LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

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\82N091024W.M
Title : SW846 8260

Signal : TIC: VN083963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1046	1056	1060	rBV	120235	291334	2.60%	0.397%
2	8.218	1060	1065	1075	rVB	238071	523406	4.67%	0.713%
3	8.571	1116	1125	1136	rBV	149629	324944	2.90%	0.443%
4	9.100	1206	1215	1227	rBV	328247	680735	6.07%	0.927%
5	10.012	1363	1370	1381	rVB	62770	125632	1.12%	0.171%
6	10.141	1381	1392	1398	rBV	94233	193642	1.73%	0.264%
7	10.494	1443	1452	1457	rBV	111742	209449	1.87%	0.285%
8	10.565	1457	1464	1472	rVV	500429	908827	8.10%	1.238%
9	11.641	1639	1647	1659	rVB3	109300	240934	2.15%	0.328%
10	11.741	1659	1664	1674	rVB	89773	158409	1.41%	0.216%
11	11.865	1674	1685	1691	rBV2	496622	1034275	9.22%	1.409%
12	11.959	1698	1701	1707	rVB	153136	243592	2.17%	0.332%
13	12.065	1711	1719	1731	rVV	1313616	2561741	22.84%	3.489%
14	12.394	1766	1775	1783	rVV	788560	1445860	12.89%	1.969%
15	12.476	1783	1789	1795	rVB	86656	158396	1.41%	0.216%
16	12.694	1820	1826	1831	rBV	338043	592504	5.28%	0.807%
17	12.823	1840	1848	1861	rVB2	616658	1863304	16.61%	2.538%
18	12.929	1861	1866	1871	rVB3	81303	153183	1.37%	0.209%
19	12.988	1871	1876	1879	rBV	198734	355276	3.17%	0.484%
20	13.035	1879	1884	1889	rVV	690172	1093114	9.75%	1.489%
21	13.094	1889	1894	1898	rVV	3356394	5712891	50.93%	7.781%
22	13.129	1898	1900	1903	rVV	1466742	1955731	17.44%	2.664%
23	13.170	1903	1907	1918	rVB	2182545	3823853	34.09%	5.208%
24	13.335	1926	1935	1942	rBV	1465920	2632594	23.47%	3.586%
25	13.423	1942	1950	1954	rBV	642175	1147154	10.23%	1.562%
26	13.482	1954	1960	1966	rBV	7256603	11216855	100.00%	15.277%
27	13.529	1966	1968	1974	rVB	283991	393416	3.51%	0.536%
28	13.641	1974	1987	1996	rBV4	758778	2296820	20.48%	3.128%
29	13.718	1996	2000	2002	rBV	131594	182745	1.63%	0.249%
30	13.753	2002	2006	2008	rBV2	102125	120570	1.07%	0.164%
31	13.823	2008	2018	2030	rVB3	2163962	6203490	55.31%	8.449%
32	13.953	2034	2040	2041	rBV3	431735	672330	5.99%	0.916%
33	13.988	2041	2046	2049	rBV2	1396066	2861930	25.51%	3.898%
34	14.106	2062	2066	2070	rBV2	204046	299735	2.67%	0.408%
35	14.182	2074	2079	2084	rVB	517197	899259	8.02%	1.225%
36	14.241	2084	2089	2092	rBV	811357	1373540	12.25%	1.871%

LSC Area Percent Report

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Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

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\82N091024W.M
Title : SW846 8260

37	14.270	2092	2094	2099	rVV	736427	951358	8.48%	1.296%
38	14.329	2099	2104	2113	rVB	1478802	2353472	20.98%	3.205%
39	14.441	2118	2123	2128	rVB3	362705	612481	5.46%	0.834%
40	14.576	2140	2146	2151	rBV	321777	536242	4.78%	0.730%
41	14.653	2151	2159	2162	rBV	990225	1694934	15.11%	2.308%
42	14.694	2162	2166	2170	rVV	1174534	1817981	16.21%	2.476%
43	14.735	2170	2173	2177	rVB3	434033	601330	5.36%	0.819%
44	14.806	2182	2185	2192	rVB	194775	292076	2.60%	0.398%
45	14.876	2192	2197	2200	rBV2	176986	245181	2.19%	0.334%
46	14.923	2200	2205	2209	rBV	525684	966117	8.61%	1.316%
47	15.047	2216	2226	2232	rBV4	783022	2594972	23.13%	3.534%
48	15.206	2249	2253	2261	rVB4	92569	190337	1.70%	0.259%
49	15.317	2261	2272	2284	rVV3	292594	875645	7.81%	1.193%
50	15.429	2285	2291	2300	rVB5	199059	496397	4.43%	0.676%
51	15.641	2313	2327	2334	rVB	805355	1796929	16.02%	2.447%
52	15.747	2340	2345	2349	rBV4	103870	198451	1.77%	0.270%
53	15.829	2354	2359	2370	rVB2	182582	398949	3.56%	0.543%
54	15.941	2370	2378	2387	rBV	153575	380473	3.39%	0.518%
55	16.123	2404	2409	2424	rVB3	77600	241882	2.16%	0.329%
56	16.253	2425	2431	2437	rVV4	71200	164942	1.47%	0.225%
57	16.335	2438	2445	2453	rVB3	122068	289154	2.58%	0.394%
58	16.776	2513	2520	2522	rBV	443737	771356	6.88%	1.051%

