LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

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\82N111623W.M
Title : SW846 8260

Signal : TIC: VN080286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	51	57	63	rBV2	14576	28421	2.71%	0.329%
2	8.171	1047	1057	1061	rBV	168274	391554	37.34%	4.533%
3	8.229	1061	1067	1078	rVB	223883	511715	48.80%	5.924%
4	8.582	1116	1127	1137	rBV	159439	358498	34.19%	4.150%
5	9.106	1206	1216	1226	rBV	340242	709479	67.65%	8.213%
6	10.570	1457	1465	1474	rBV	570040	1048695	100.00%	12.140%
7	11.870	1677	1686	1697	rBV	547567	979533	93.40%	11.340%
8	11.964	1697	1702	1709	rVV	22967	39508	3.77%	0.457%
9	12.070	1713	1720	1730	rVB	87989	162325	15.48%	1.879%
10	12.394	1772	1775	1782	rVB3	14737	23990	2.29%	0.278%
11	12.853	1845	1853	1863	rBV	459336	785576	74.91%	9.094%
12	13.035	1879	1884	1889	rBV	13535	21146	2.02%	0.245%
13	13.100	1889	1895	1899	rVV	56171	105312	10.04%	1.219%
14	13.135	1899	1901	1904	rVV2	24853	30680	2.93%	0.355%
15	13.176	1904	1908	1914	rVB	33505	52541	5.01%	0.608%
16	13.335	1929	1935	1940	rBV2	27896	45406	4.33%	0.526%
17	13.482	1953	1960	1967	rBV	129668	210774	20.10%	2.440%
18	13.676	1989	1993	1997	rVB2	9207	12684	1.21%	0.147%
19	13.794	2006	2013	2024	rBV2	576973	1045643	99.71%	12.105%
20	13.994	2032	2047	2063	rBV4	63049	225992	21.55%	2.616%
21	14.182	2075	2079	2085	rBV3	14732	24204	2.31%	0.280%
22	14.247	2085	2090	2092	rBV2	25523	40228	3.84%	0.466%
23	14.276	2092	2095	2100	rVV	25726	39783	3.79%	0.461%
24	14.335	2100	2105	2111	rVB	38259	62610	5.97%	0.725%
25	14.400	2111	2116	2118	rBV3	12101	17707	1.69%	0.205%
26	14.447	2118	2124	2130	rVV2	41825	73345	6.99%	0.849%
27	14.529	2133	2138	2142	rBV5	7042	12422	1.18%	0.144%
28	14.576	2142	2146	2151	rVB2	17199	25609	2.44%	0.296%
29	14.652	2151	2159	2163	rBV2	27752	48738	4.65%	0.564%
30	14.694	2163	2166	2171	rVV	39764	61589	5.87%	0.713%
31	14.735	2171	2173	2177	rVV2	15240	15712	1.50%	0.182%
32	14.876	2189	2197	2201	rBV4	11660	23733	2.26%	0.275%
33	14.929	2201	2206	2211	rBV2	49125	90818	8.66%	1.051%
34	15.052	2217	2227	2233	rBV3	95600	221949	21.16%	2.569%
35	15.105	2233	2236	2246	rVV4	10492	23868	2.28%	0.276%
36	15.211	2248	2254	2261	rVV3	83723	155688	14.85%	1.802%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

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\82N111623W.M
Title : SW846 8260

