LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084983.D
Acq On : 20 Nov 2024 20:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-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\82N103024W.M
Title : SW846 8260

Signal : TIC: VN084983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	50	58	67	rBV3	15989	35382	3.55%	0.335%
2	2.883	150	158	159	rBV6	7444	14585	1.46%	0.138%
3	4.124	358	369	376	rBV4	3785	10443	1.05%	0.099%
4	8.165	1046	1056	1060	rBV	122408	291777	29.25%	2.766%
5	8.218	1060	1065	1079	rVB	216916	482020	48.31%	4.570%
6	8.577	1113	1126	1134	rBV	137138	321047	32.18%	3.044%
7	8.741	1134	1154	1175	rVB4	52860	404988	40.59%	3.839%
8	9.100	1206	1215	1223	rBV	318587	661877	66.34%	6.275%
9	9.177	1223	1228	1234	rVB5	6424	13288	1.33%	0.126%
10	10.153	1387	1394	1397	rVB2	6331	11908	1.19%	0.113%
11	10.565	1455	1464	1470	rBV	473299	855439	85.74%	8.110%
12	10.630	1470	1475	1486	rVB	221786	406737	40.77%	3.856%
13	11.865	1677	1685	1694	rBV	435372	763125	76.49%	7.235%
14	11.959	1694	1701	1709	rVB	94837	161505	16.19%	1.531%
15	12.065	1711	1719	1730	rBV	374456	703877	70.55%	6.673%
16	12.400	1768	1776	1783	rBV	187006	329656	33.04%	3.125%
17	12.694	1819	1826	1832	rBV	32960	53190	5.33%	0.504%
18	12.847	1842	1852	1862	rBV	369676	623583	62.50%	5.912%
19	13.035	1878	1884	1889	rVV	63507	101022	10.13%	0.958%
20	13.094	1889	1894	1898	rVV	230368	389949	39.09%	3.697%
21	13.129	1898	1900	1903	rVV	101131	128542	12.88%	1.219%
22	13.171	1903	1907	1913	rVV	146425	236610	23.72%	2.243%
23	13.335	1926	1935	1944	rBV	98960	159918	16.03%	1.516%
24	13.482	1953	1960	1967	rVB	544287	837477	83.94%	7.940%
25	13.606	1975	1981	1988	rBV4	10730	26899	2.70%	0.255%
26	13.671	1988	1992	1997	rVV2	12062	16423	1.65%	0.156%
27	13.729	1997	2002	2006	rVV3	10215	16152	1.62%	0.153%
28	13.788	2006	2012	2030	rVB2	459395	997672	100.00%	9.458%
29	13.988	2040	2046	2049	rBV2	89497	172996	17.34%	1.640%
30	14.112	2062	2067	2072	rVB4	7366	12172	1.22%	0.115%
31	14.182	2072	2079	2084	rBV	25514	40171	4.03%	0.381%
32	14.241	2084	2089	2092	rVV	51555	88424	8.86%	0.838%
33	14.270	2092	2094	2099	rVV2	49687	70856	7.10%	0.672%
34	14.329	2099	2104	2110	rVB	91658	143630	14.40%	1.362%
35	14.400	2110	2116	2118	rBV	6743	11732	1.18%	0.111%
36	14.441	2118	2123	2132	rVB3	29060	56654	5.68%	0.537%

LSC Area Percent Report

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Acq On : 20 Nov 2024 20:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-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\82N103024W.M
Title : SW846 8260

37	14.570	2140	2145	2151	rVB2	18912	31064	3.11%	0.295%
38	14.653	2151	2159	2162	rBV	59576	96853	9.71%	0.918%
39	14.694	2162	2166	2170	rVV	91386	147129	14.75%	1.395%
40	14.729	2170	2172	2177	rVV3	15570	24581	2.46%	0.233%
41	14.776	2177	2180	2181	rVV	10061	11745	1.18%	0.111%
42	14.806	2181	2185	2193	rVV4	13175	23272	2.33%	0.221%
43	14.876	2193	2197	2201	rVV4	8281	12999	1.30%	0.123%
44	14.923	2201	2205	2210	rVV	34811	66301	6.65%	0.629%
45	14.965	2210	2212	2217	rVV2	11422	14554	1.46%	0.138%
46	15.047	2217	2226	2232	rVV3	64498	186071	18.65%	1.764%
47	15.100	2232	2235	2245	rVB6	9091	21516	2.16%	0.204%
48	15.212	2249	2254	2260	rBV6	6904	14144	1.42%	0.134%
49	15.323	2266	2273	2281	rBV3	17239	41576	4.17%	0.394%
50	15.435	2287	2292	2299	rVB6	13232	28988	2.91%	0.275%
51	15.641	2320	2327	2334	rBV	59867	117779	11.81%	1.117%
52	15.759	2341	2347	2350	rBV6	6683	13072	1.31%	0.124%
53	15.947	2372	2379	2388	rBV3	6850	14976	1.50%	0.142%
54	16.782	2513	2521	2522	rBV2	18032	29669	2.97%	0.281%