Sum of corrected areas: 73422129

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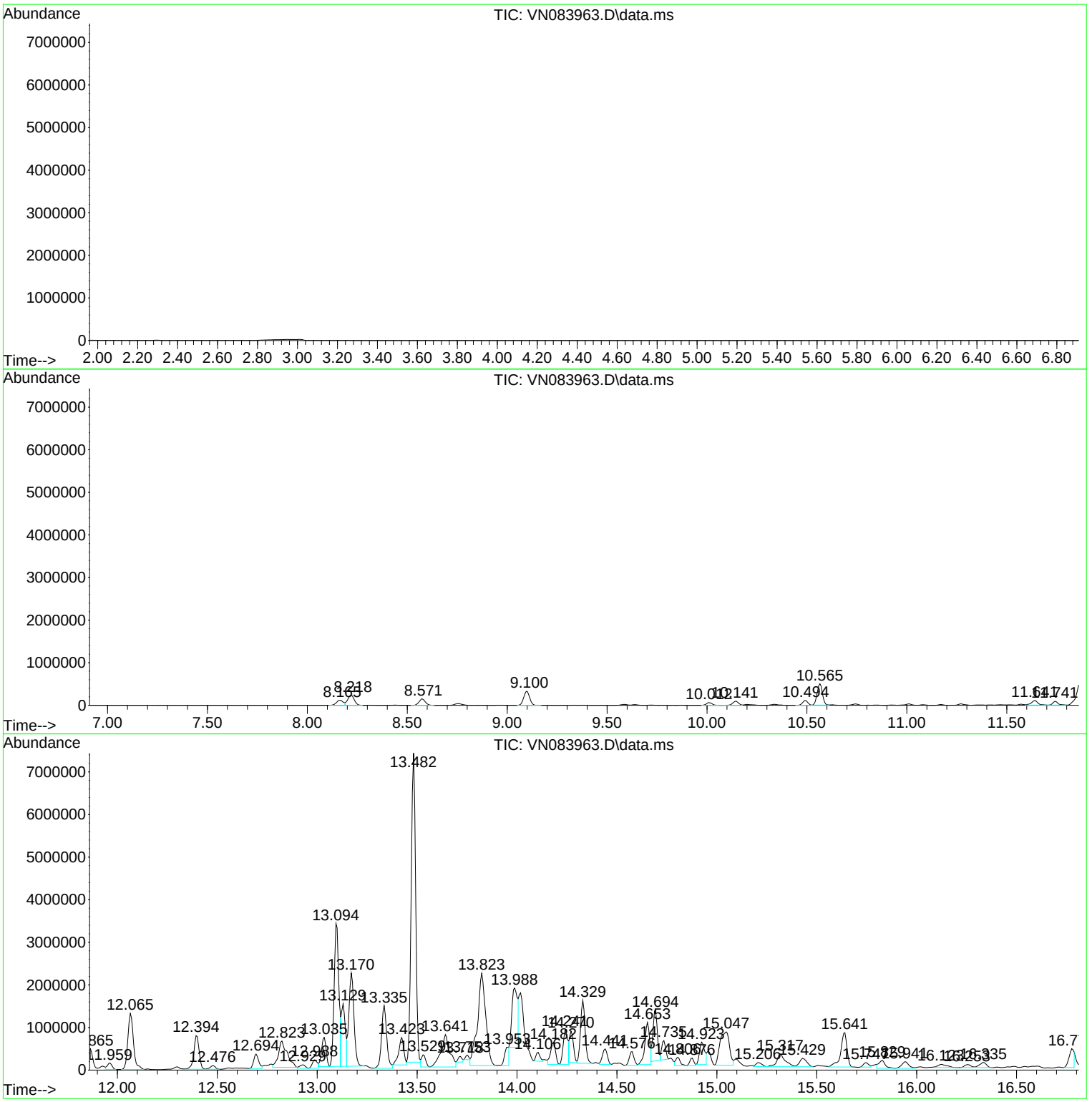
Instrument :
MSVOA_N
ClientSampleId :
FDF-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



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Data File : VN083963.D
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Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
FDF-1

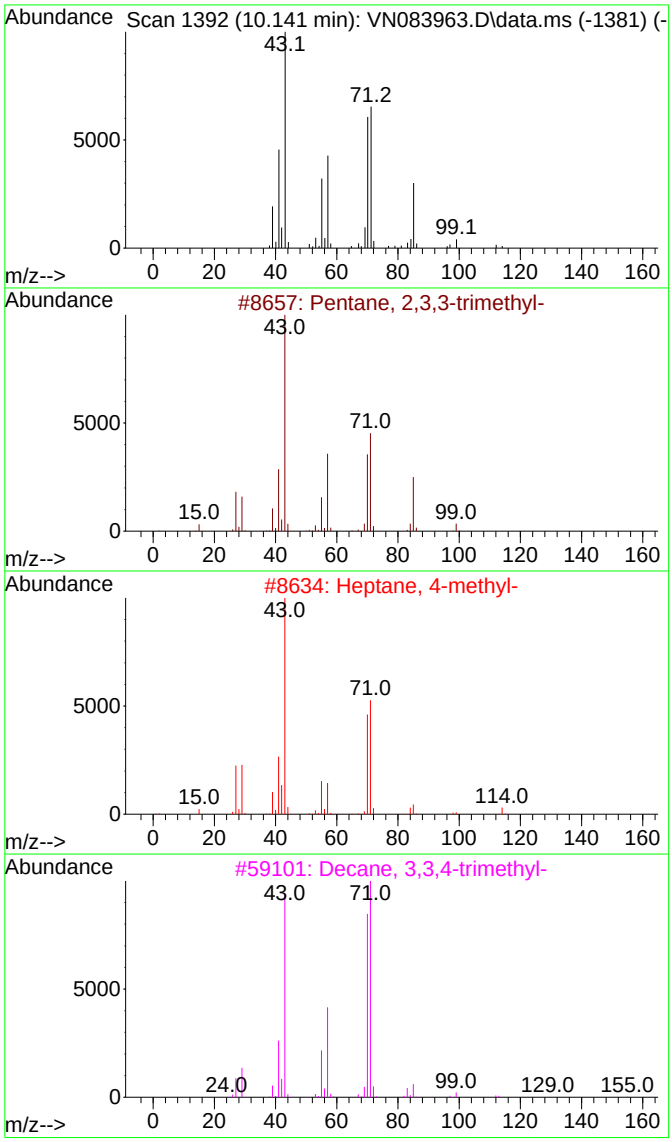
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

