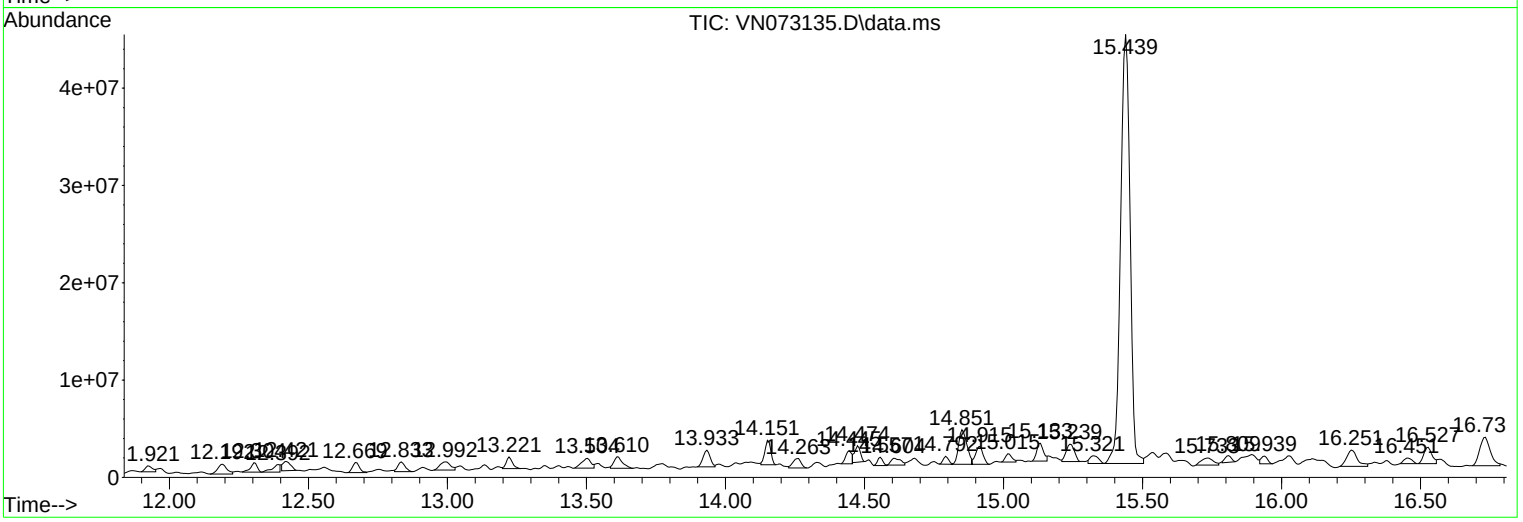
SP-EXC-1-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073135.D
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Operator : JC\MD
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Instrument :
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ClientSampleId :
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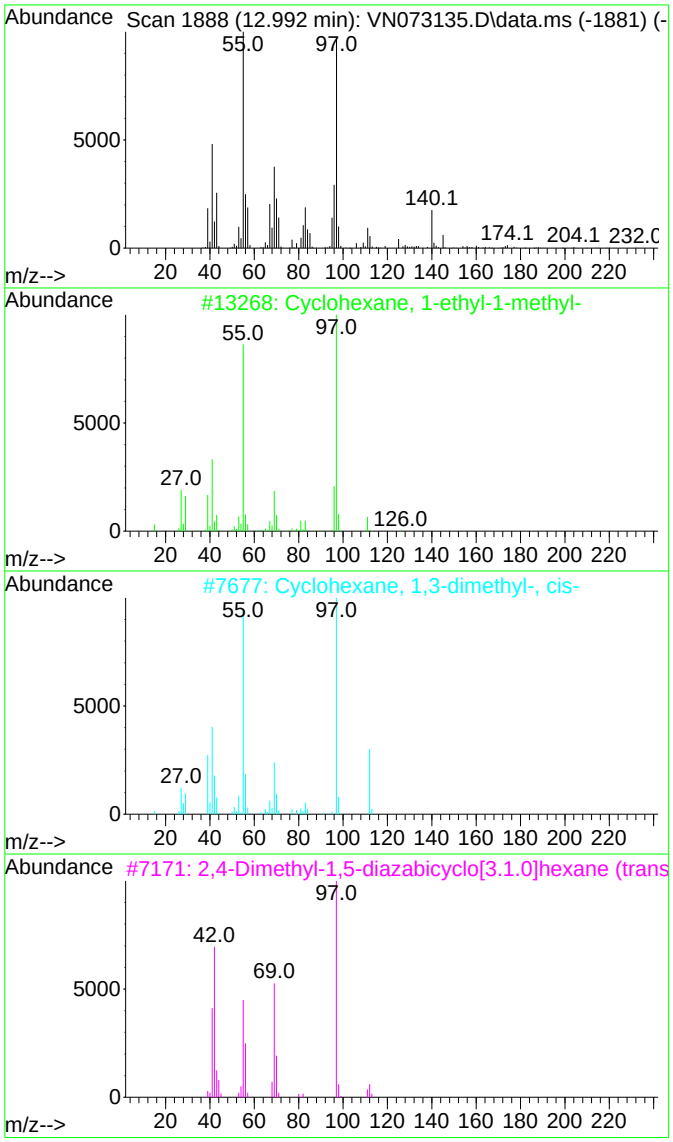
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