37	15.323	2262	2273	2277	rVV3	38770	102810	9.80%	1.190%
38	15.364	2277	2280	2285	rVV5	23027	40682	3.88%	0.471%
39	15.441	2285	2293	2302	rVB6	35746	92616	8.83%	1.072%
40	15.641	2321	2327	2332	rVV2	22936	48499	4.62%	0.561%
41	15.699	2332	2337	2342	rVV2	31963	61422	5.86%	0.711%
42	15.752	2342	2346	2347	rVV4	18881	26309	2.51%	0.305%
43	15.788	2348	2352	2365	rVB5	26250	72808	6.94%	0.843%
44	15.952	2372	2380	2388	rBV3	24546	51759	4.94%	0.599%
45	16.129	2400	2410	2411	rBV4	19556	34990	3.34%	0.405%
46	16.170	2411	2417	2426	rVB3	73655	161308	15.38%	1.867%
47	16.346	2439	2447	2453	rVV6	14988	32896	3.14%	0.381%
48	16.511	2464	2475	2486	rBV3	44560	109224	10.42%	1.264%
49	16.717	2497	2510	2516	rBV5	28541	75418	7.19%	0.873%

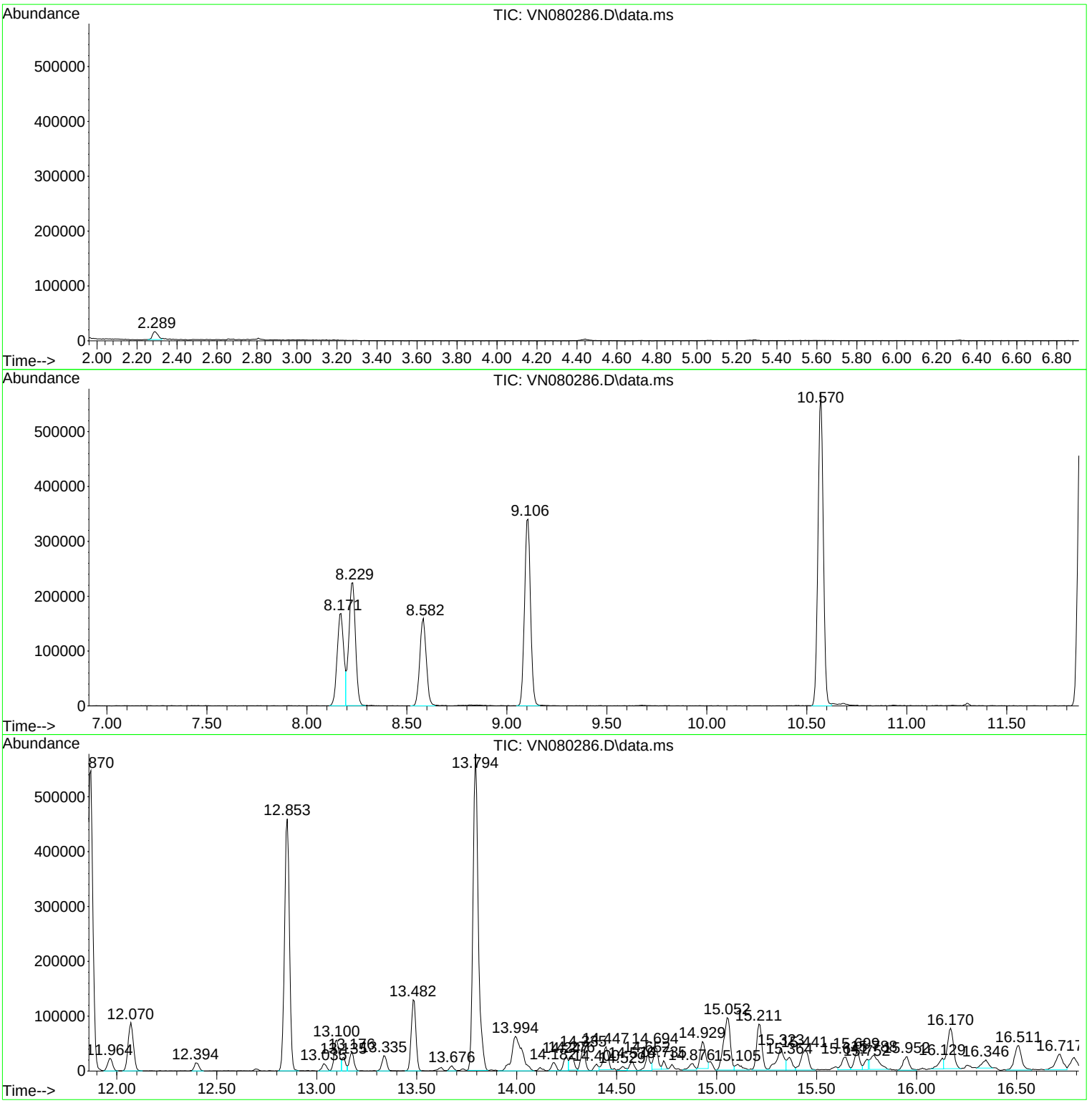
Sum of corrected areas: 8638216

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

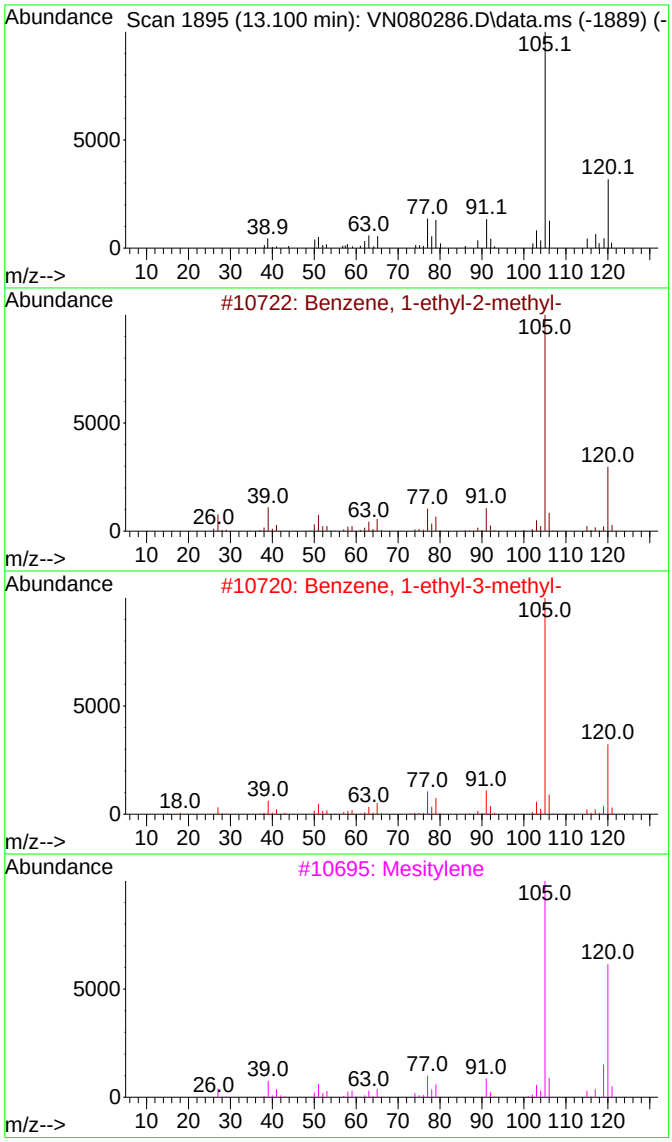
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

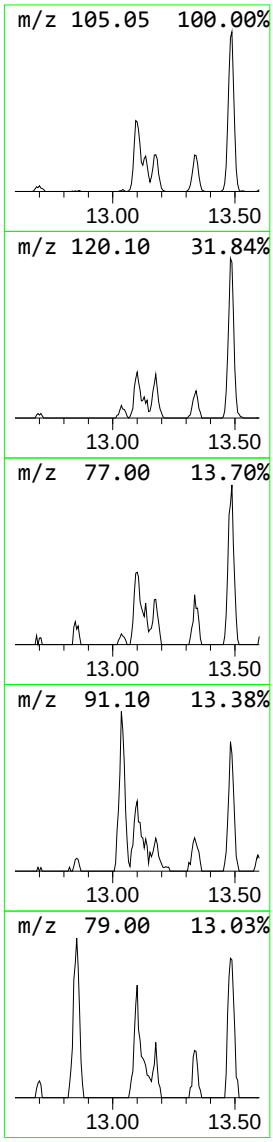
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	5.04 ug/l	105312	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	91
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Mesitylene	120	C9H12	000108-67-8	87
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	86
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