Sum of corrected areas: 10548015

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Instrument :
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ClientSampleId :
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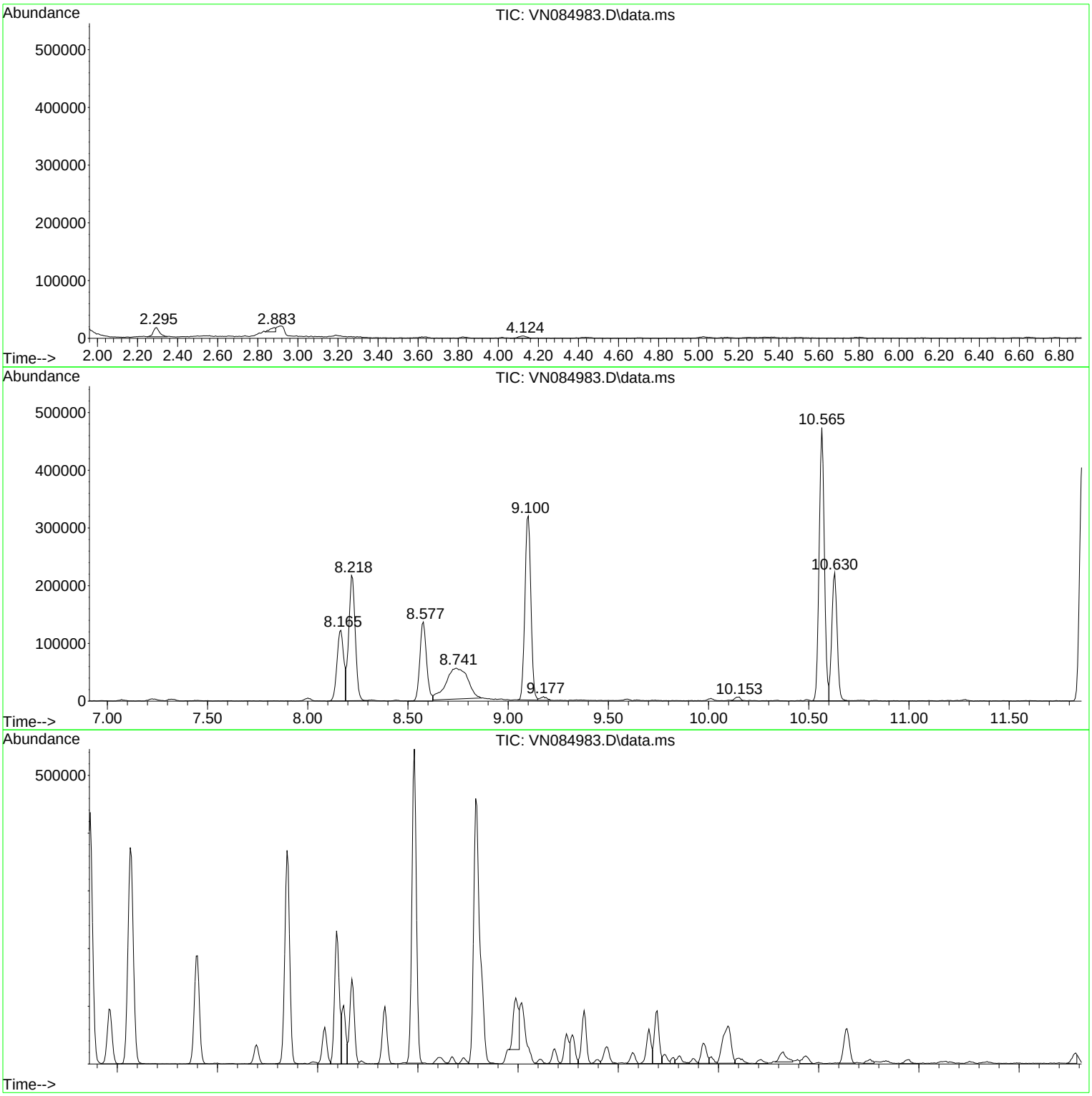