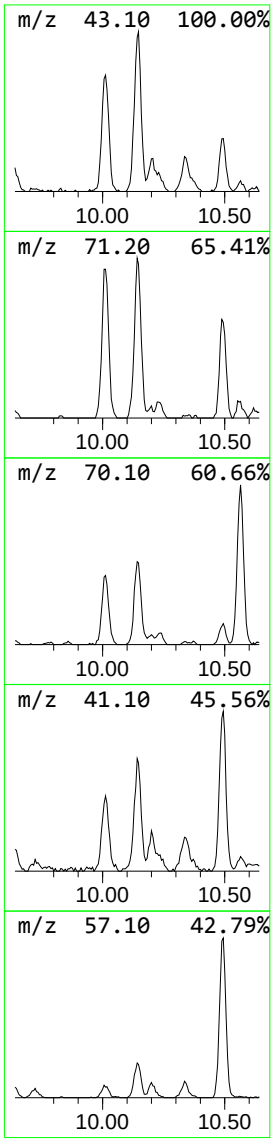
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.141	14.22 ug/l	193642	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

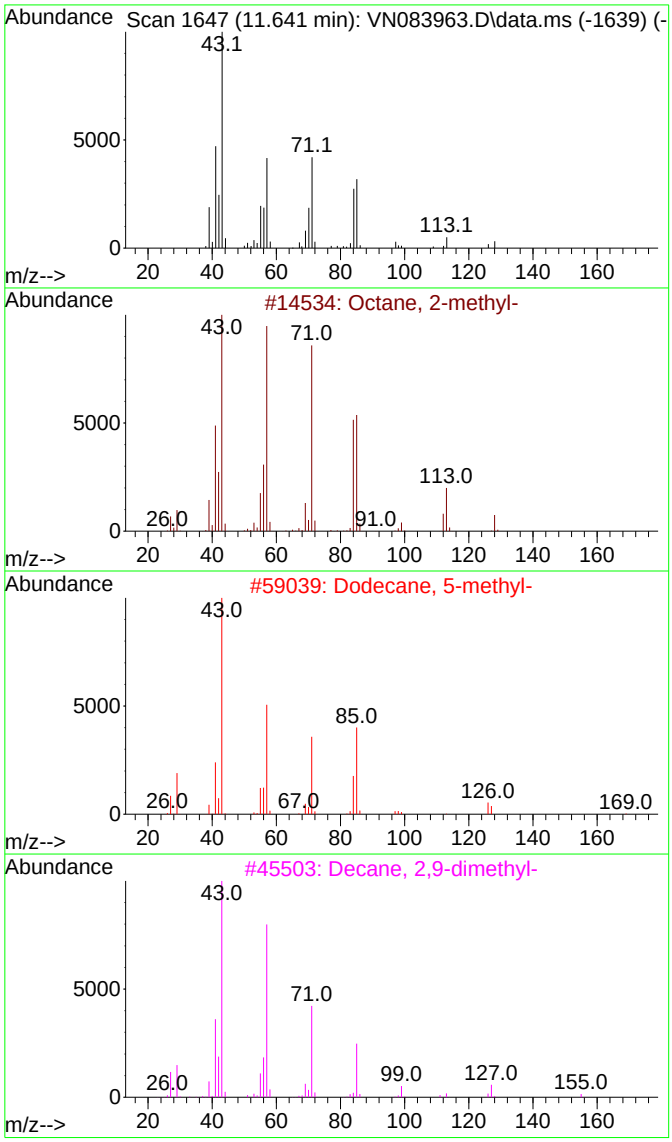
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

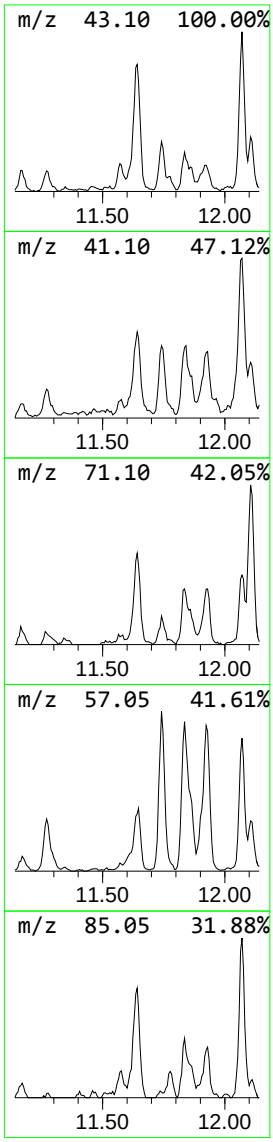
****

Peak Number 2 Octane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	11.65 ug/l	240934	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	59
2	Dodecane, 5-methyl-	184	C13H28	017453-93-9	59
3	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	59
4	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	53
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