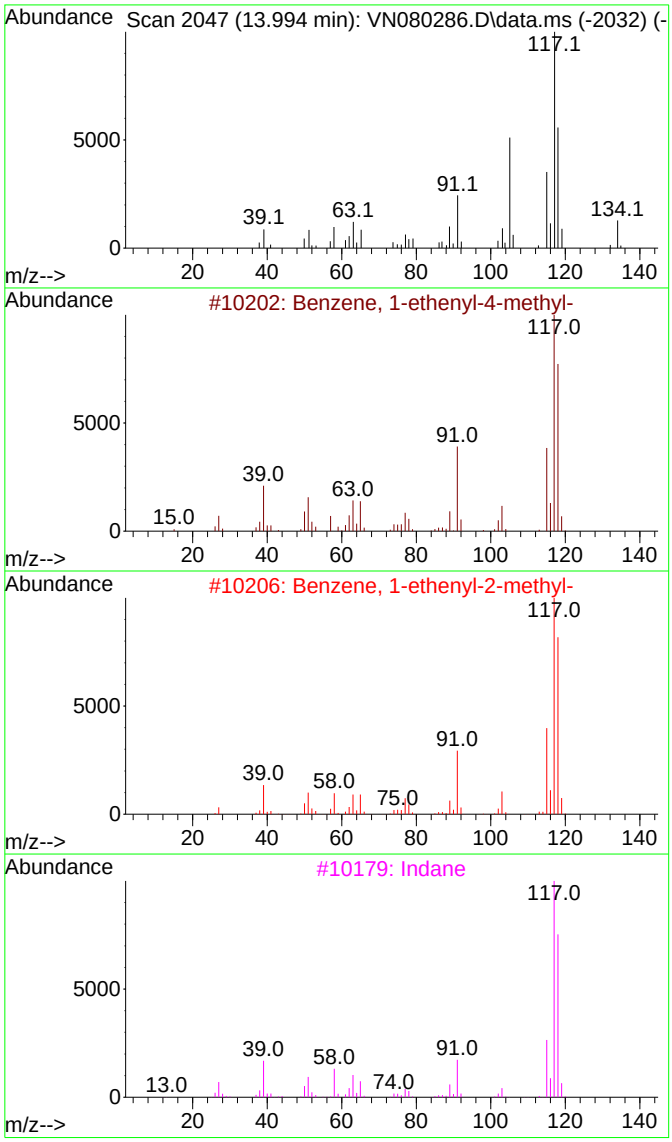
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

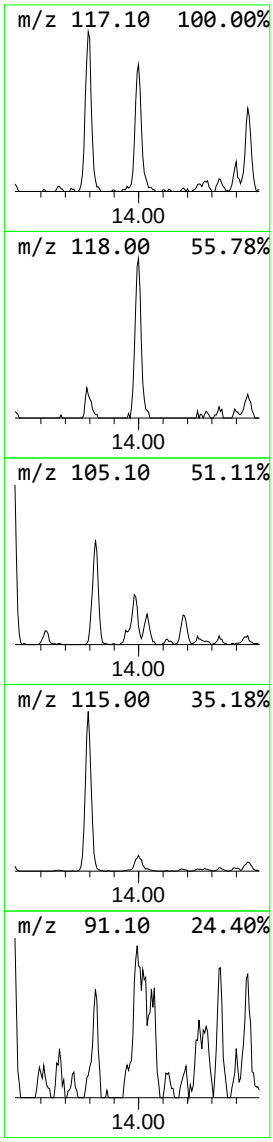
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	10.81 ug/l	225992	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	95
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3	Indane	118	C9H10	000496-11-7	93
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