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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Data File : VN084983.D
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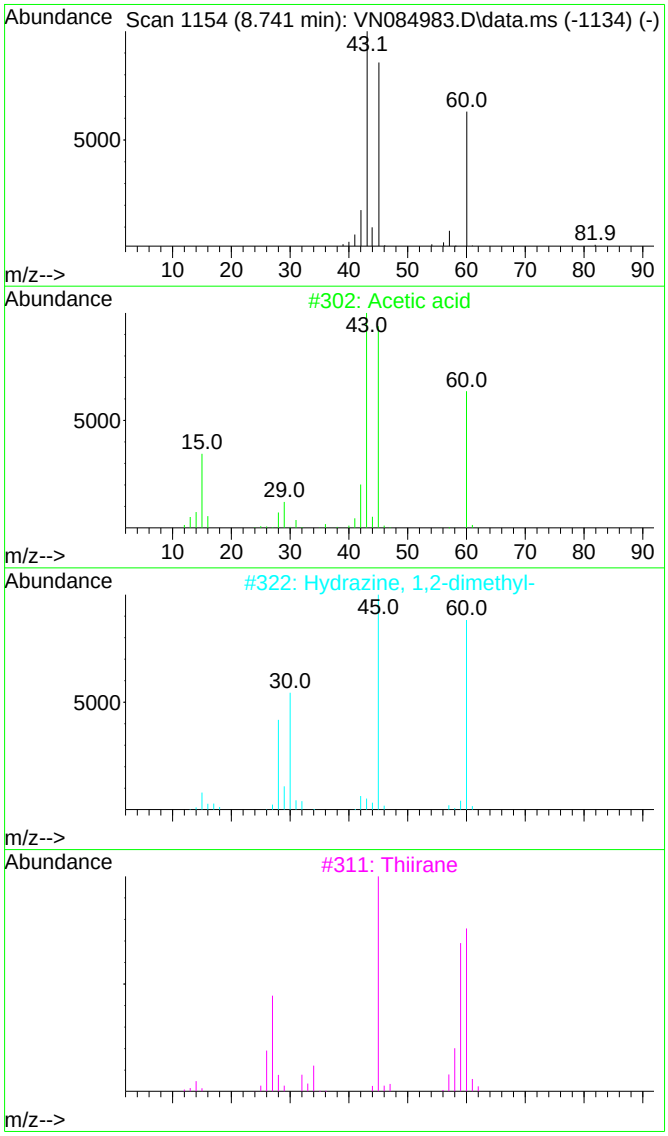
Quant Title : SW846 8260