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Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

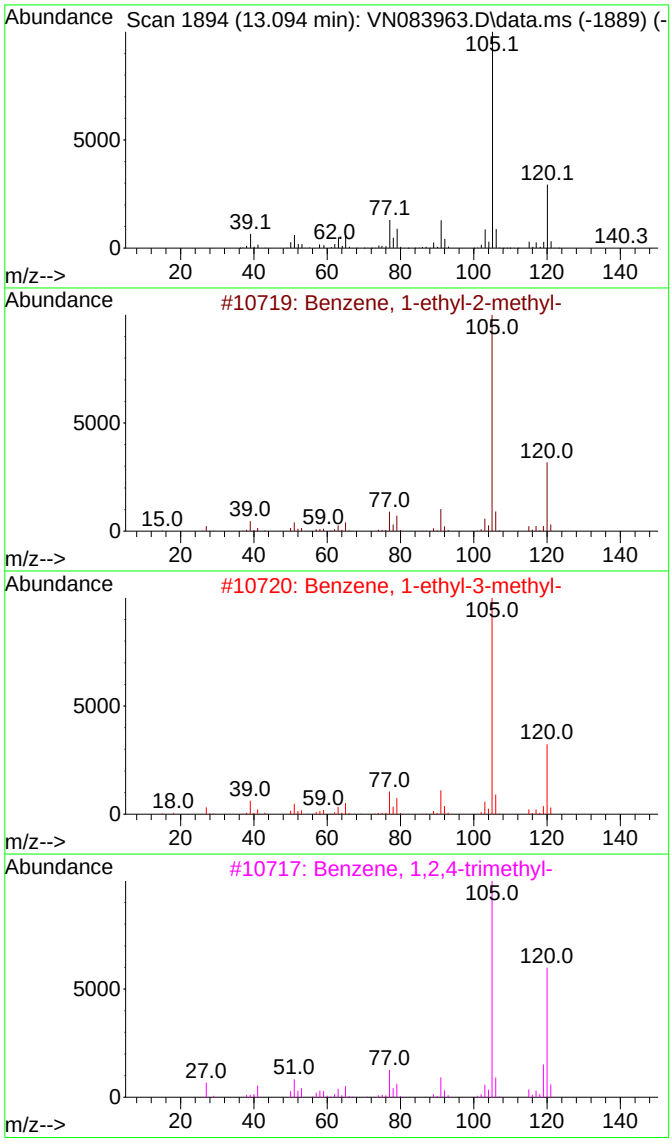
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

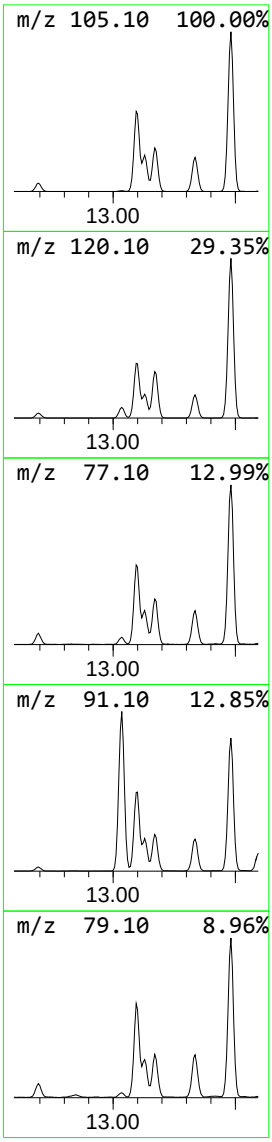
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	46.05 ug/l	5712890	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083963.D
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Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

