LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

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\82N112122W.M
Title : SW846 8260

Signal : TIC: VN075376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.106	178	179	191	rVB5	21628	45591	1.25%	0.389%
2	8.165	1030	1039	1043	rBV2	65736	152452	4.16%	1.301%
3	8.224	1043	1049	1062	rVB	195799	449903	12.29%	3.839%
4	8.583	1101	1110	1123	rVB	49890	113731	3.11%	0.970%
5	8.712	1123	1132	1136	rBV4	15687	45554	1.24%	0.389%
6	9.100	1190	1198	1208	rBV	283178	566789	15.48%	4.836%
7	10.565	1439	1447	1452	rBV	159363	299387	8.18%	2.555%
8	10.630	1452	1458	1473	rVV	2049468	3661570	100.00%	31.244%
9	11.865	1660	1668	1672	rBV	366625	678391	18.53%	5.789%
10	11.906	1672	1675	1680	rVV	195423	291810	7.97%	2.490%
11	11.965	1680	1685	1692	rVV	49135	83860	2.29%	0.716%
12	12.071	1695	1703	1714	rVB	189104	361675	9.88%	3.086%
13	12.400	1748	1759	1766	rBV	45631	93436	2.55%	0.797%
14	12.853	1829	1836	1846	rVB	230810	423550	11.57%	3.614%
15	13.035	1861	1867	1872	rBV	52996	85195	2.33%	0.727%
16	13.100	1872	1878	1881	rVV	103635	171489	4.68%	1.463%
17	13.129	1881	1883	1887	rVV	71301	118660	3.24%	1.013%
18	13.171	1887	1890	1897	rVB	93292	159963	4.37%	1.365%
19	13.335	1909	1918	1925	rBV	55420	107549	2.94%	0.918%
20	13.482	1937	1943	1950	rBV	290846	481132	13.14%	4.105%
21	13.794	1989	1996	2015	rVB2	384475	819520	22.38%	6.993%
22	13.953	2018	2023	2024	rBV	33908	41879	1.14%	0.357%
23	13.988	2024	2029	2032	rVV2	108760	217503	5.94%	1.856%
24	14.023	2032	2035	2045	rVV4	102627	251060	6.86%	2.142%
25	14.182	2055	2062	2067	rVB	28732	48280	1.32%	0.412%
26	14.247	2067	2073	2075	rBV	48709	81465	2.22%	0.695%
27	14.276	2075	2078	2082	rVV	53261	77438	2.11%	0.661%
28	14.335	2082	2088	2094	rVV	122703	197703	5.40%	1.687%
29	14.447	2102	2107	2113	rVB3	59238	103990	2.84%	0.887%
30	14.576	2123	2129	2134	rBV2	24299	45159	1.23%	0.385%
31	14.659	2134	2143	2146	rVV	77332	146652	4.01%	1.251%
32	14.694	2146	2149	2153	rVV	77482	115924	3.17%	0.989%
33	14.735	2153	2156	2160	rVV2	46304	64971	1.77%	0.554%
34	14.876	2176	2180	2184	rVB3	30960	43367	1.18%	0.370%
35	14.929	2184	2189	2193	rBV2	89575	176199	4.81%	1.503%
36	15.053	2201	2210	2215	rBV4	109303	293445	8.01%	2.504%

LSC Area Percent Report

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

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\82N112122W.M
Title : SW846 8260

37	15.100	2215	2218	2232	rVB2	40826	83725	2.29%	0.714%
38	15.323	2244	2256	2262	rBV3	58042	164747	4.50%	1.406%
39	15.435	2268	2275	2283	rVB4	38173	94079	2.57%	0.803%
40	15.641	2295	2310	2317	rBV	78207	171771	4.69%	1.466%
41	15.747	2323	2328	2334	rBV5	20544	39863	1.09%	0.340%
42	15.947	2354	2362	2369	rBV4	20707	48832	1.33%	0.417%