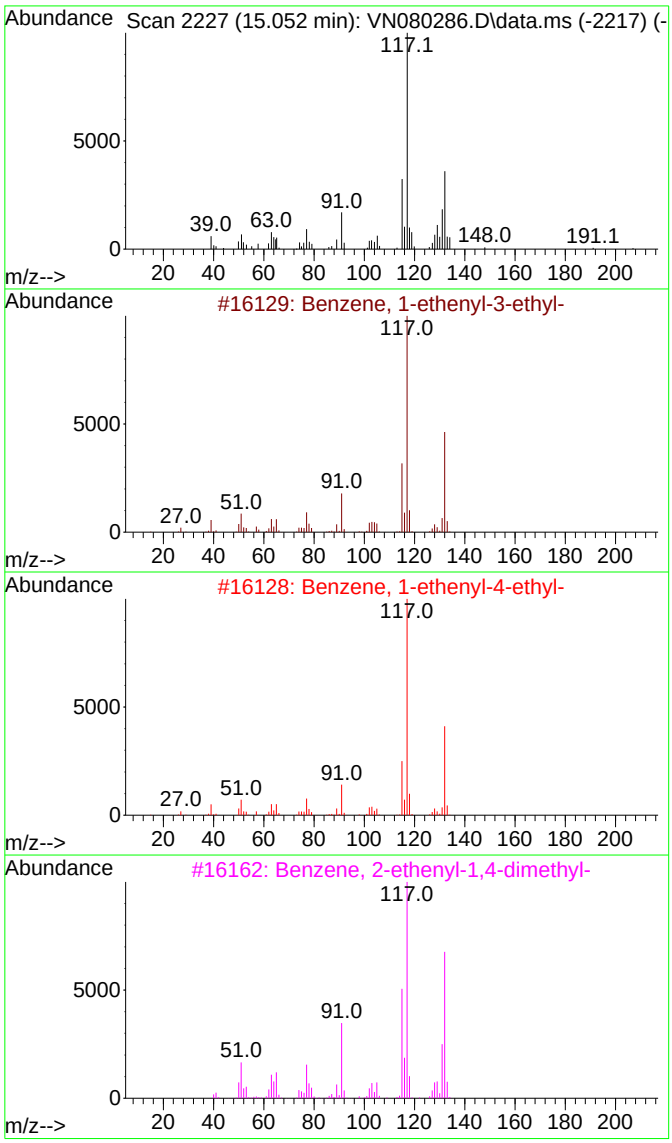
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

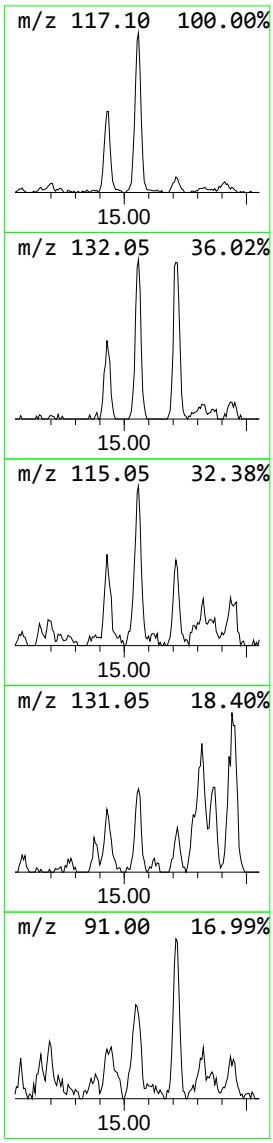
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	10.61 ug/l	221949	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	94
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