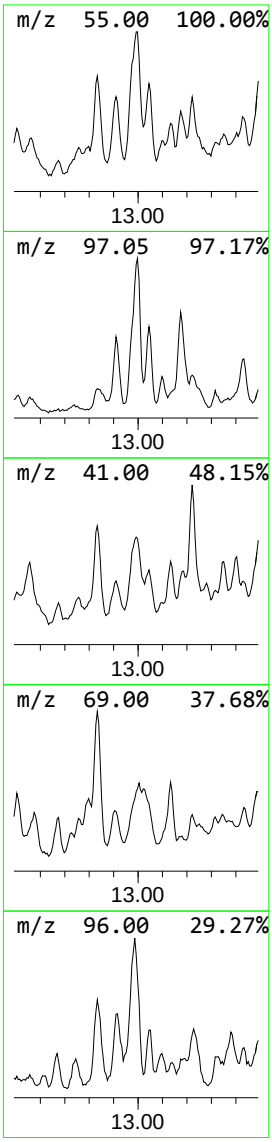
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	45.11 ug/l	2270140	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	53
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	52
3	2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	1000283-20-9	52
4	2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	52
5	Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	006294-39-9	50





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ClientSampleId :
SP-EXC-1-3

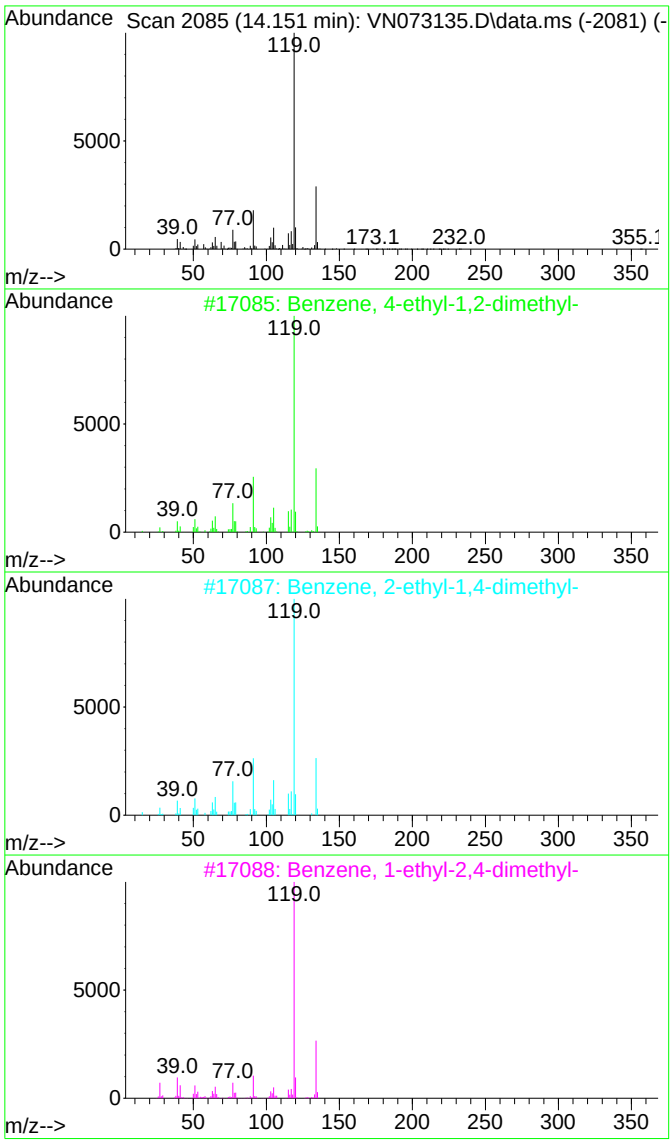
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

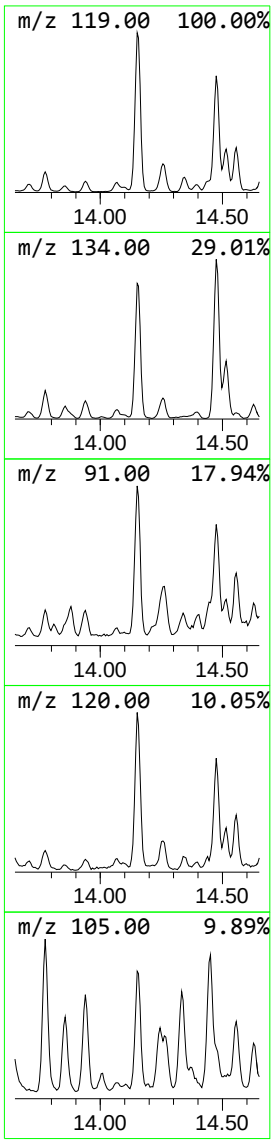
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	73.34 ug/l	3690710	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	97
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	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\VN062522\
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Operator : JC\MD
Sample : N3494-21
Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