Sum of corrected areas: 11719259

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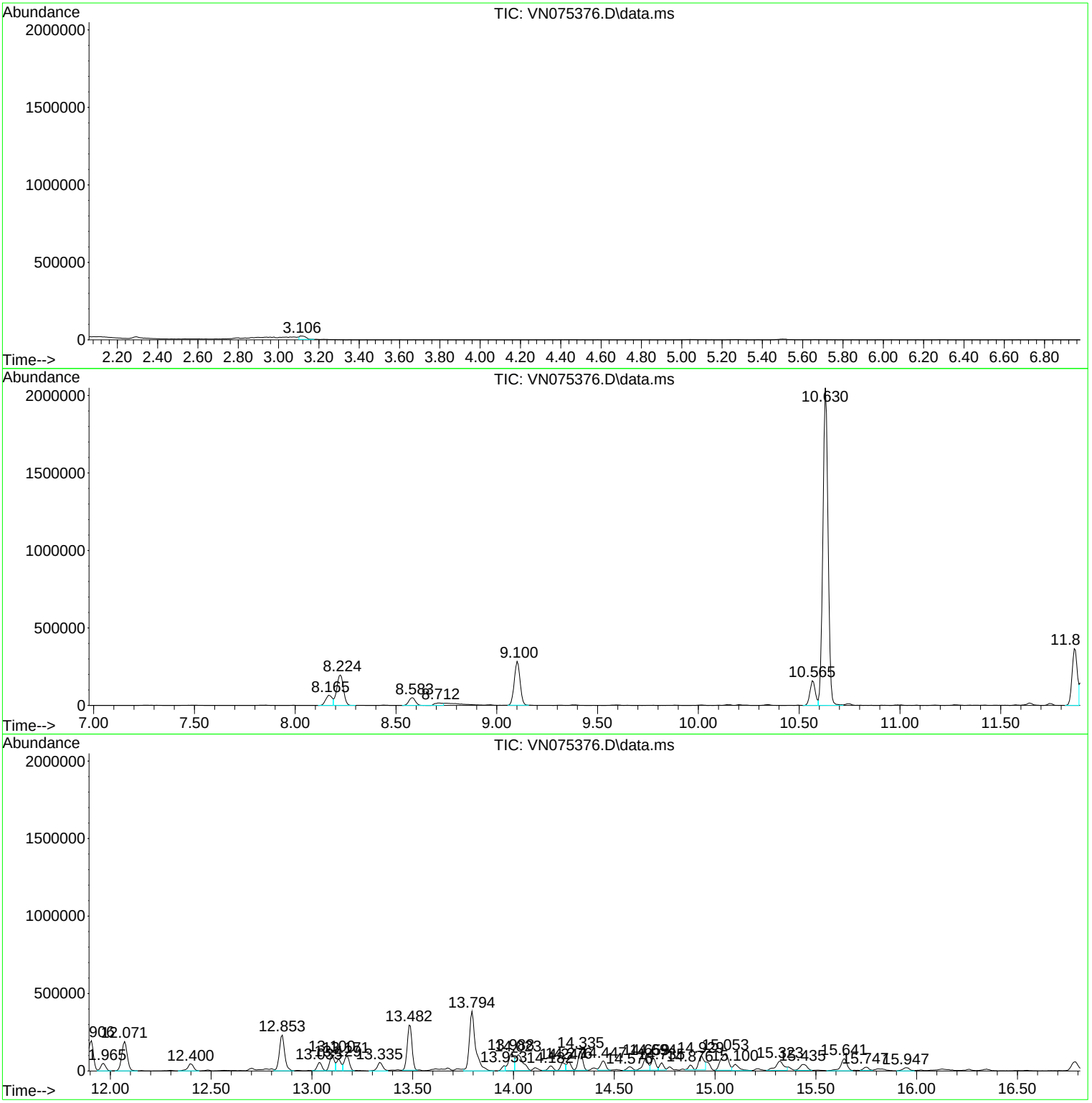
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

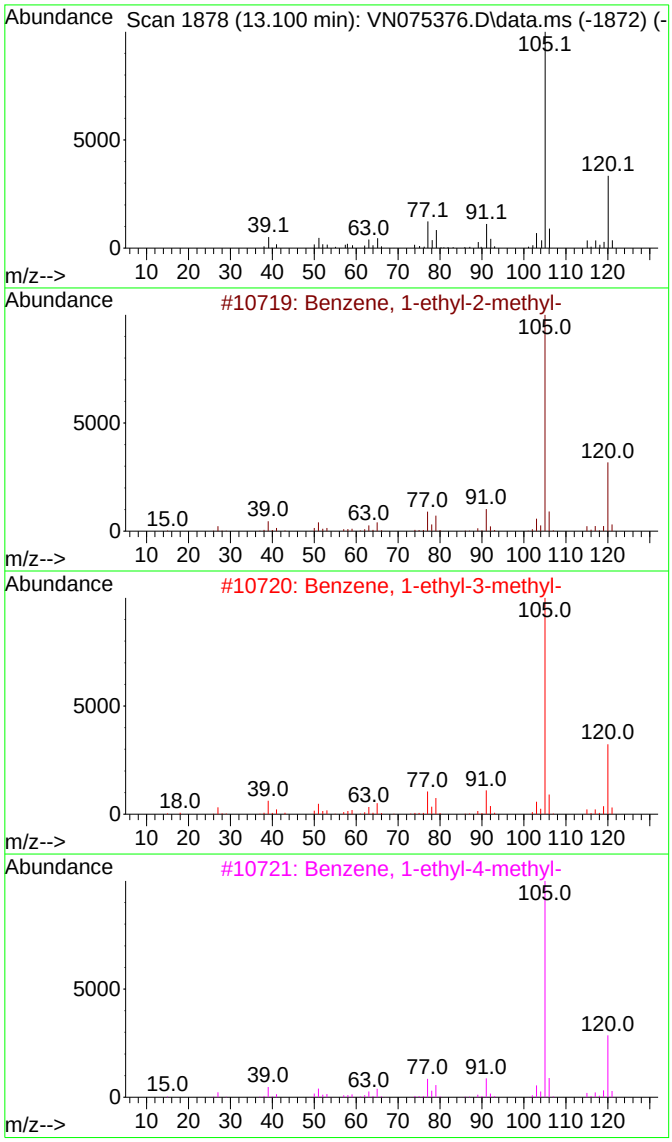
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

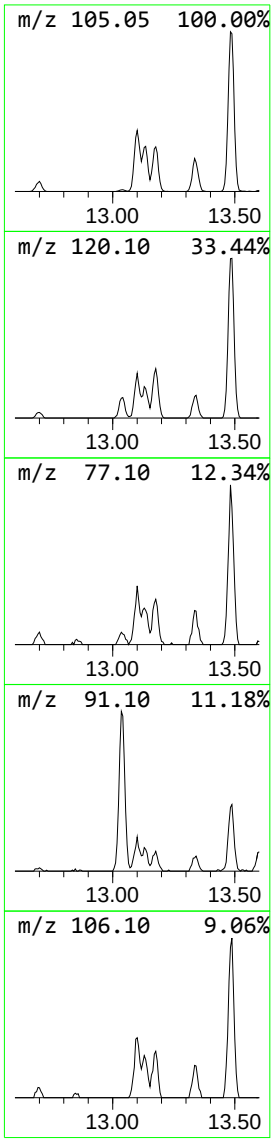
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	10.46 ug/l	171489	1,4-Dichlorobenzene-d4	13.794