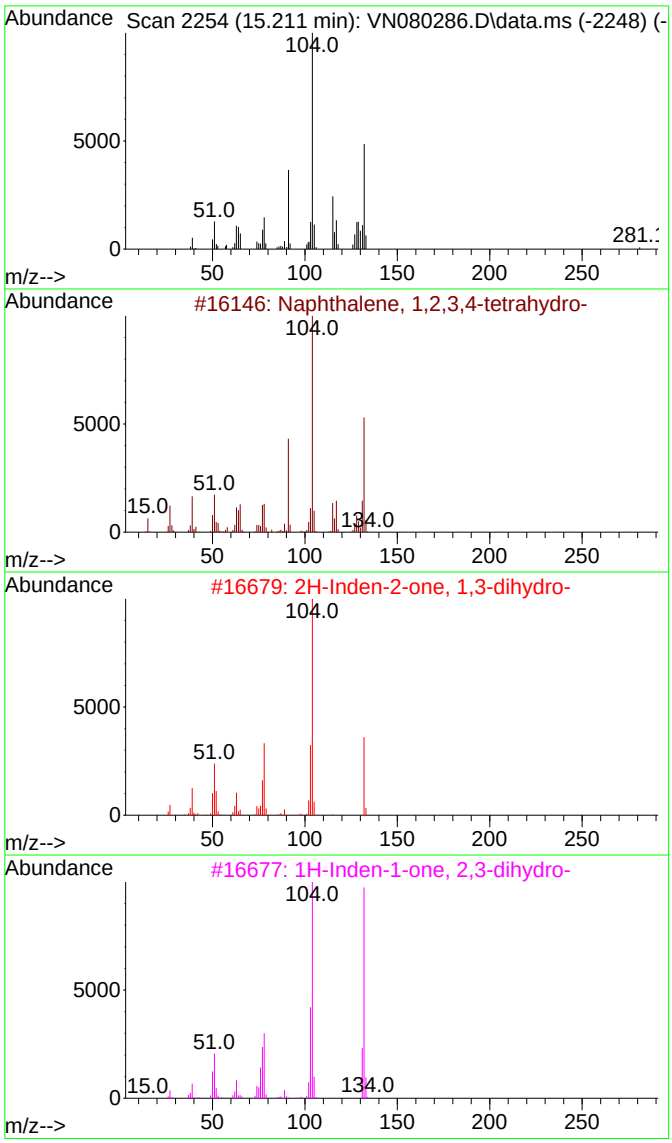
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

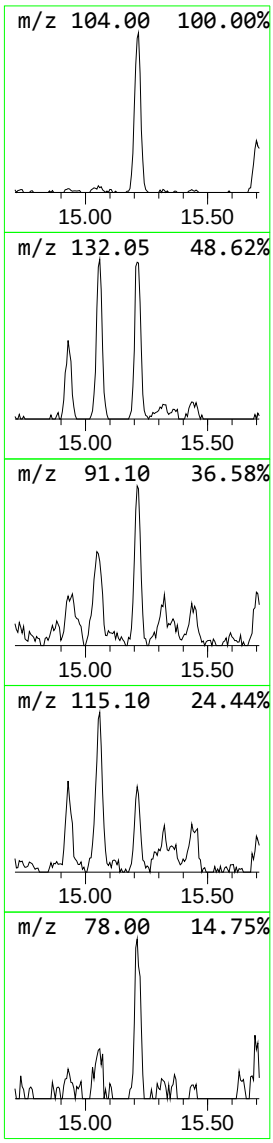
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	7.44 ug/l	155688	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
3	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	50
4	Indan, epoxide	132	C9H8O	000768-22-9	49
5	6-Dimethylaminomethyltricyclo[8....	281	C19H23NO	1000306-67-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