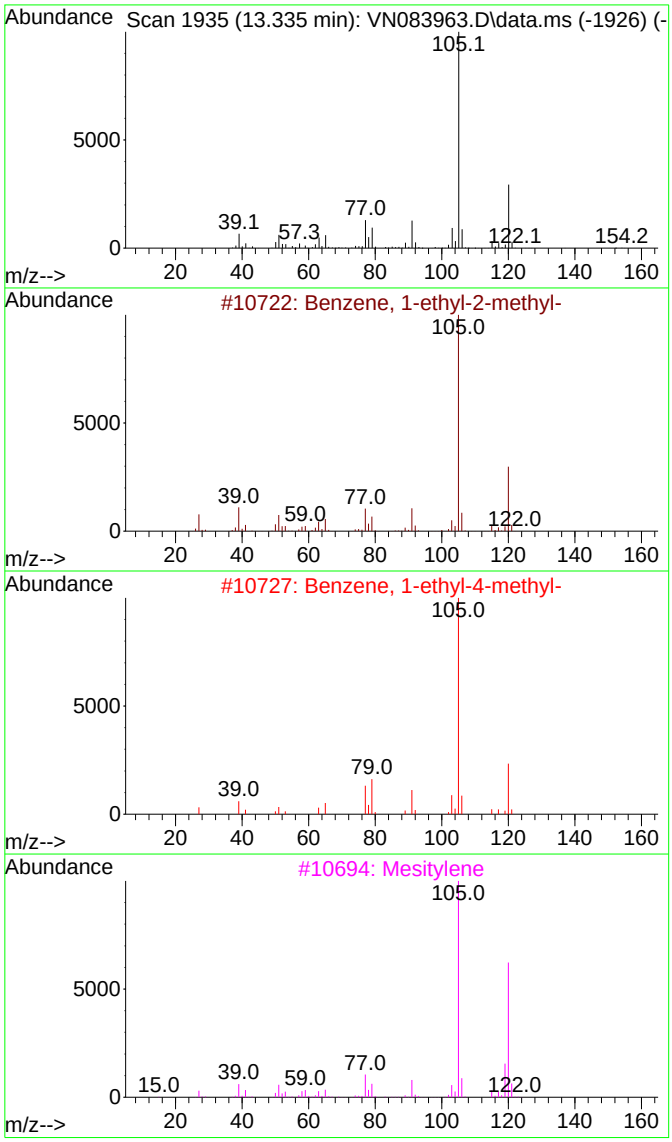
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

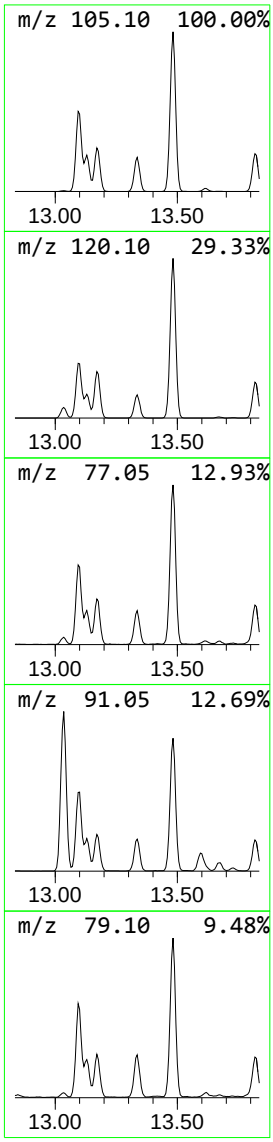
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	21.22 ug/l	2632590	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	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
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Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

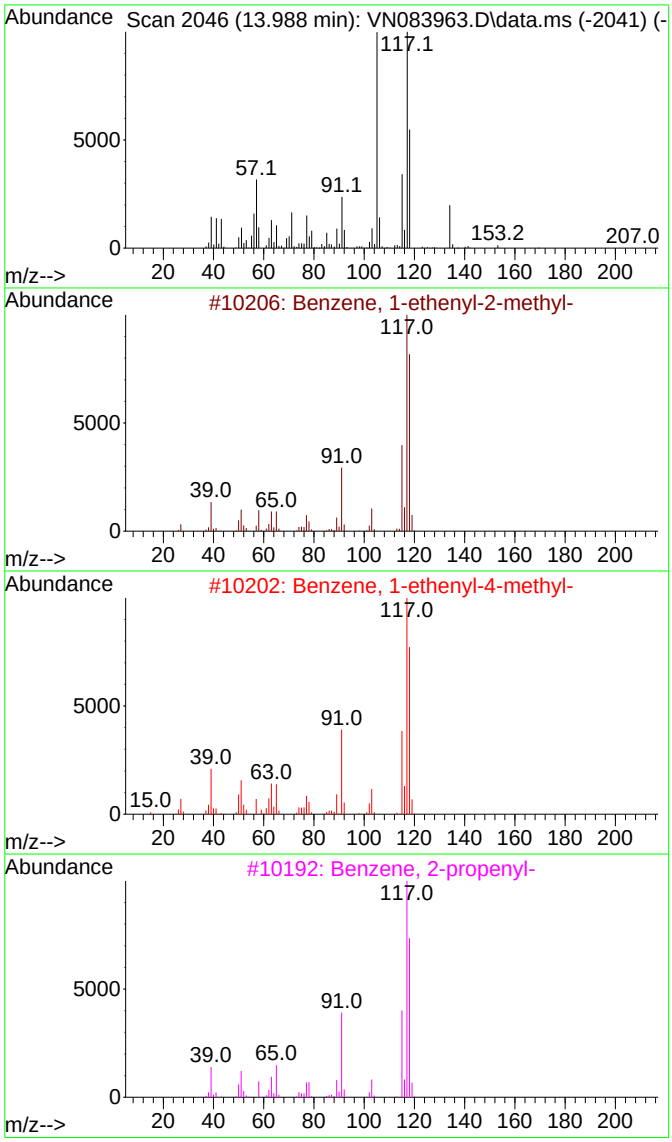
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