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	94
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	Mesitylene	120	C9H12	000108-67-8	91





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Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

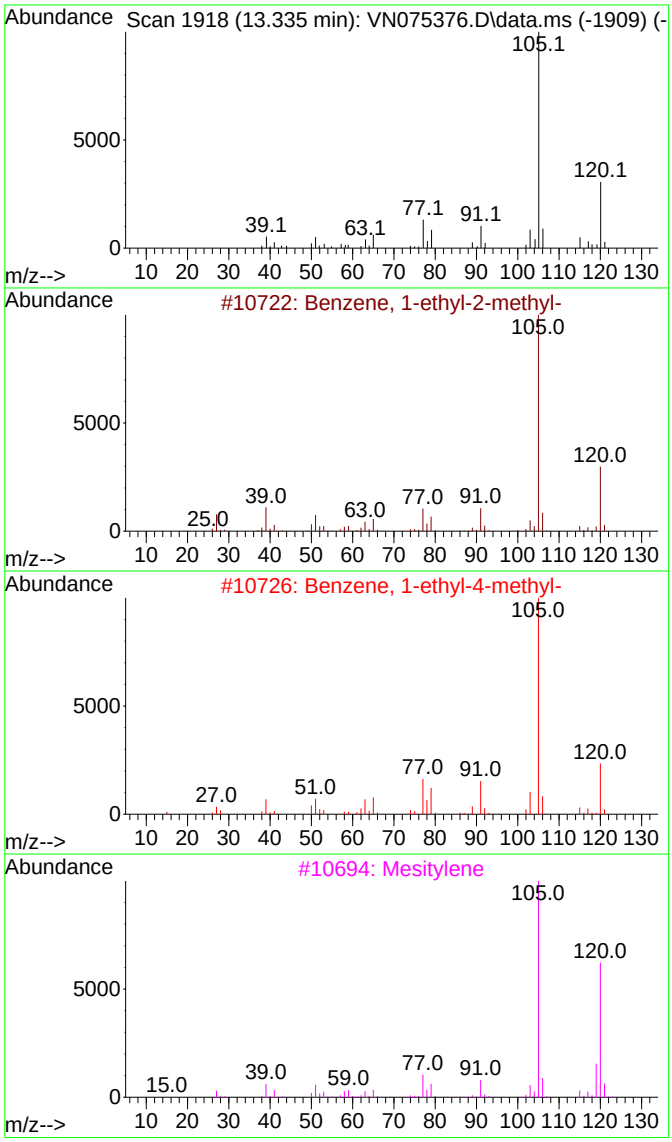
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

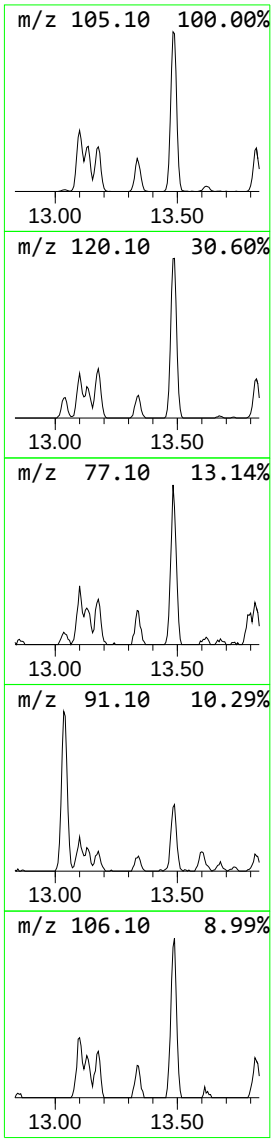
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	6.56 ug/l	107549	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

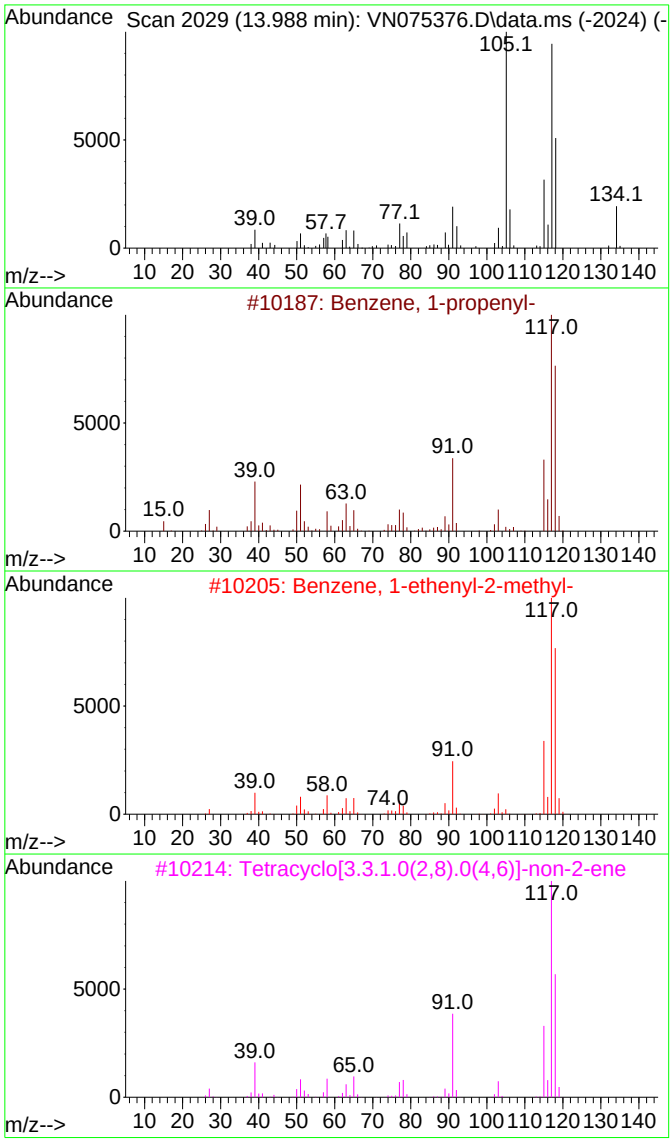
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