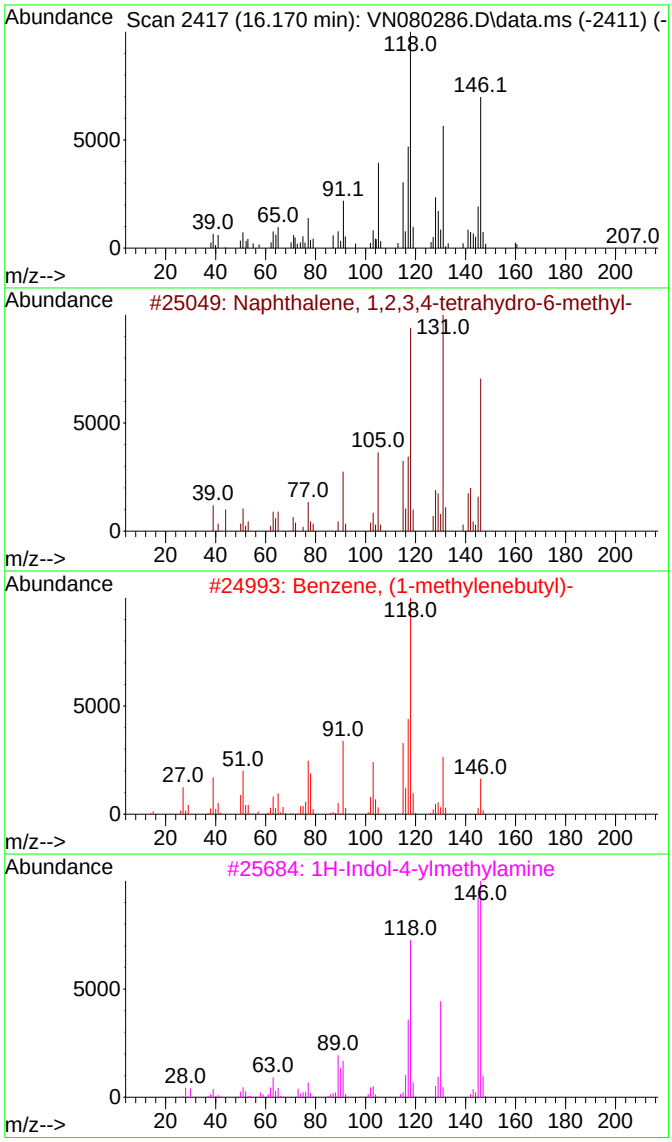
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

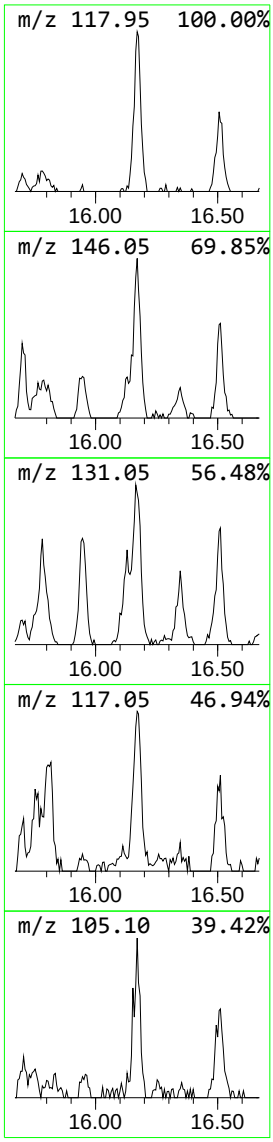
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	7.71 ug/l	161308	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	87
2	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	83
3	1H-Indol-4-ylmethylamine	146	C9H10N2	003468-18-6	58
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	53
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