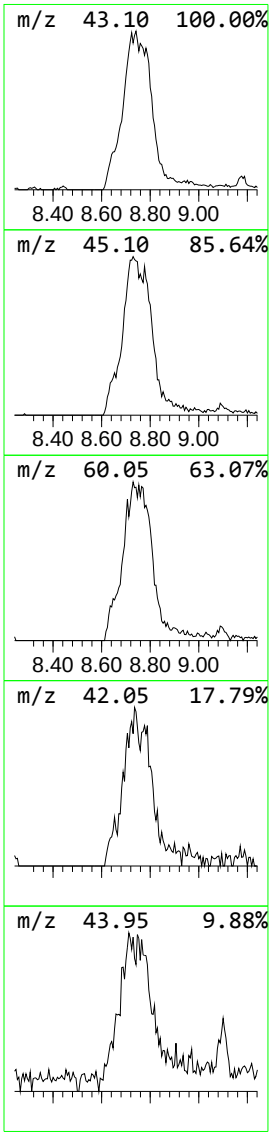
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.741	30.59 ug/l	404988	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	64
3	Thiirane	60	C2H4S	000420-12-2	38
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9





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Instrument :
MSVOA_N
ClientSampleId :
MW-1

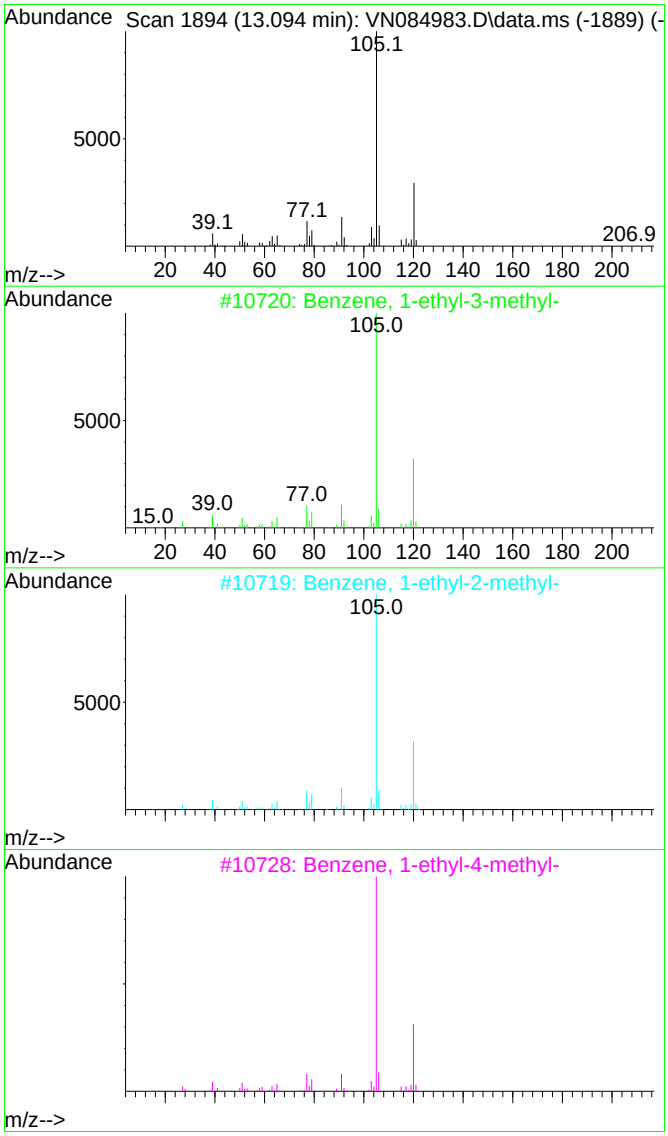
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

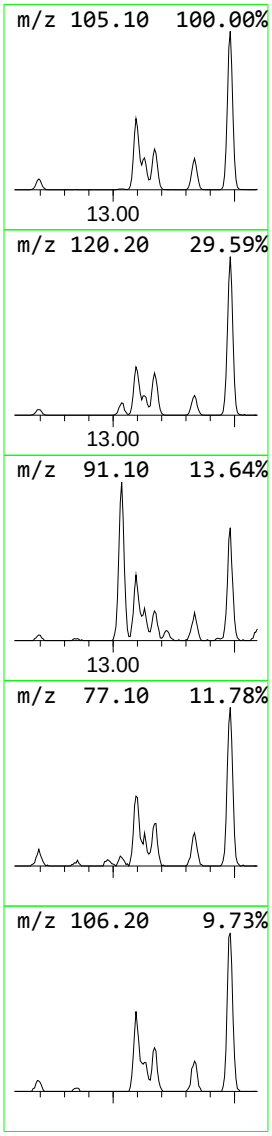
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	19.54 ug/l	389949	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