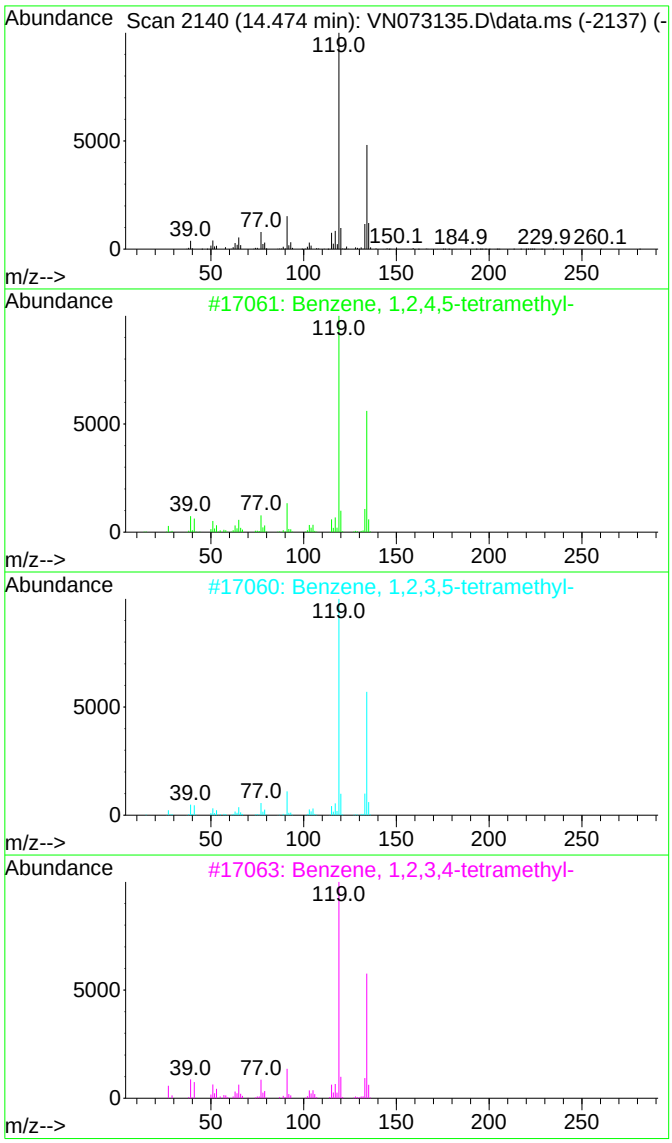
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

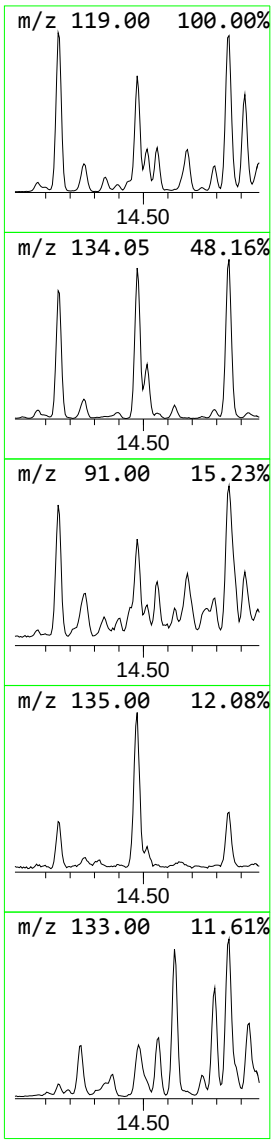
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	46.53 ug/l	2341390	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
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Operator : JC\MD
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Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

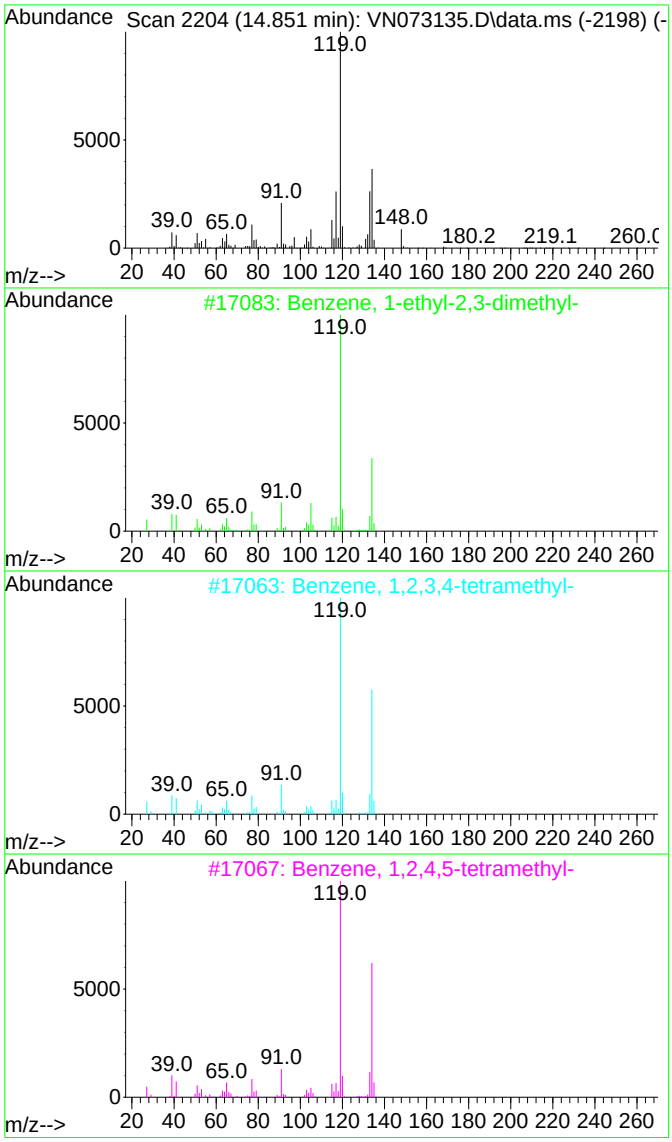
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