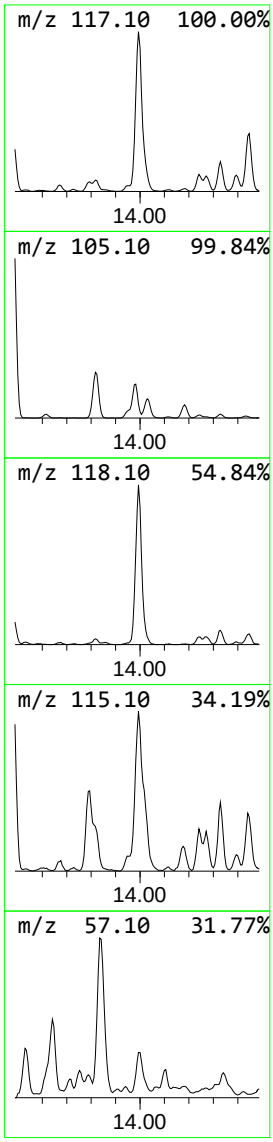
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	23.07 ug/l	2861930	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	92
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Indane	118	C9H10	000496-11-7	64





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Operator : JC\MD
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ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

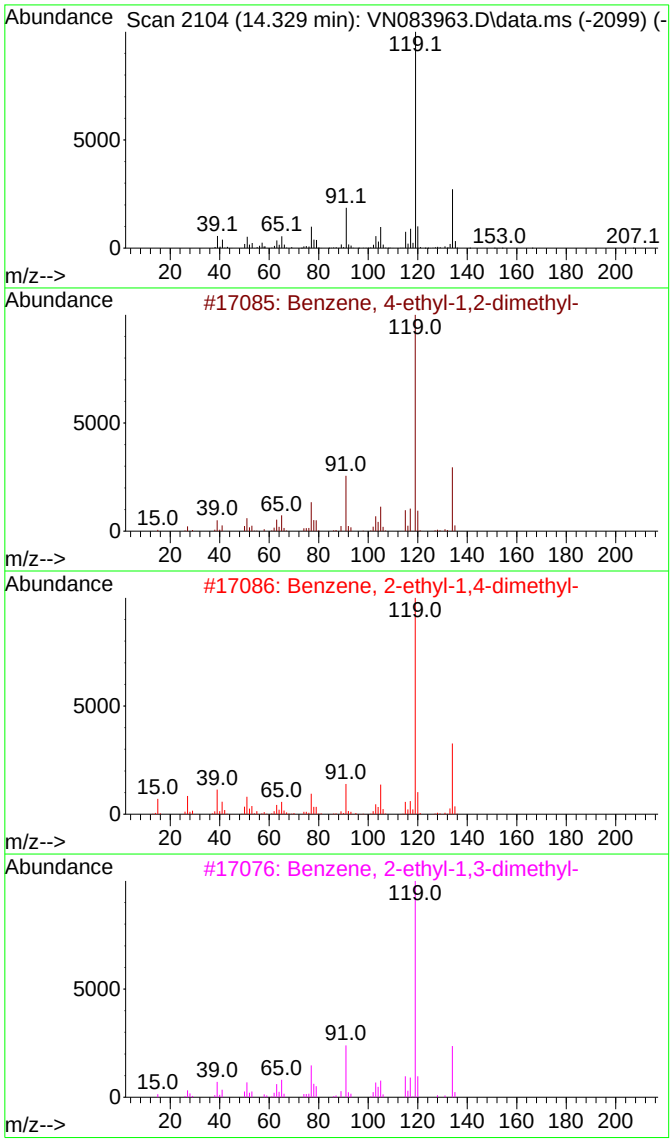
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

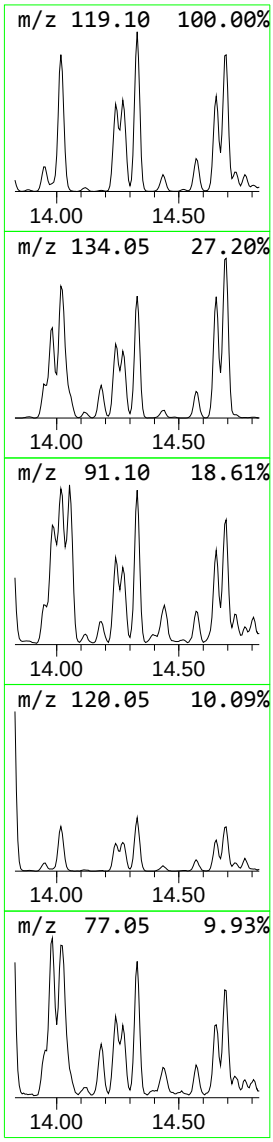
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	18.97 ug/l	2353470	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	p-Cymene	134	C10H14	000099-87-6	95





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Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