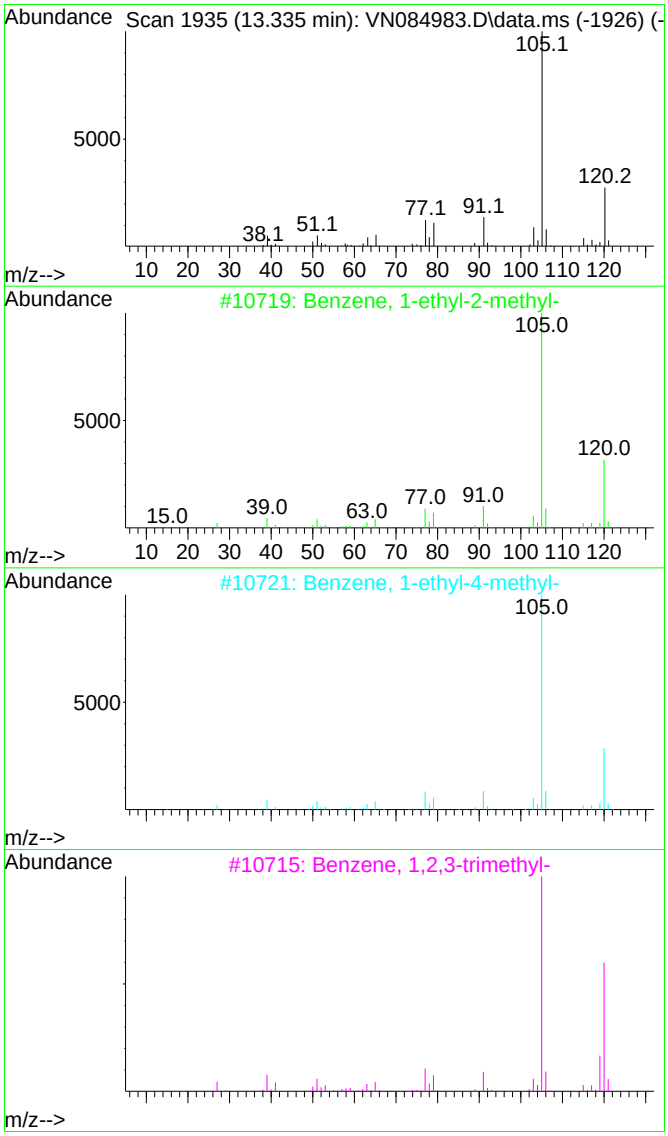
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

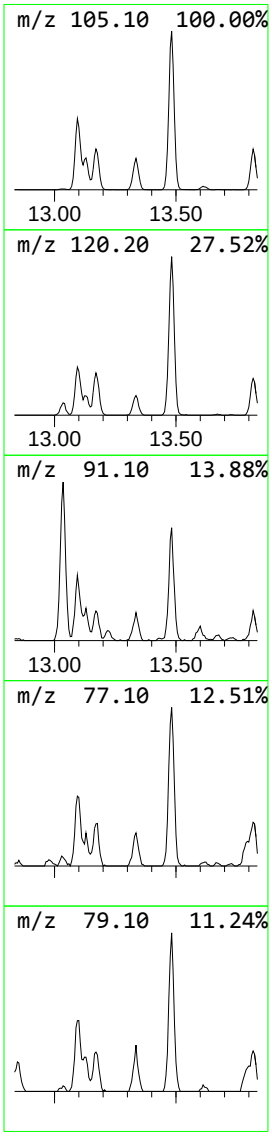
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	8.01 ug/l	159918	1,4-Dichlorobenzene-d4	13.788

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-4-methyl-	120	C9H12	000622-96-8	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

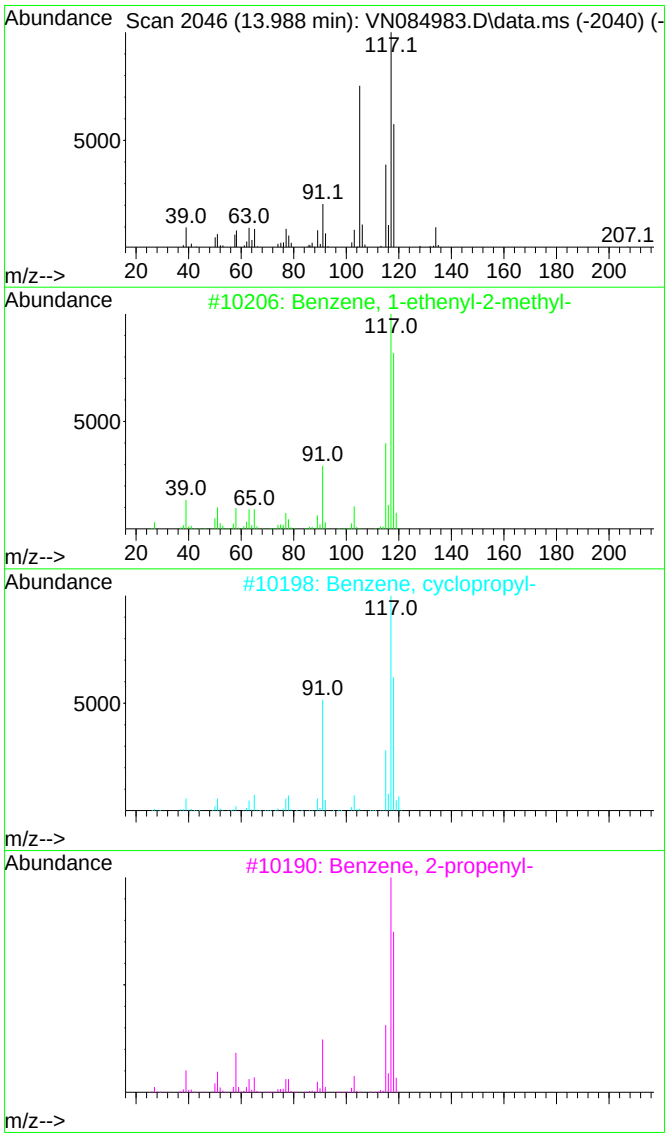
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