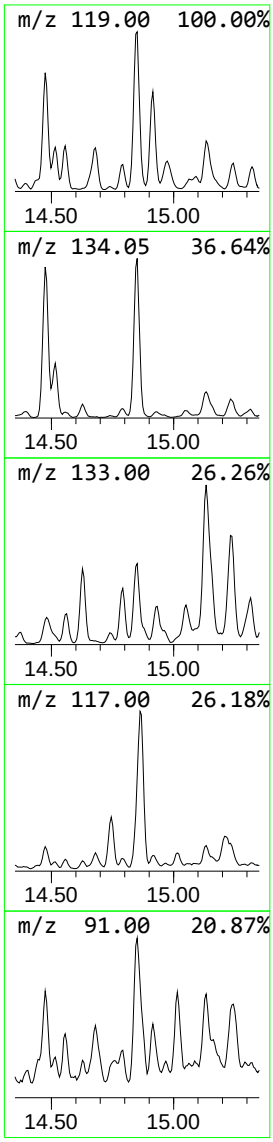
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	146.69 ug/l	7381910	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	76
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	76
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	70





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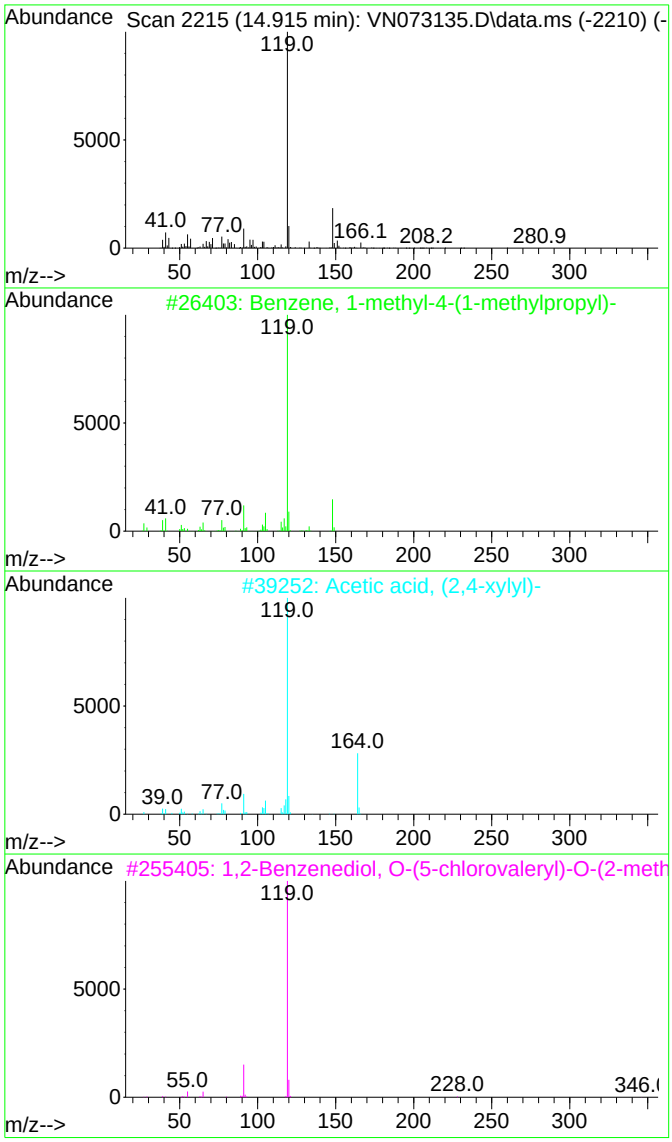
Quant Title : SW846 8260

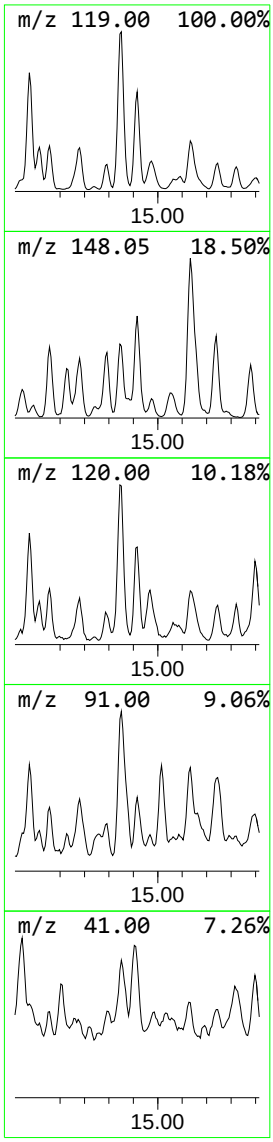
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-methyl-4-(1-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.915	68.06 ug/l	3425280	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	72
2	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	59
3	1,2-Benzenediol, O-(5-chlorovale...	346	C19H19ClO4	1000329-74-2	59
4	o-Toluic acid, 4-nitrophenyl ester	257	C14H11NO4	1000307-46-0	59
5	m-Toluic acid, 4-cyanophenyl ester	237	C15H11NO2	1000307-56-9	59