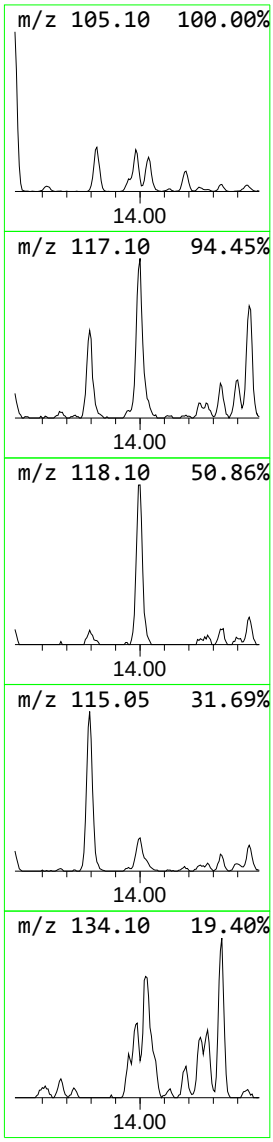
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-propenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	13.27 ug/l	217503	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5	Indane	118	C9H10	000496-11-7	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

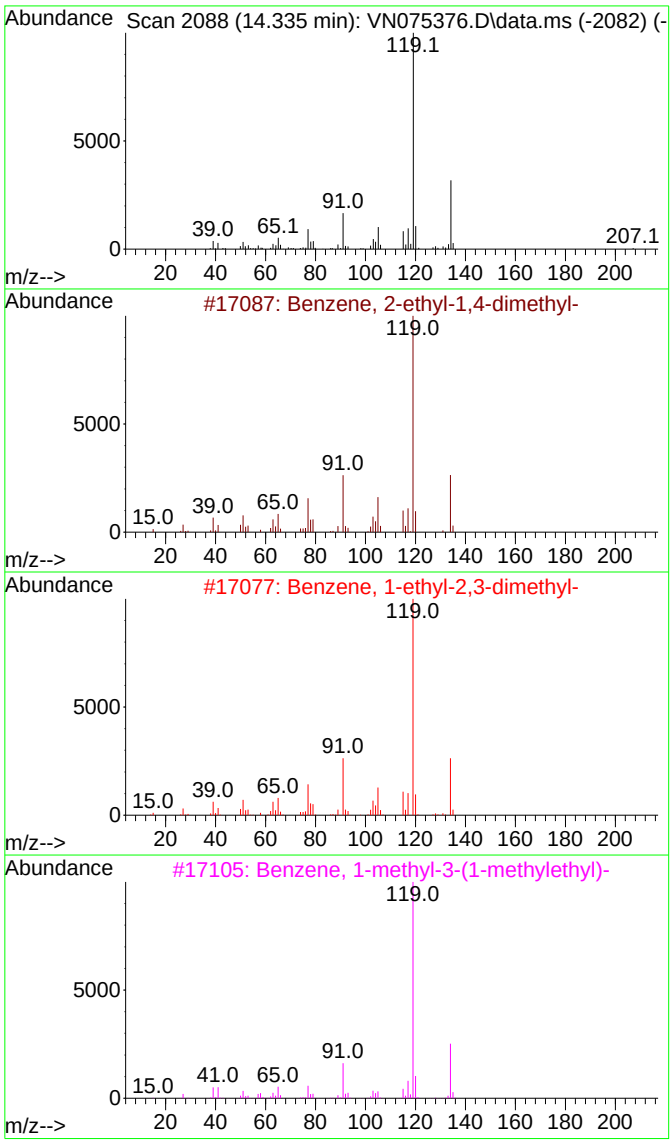
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

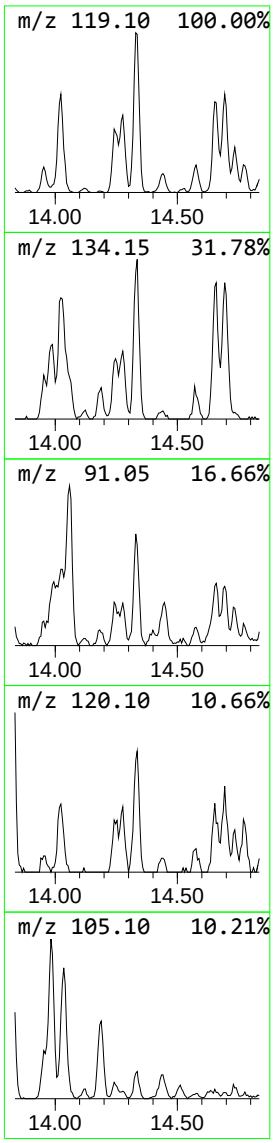
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	12.06 ug/l	197703	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94





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Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