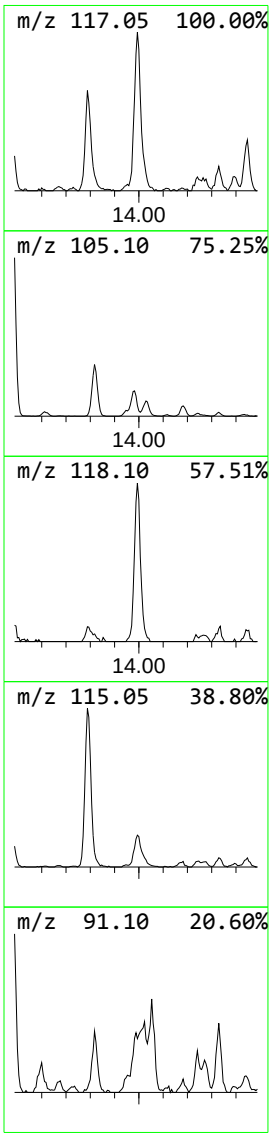
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	8.67 ug/l	172996	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4	Indane	118	C9H10	000496-11-7	60
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	60





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Instrument :
MSVOA_N
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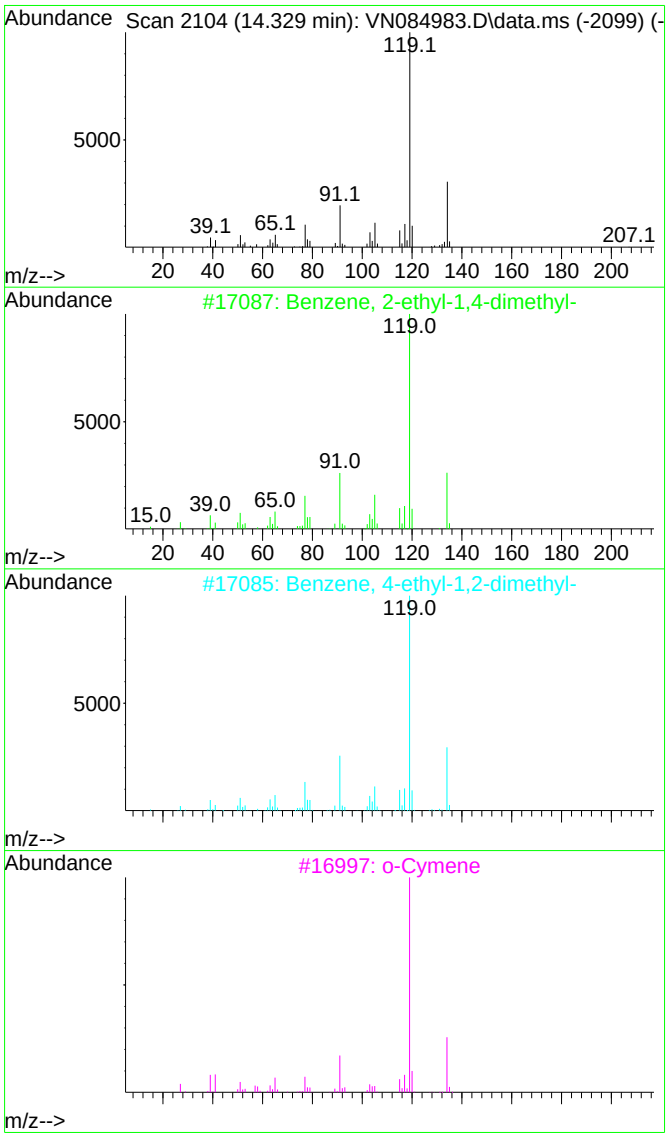
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