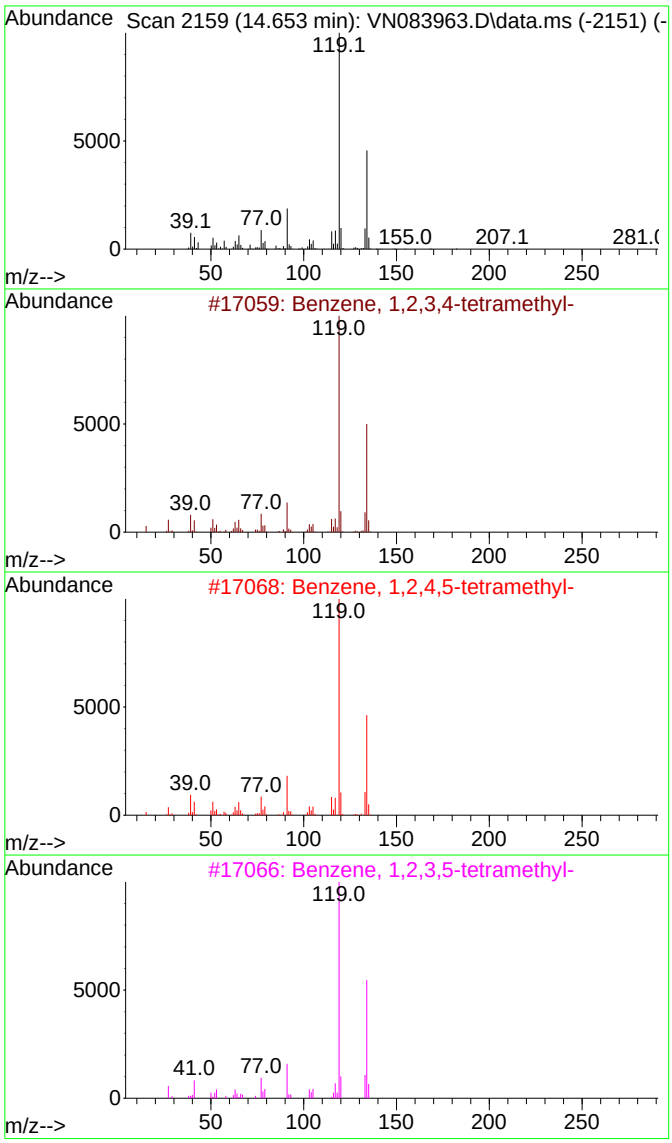
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

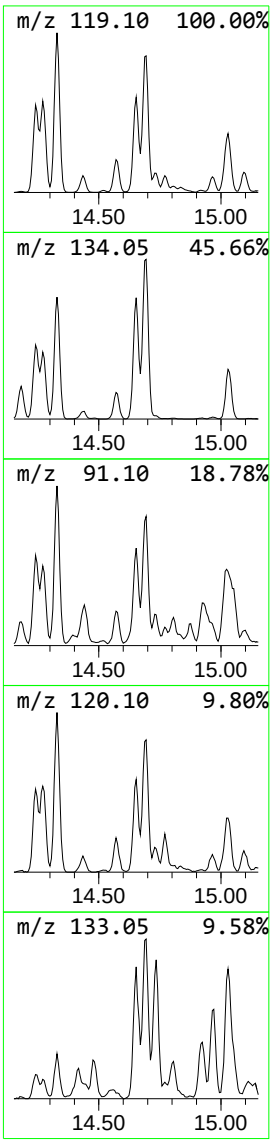
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.653	13.66 ug/l	1694930	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94





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Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

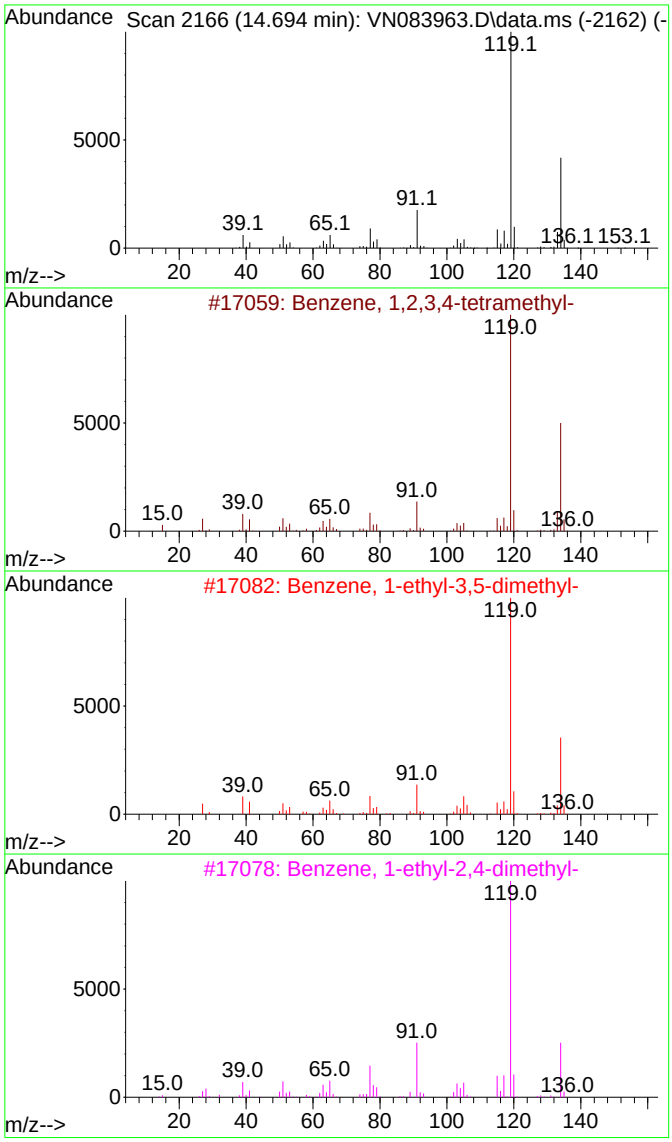
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