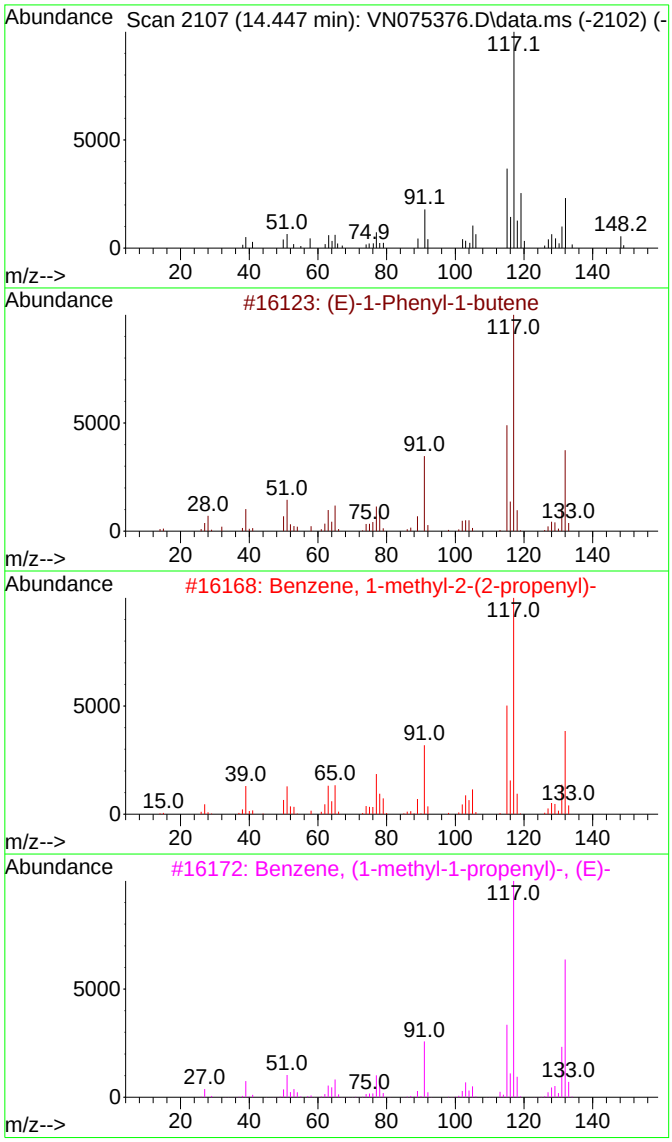
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

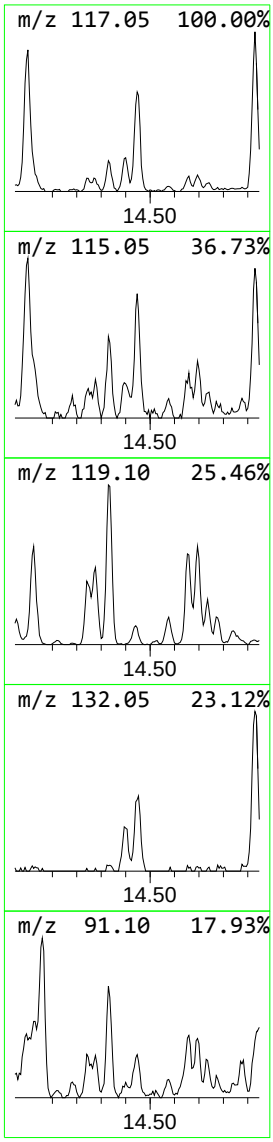
****

Peak Number 5 (E)-1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	6.34 ug/l	103990	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	81
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	74
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	72
4	Indan, 1-methyl-	132	C10H12	000767-58-8	72
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	68





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Operator : JC\MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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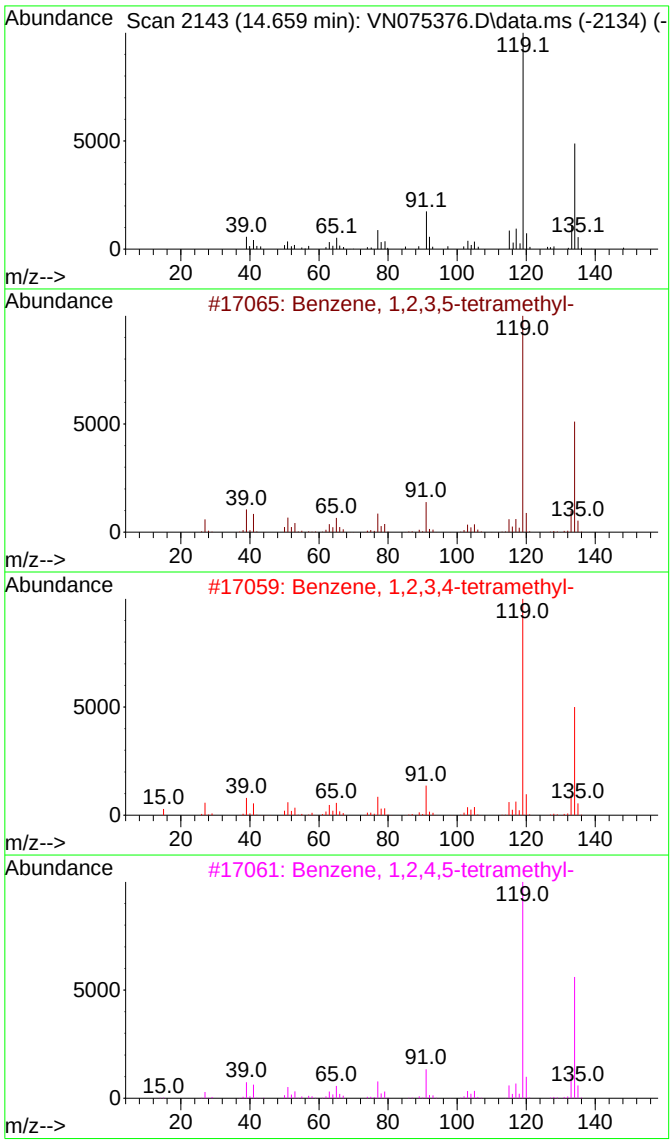
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