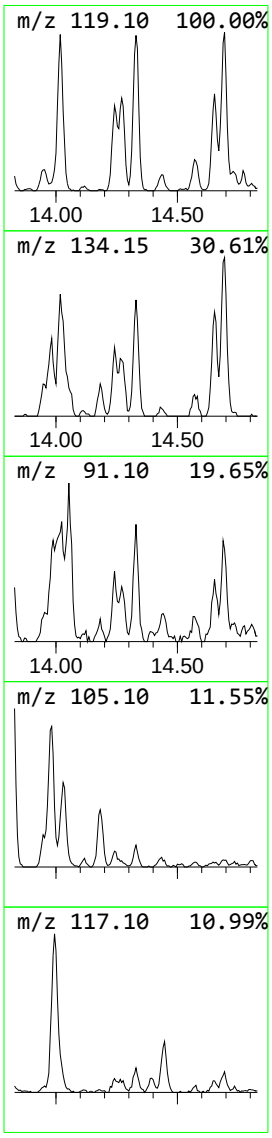
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	7.20 ug/l	143630	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





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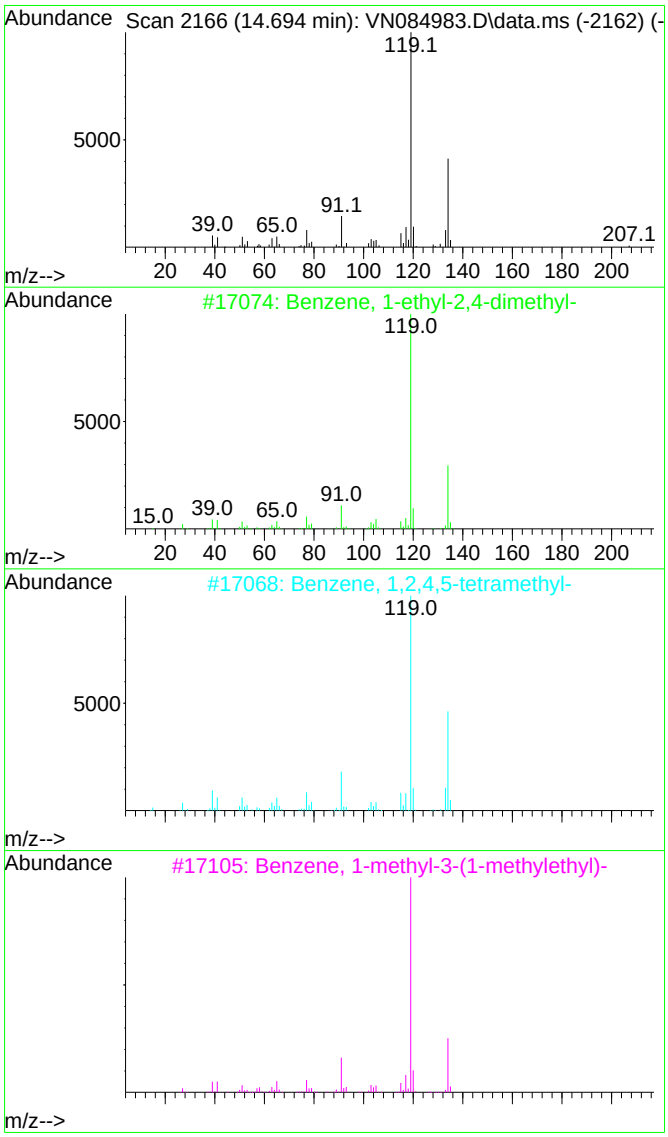
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

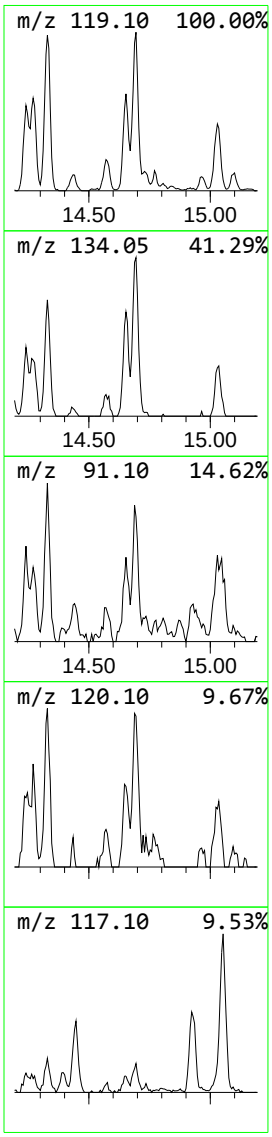
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	7.37 ug/l	147129	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91