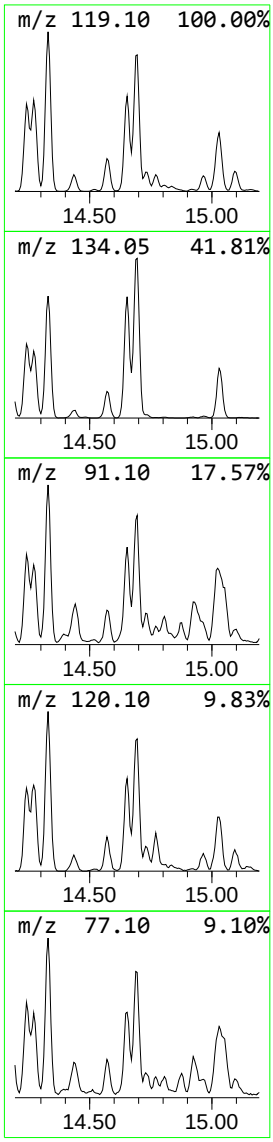
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	14.65 ug/l	1817980	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

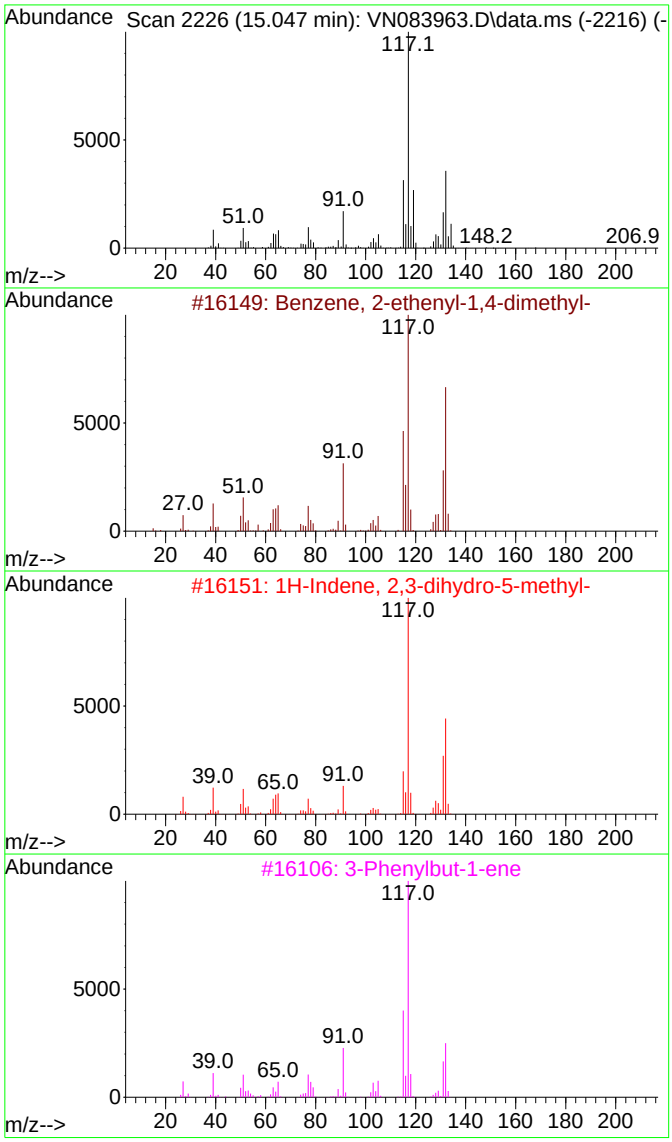
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

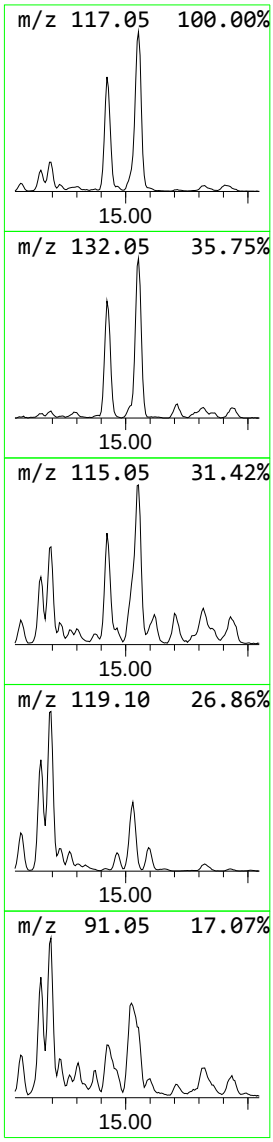
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	20.92 ug/l	2594970	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	95
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
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\VN091724\
Data File : VN083963.D
Acq On : 18 Sep 2024 05:33
Operator : JC\MD
Sample : P3964-01
Misc : 4.16g/10mL/100uL/5.00ml/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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
Pentane, 2,3,3-...	10.141	14.2	ug/l	193642	2	9.100	680735	50.0
Octane, 2-methyl-	11.641	11.7	ug/l	240934	3	11.865	1034280	50.0
Benzene, 1-ethy...	13.094	46.0	ug/l	5712890	4	13.794	6203490	50.0
Benzene, 1-ethy...	13.335	21.2	ug/l	2632590	4	13.794	6203490	50.0
Benzene, 1-ethe...	13.988	23.1	ug/l	2861930	4	13.794	6203490	50.0
Benzene, 4-ethy...	14.329	19.0	ug/l	2353470	4	13.794	6203490	50.0
Benzene, 1,2,3,...	14.653	13.7	ug/l	1694930	4	13.794	6203490	50.0
Benzene, 1-ethy...	14.694	14.7	ug/l	1817980	4	13.794	6203490	50.0
Benzene, 2-ethe...	15.047	20.9	ug/l	2594970	4	13.794	6203490	50.0