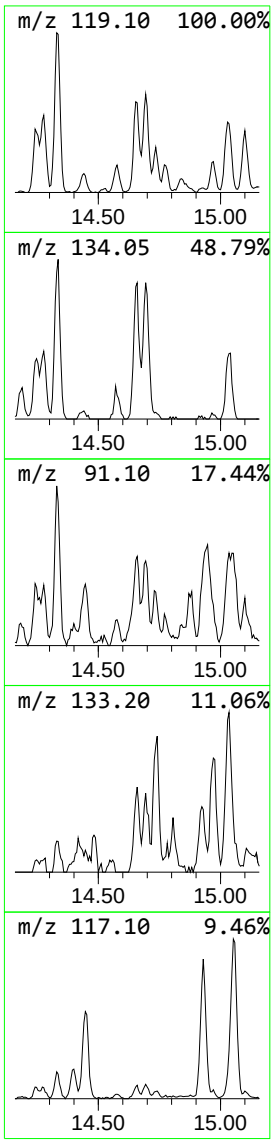
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	8.95 ug/l	146652	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	91





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Instrument :
MSVOA_N
ClientSampleId :
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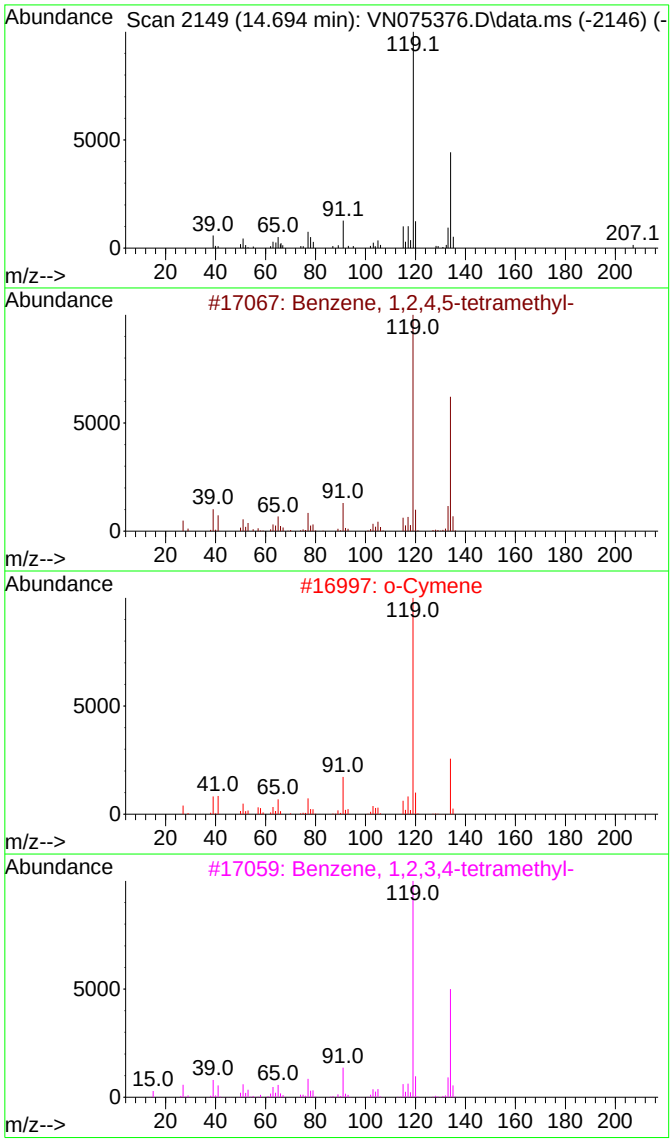
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

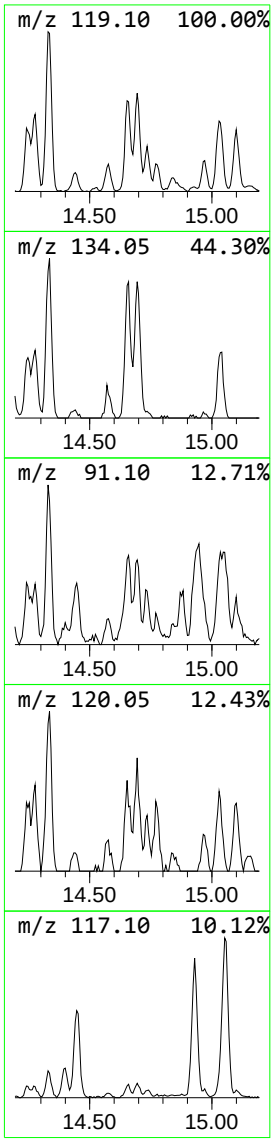
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	7.07 ug/l	115924	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
2	o-Cymene	134	C10H14	000527-84-4	93
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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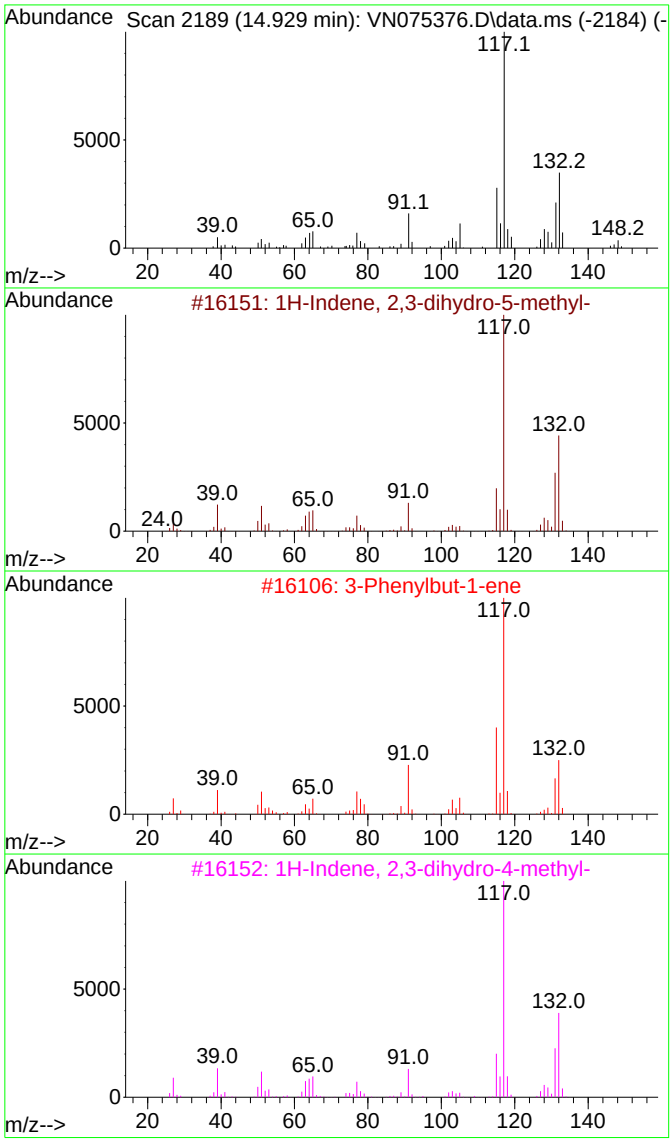
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