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ClientSampleId :
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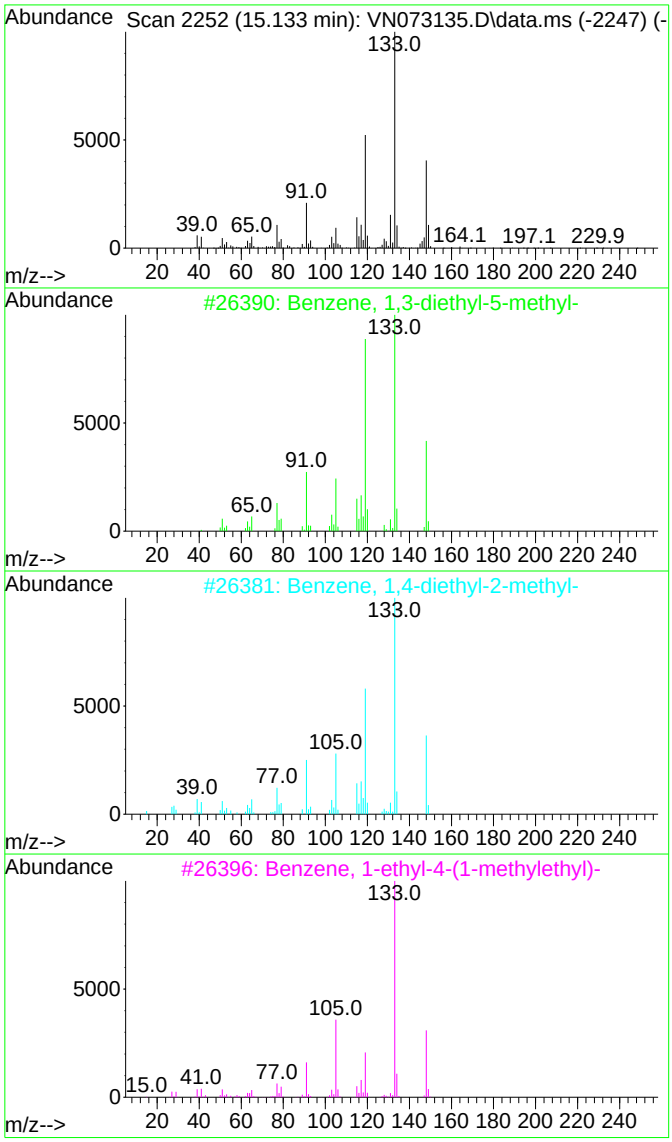
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

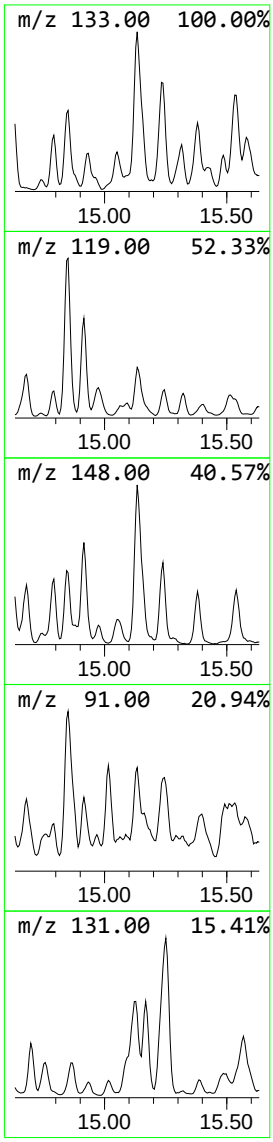
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,3-diethyl-5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	64.02 ug/l	3221730	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	90
2	Benzene, 1,4-diethyl-2-methyl-	148	C11H16	013632-94-5	90
3	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	72
4	Benzene, pentamethyl-	148	C11H16	000700-12-9	70
5	6-Methyl-4-indanol	148	C10H12O	020294-32-0	70





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Operator : JC\MD
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Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