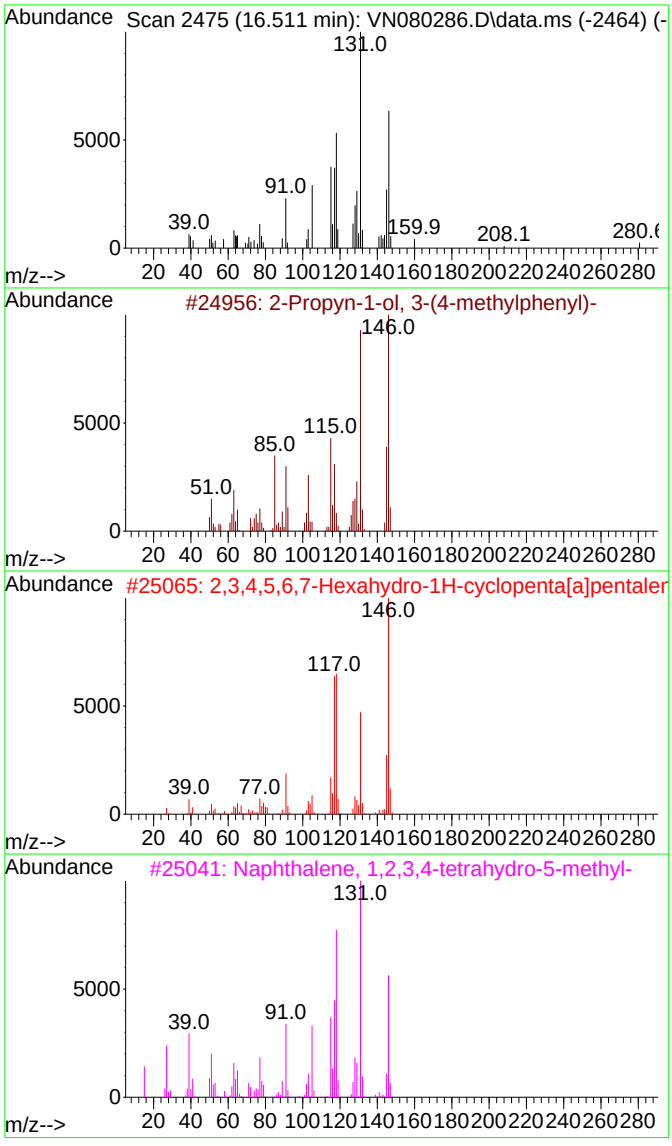
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

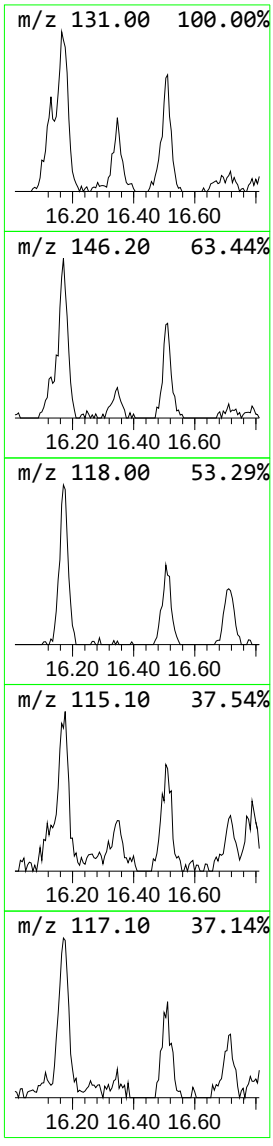
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Propyn-1-ol, 3-(4-methylp... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	5.22 ug/l	109224	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	81
2	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	81
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	74
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	68
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112723\
Data File : VN080286.D
Acq On : 27 Nov 2023 19:34
Operator : JC\MD
Sample : 05550-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A591

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.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	5.0	ug/l	105312	4	13.794	1045640	50.0
Benzene, 1-ethe...	13.994	10.8	ug/l	225992	4	13.794	1045640	50.0
Benzene, 1-ethe...	15.053	10.6	ug/l	221949	4	13.794	1045640	50.0
Naphthalene, 1,...	15.211	7.4	ug/l	155688	4	13.794	1045640	50.0
Naphthalene, 1,...	16.170	7.7	ug/l	161308	4	13.794	1045640	50.0
2-Propyn-1-ol, ...	16.511	5.2	ug/l	109224	4	13.794	1045640	50.0