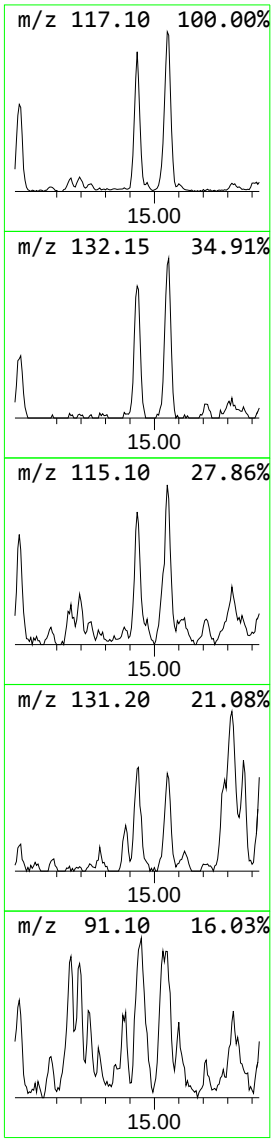
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	10.75 ug/l	176199	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	72





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Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

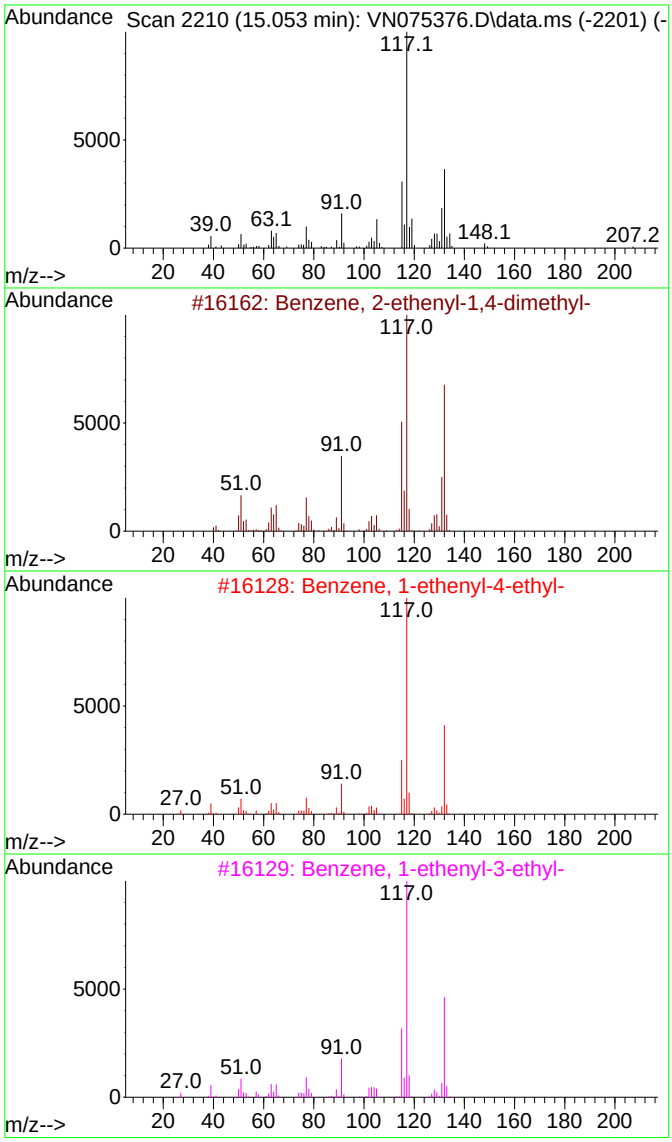
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