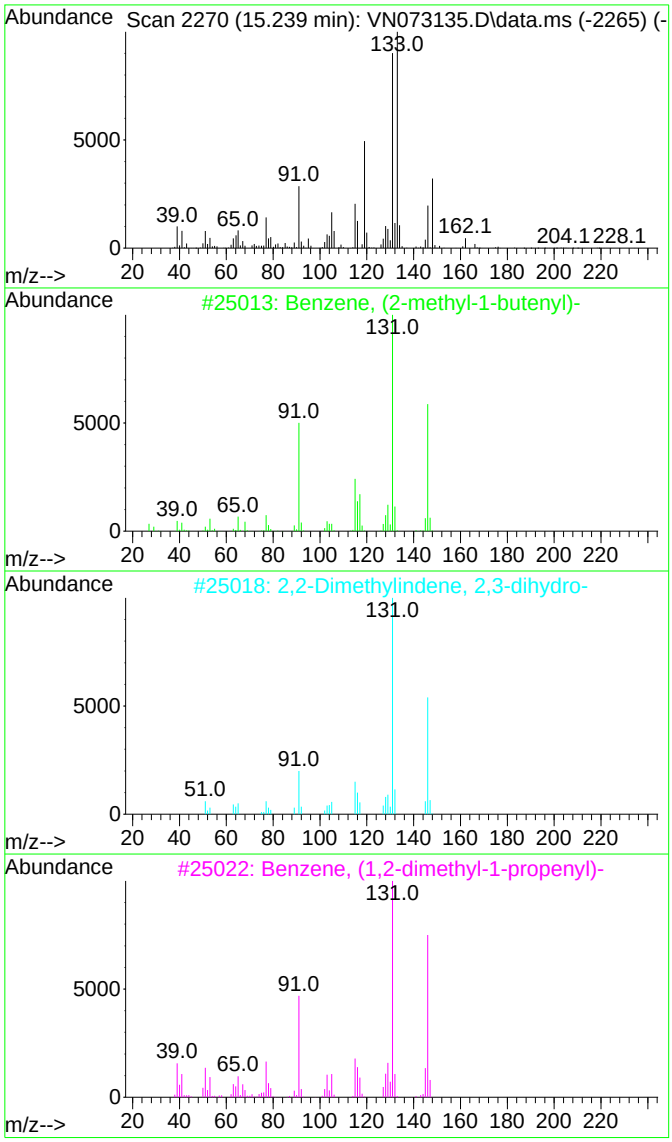
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

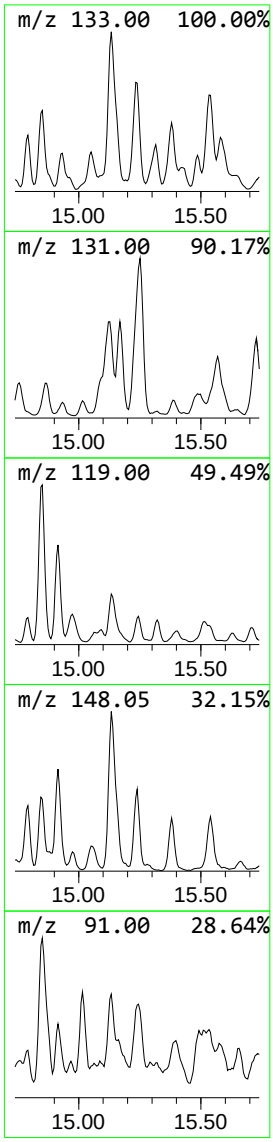
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	73.25 ug/l	3686140	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	86
2	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	64
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	50
4	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	50
5	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	46





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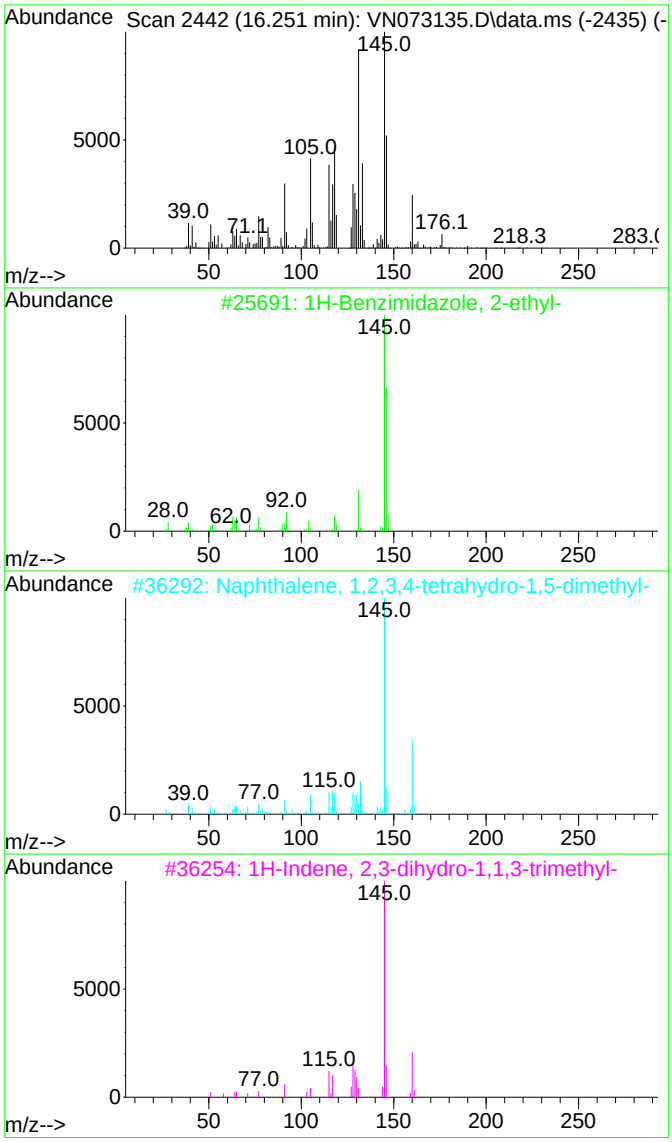
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