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MSVOA_N
ClientSampleId :
MW-1

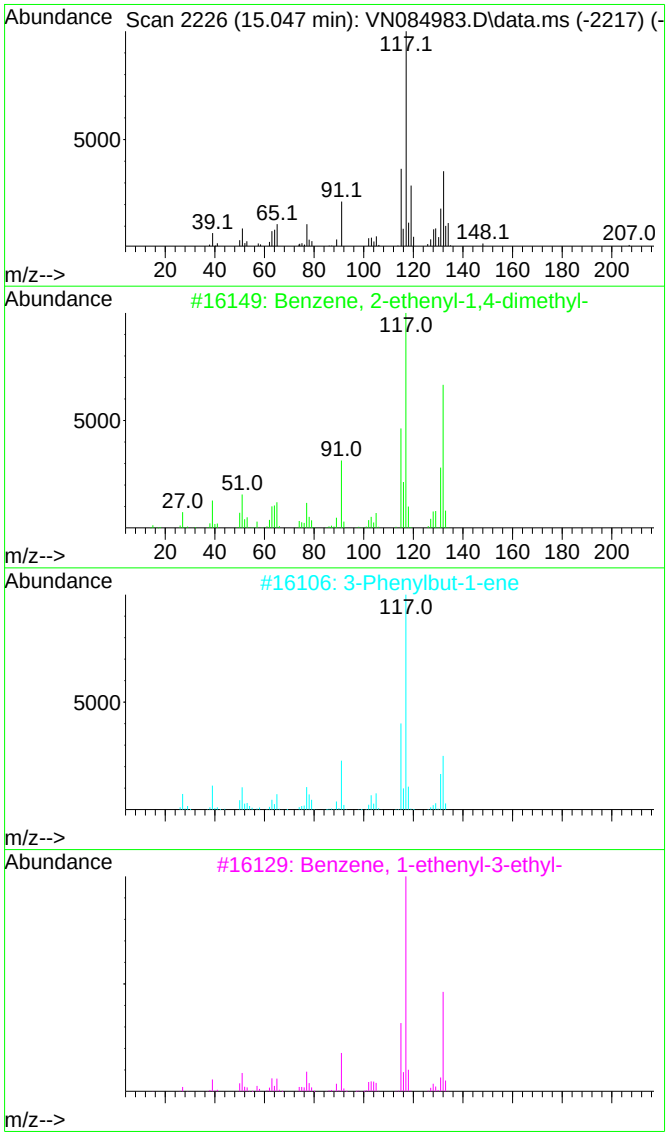
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

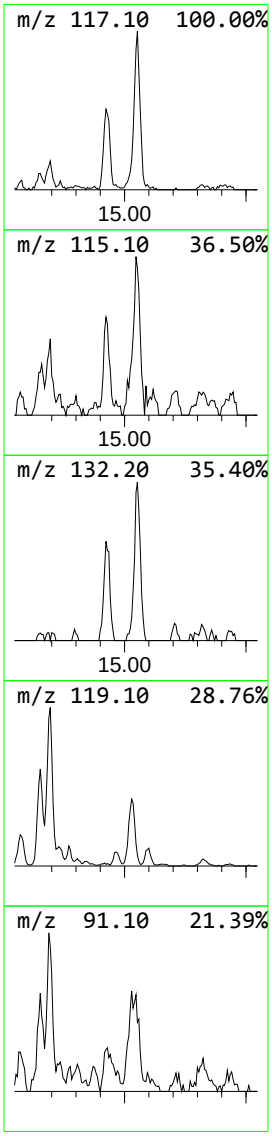
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	9.33 ug/l	186071	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	89
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	68





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
Acetic acid	8.741	30.6	ug/l	404988	2	9.100	661877	50.0
Benzene, 1-ethy...	13.094	19.5	ug/l	389949	4	13.788	997672	50.0
Benzene, 1-ethy...	13.335	8.0	ug/l	159918	4	13.788	997672	50.0
Benzene, 1-ethe...	13.988	8.7	ug/l	172996	4	13.788	997672	50.0
Benzene, 2-ethy...	14.329	7.2	ug/l	143630	4	13.788	997672	50.0
Benzene, 1-ethy...	14.694	7.4	ug/l	147129	4	13.788	997672	50.0
Benzene, 2-ethe...	15.047	9.3	ug/l	186071	4	13.788	997672	50.0