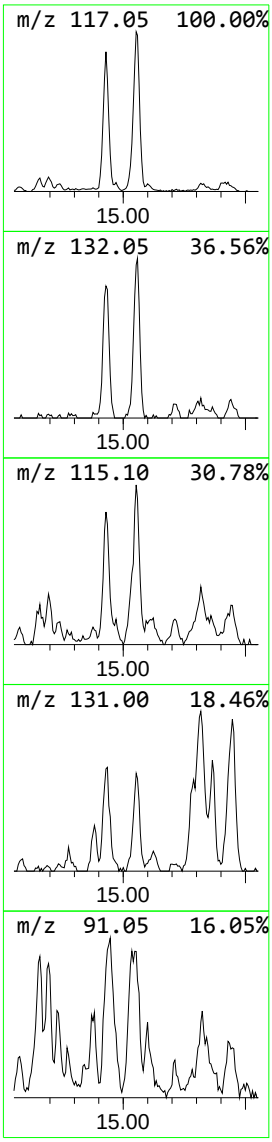
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	17.90 ug/l	293445	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	92





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

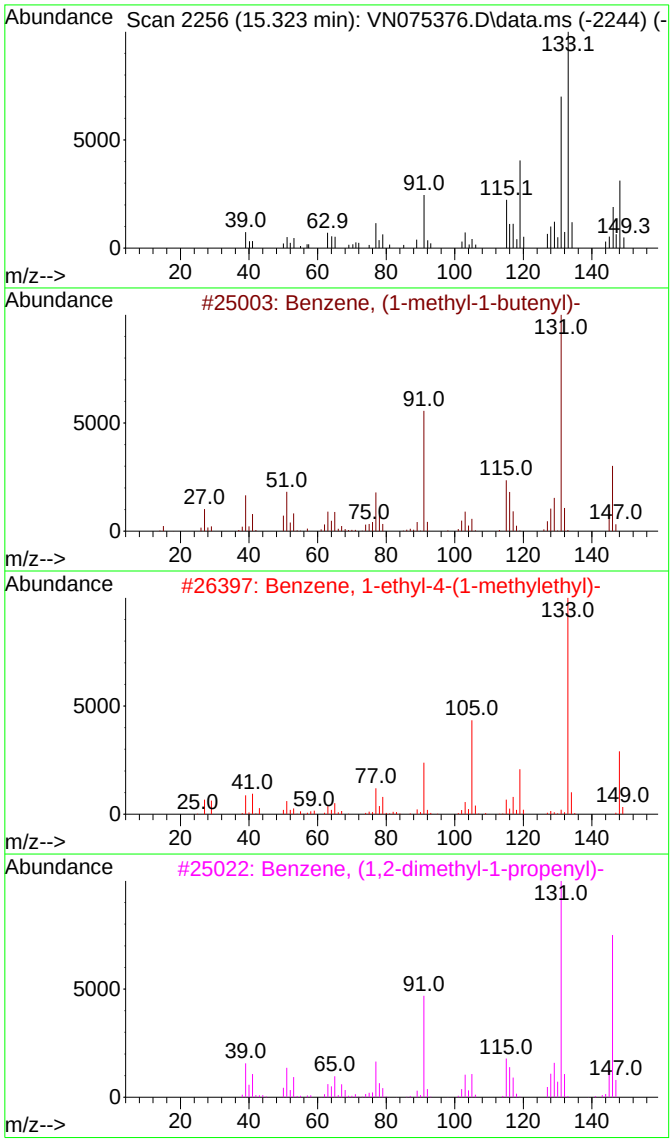
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

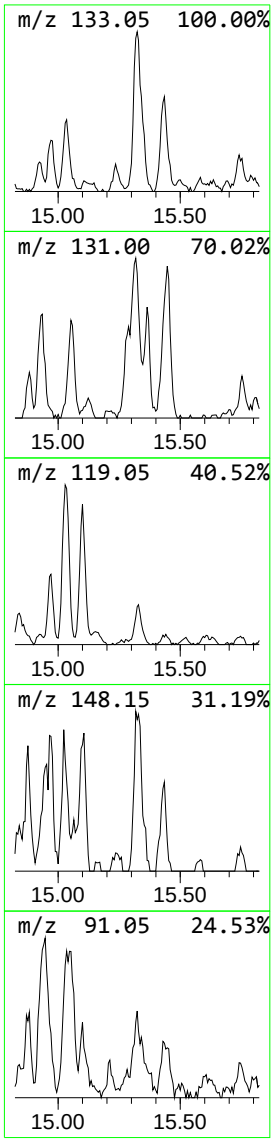
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, (1-methyl-1-butenyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	10.05 ug/l	164747	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	70
2	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	49
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	47
4	1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	46
5	Benzene, pentamethyl-	148	C11H16	000700-12-9	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075376.D
Acq On : 22 Nov 2022 18:31
Operator : JC\MD
Sample : N5644-02
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
110222

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.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-ethy...	13.100	10.5	ug/l	171489	4	13.794	819520	50.0
Benzene, 1-ethy...	13.335	6.6	ug/l	107549	4	13.794	819520	50.0
Benzene, 1-prop...	13.988	13.3	ug/l	217503	4	13.794	819520	50.0
Benzene, 2-ethy...	14.335	12.1	ug/l	197703	4	13.794	819520	50.0
(E)-1-Phenyl-1-...	14.447	6.3	ug/l	103990	4	13.794	819520	50.0
Benzene, 1,2,3,...	14.659	8.9	ug/l	146652	4	13.794	819520	50.0
Benzene, 1,2,4,...	14.694	7.1	ug/l	115924	4	13.794	819520	50.0
1H-Indene, 2,3-...	14.929	10.8	ug/l	176199	4	13.794	819520	50.0
Benzene, 2-ethe...	15.053	17.9	ug/l	293445	4	13.794	819520	50.0
Benzene, (1-met...	15.323	10.1	ug/l	164747	4	13.794	819520	50.0