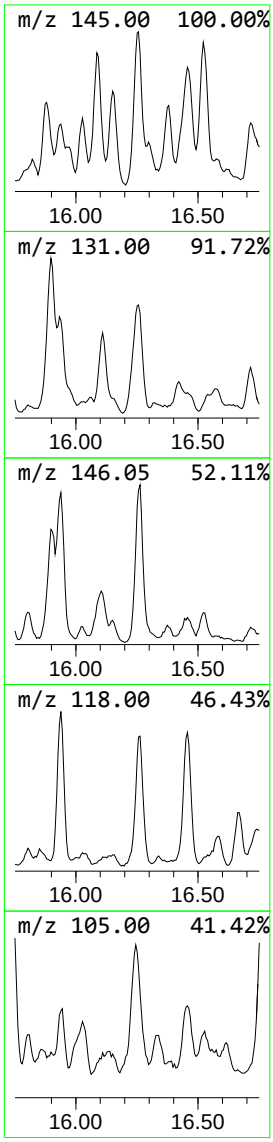
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Benzimidazole, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.251	88.45 ug/l	4451170	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	60
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	55
3	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	50
4	1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	46
5	1H-Indene, 2,3-dihydro-1,4,7-tri...	160	C12H16	054340-87-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073135.D
Acq On : 26 Jun 2022 03:19
Operator : JC\MD
Sample : N3494-21
Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

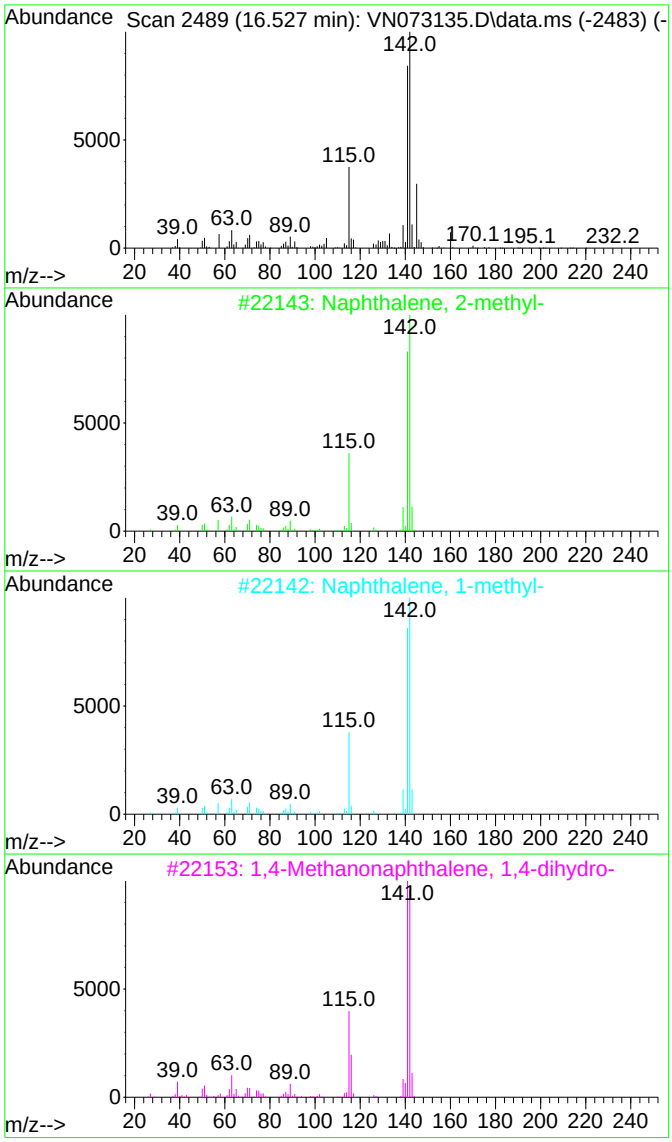
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

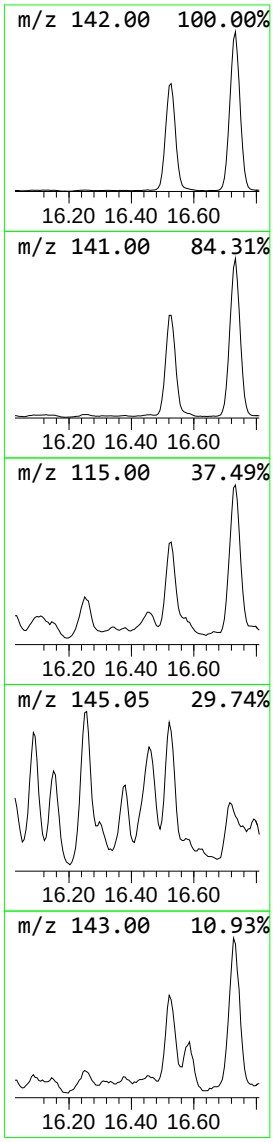
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	69.80 ug/l	3512470	1,4-Dichlorobenzene-d4	13.610

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	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	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073135.D
Acq On : 26 Jun 2022 03:19
Operator : JC\MD
Sample : N3494-21
Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

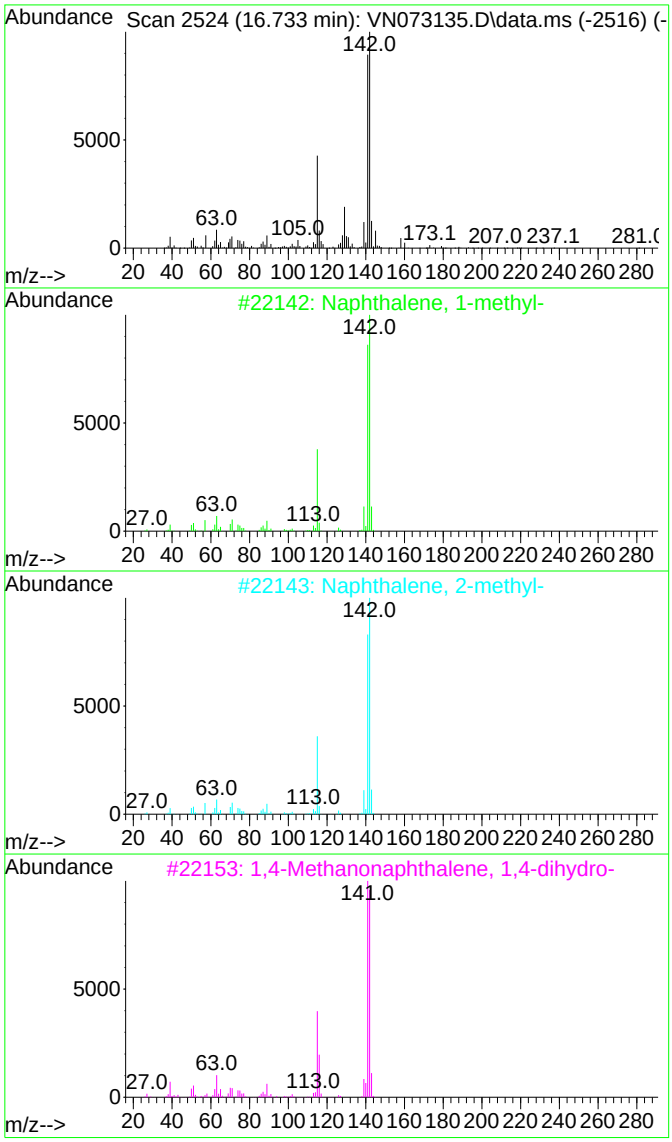
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

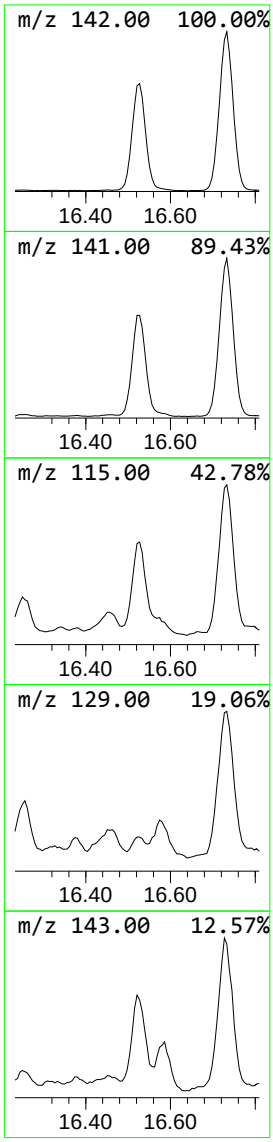
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	154.05 ug/l	7752430	1,4-Dichlorobenzene-d4	13.610

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	95
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	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073135.D
Acq On : 26 Jun 2022 03:19
Operator : JC\MD
Sample : N3494-21
Misc : 3.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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
Cyclohexane, 1-...	12.992	45.1	ug/l	2270140	4	13.610	2516220	50.0
Benzene, 4-ethy...	14.151	73.3	ug/l	3690710	4	13.610	2516220	50.0
Benzene, 1,2,4,...	14.474	46.5	ug/l	2341390	4	13.610	2516220	50.0
Benzene, 1-ethy...	14.851	146.7	ug/l	7381910	4	13.610	2516220	50.0
Benzene, 1-meth...	14.915	68.1	ug/l	3425280	4	13.610	2516220	50.0
Benzene, 1,3-di...	15.133	64.0	ug/l	3221730	4	13.610	2516220	50.0
Benzene, (2-met...	15.239	73.3	ug/l	3686140	4	13.610	2516220	50.0
1H-Benzimidazol...	16.251	88.5	ug/l	4451170	4	13.610	2516220	50.0
Naphthalene, 1-...	16.527	69.8	ug/l	3512470	4	13.610	2516220	50.0
1,4-Methanonaph...	16.733	154.1	ug/l	7752430	4	13.610	2516220	50.0