LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

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\82N112224W.M
Title : SW846 8260

Signal : TIC: VN085200.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.318	52	62	76	rBV	176360	548459	2.96%	0.532%
2	8.165	1043	1056	1060	rBV	118514	280855	1.51%	0.273%
3	8.224	1060	1066	1079	rVB	205463	465421	2.51%	0.452%
4	8.577	1117	1126	1137	rBV2	131742	351201	1.89%	0.341%
5	9.100	1206	1215	1230	rBV	311932	629332	3.39%	0.611%
6	9.600	1288	1300	1315	rVB	169518	390928	2.11%	0.379%
7	10.565	1454	1464	1471	rBV	518803	1038668	5.60%	1.008%
8	10.994	1529	1537	1547	rBV5	78495	226887	1.22%	0.220%
9	11.865	1678	1685	1691	rBV	458950	828282	4.47%	0.804%
10	11.959	1694	1701	1712	rVV	3596214	6074471	32.75%	5.895%
11	12.071	1712	1720	1738	rVB	177791	424444	2.29%	0.412%
12	12.394	1765	1775	1784	rBV	186927	368889	1.99%	0.358%
13	12.694	1818	1826	1842	rVB	1125690	1878773	10.13%	1.823%
14	12.847	1842	1852	1863	rVB	365435	636059	3.43%	0.617%
15	13.029	1875	1883	1890	rBV	1235832	2031132	10.95%	1.971%
16	13.129	1890	1900	1903	rVV	499559	856465	4.62%	0.831%
17	13.170	1903	1907	1913	rVB	497757	771404	4.16%	0.749%
18	13.335	1927	1935	1943	rBV	1902300	3185359	17.17%	3.092%
19	13.476	1947	1959	1966	rBV	4112011	6919542	37.30%	6.716%
20	13.600	1973	1980	1987	rBV3	76688	186778	1.01%	0.181%
21	13.670	1987	1992	1997	rBV	273715	427809	2.31%	0.415%
22	13.729	1997	2002	2007	rVB2	168776	272543	1.47%	0.265%
23	13.817	2007	2017	2022	rBV2	2180051	4279145	23.07%	4.153%
24	13.947	2032	2039	2041	rBV	804239	1197622	6.46%	1.162%
25	13.994	2041	2047	2059	rVB	6533799	11886094	64.08%	11.536%
26	14.176	2072	2078	2083	rVB2	219492	362776	1.96%	0.352%
27	14.241	2083	2089	2092	rBV	465881	823843	4.44%	0.800%
28	14.323	2098	2103	2110	rVB	666662	1098593	5.92%	1.066%
29	14.394	2110	2115	2117	rBV	179222	272370	1.47%	0.264%
30	14.441	2117	2123	2134	rVB	3213575	5724870	30.86%	5.556%
31	14.570	2138	2145	2150	rBV	296344	462824	2.50%	0.449%
32	14.653	2150	2159	2161	rBV	493357	821527	4.43%	0.797%
33	14.688	2161	2165	2170	rVV	1120317	1745653	9.41%	1.694%
34	14.794	2177	2183	2194	rVB2	206405	513995	2.77%	0.499%
35	14.923	2198	2205	2216	rVB	2127308	3536096	19.06%	3.432%
36	15.035	2216	2224	2232	rBV2	1882837	4446075	23.97%	4.315%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

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\82N112224W.M
Title : SW846 8260

37	15.112	2232	2237	2245	rVB	1575152	2741538	14.78%	2.661%
38	15.200	2245	2252	2261	rVB	4093047	7461109	40.22%	7.241%
39	15.306	2261	2270	2277	rBV2	684299	1478652	7.97%	1.435%
40	15.441	2285	2293	2301	rVB3	200284	504320	2.72%	0.489%
41	15.564	2304	2314	2318	rVV6	95248	284723	1.53%	0.276%
42	15.635	2318	2326	2339	rVV	9560925	18549287	100.00%	18.003%
43	15.747	2339	2345	2362	rVB6	129820	442801	2.39%	0.430%
44	15.941	2370	2378	2381	rBV2	125364	269055	1.45%	0.261%
45	16.141	2405	2412	2417	rBV	283145	648470	3.50%	0.629%
46	16.194	2417	2421	2427	rVB2	191283	367768	1.98%	0.357%
47	16.276	2427	2435	2452	rVB2	427049	1540229	8.30%	1.495%
48	16.494	2465	2472	2478	rBV3	81625	202922	1.09%	0.197%
49	16.564	2478	2484	2500	rVB	186604	526587	2.84%	0.511%
50	16.776	2512	2520	2522	rBV	1095940	2053301	11.07%	1.993%

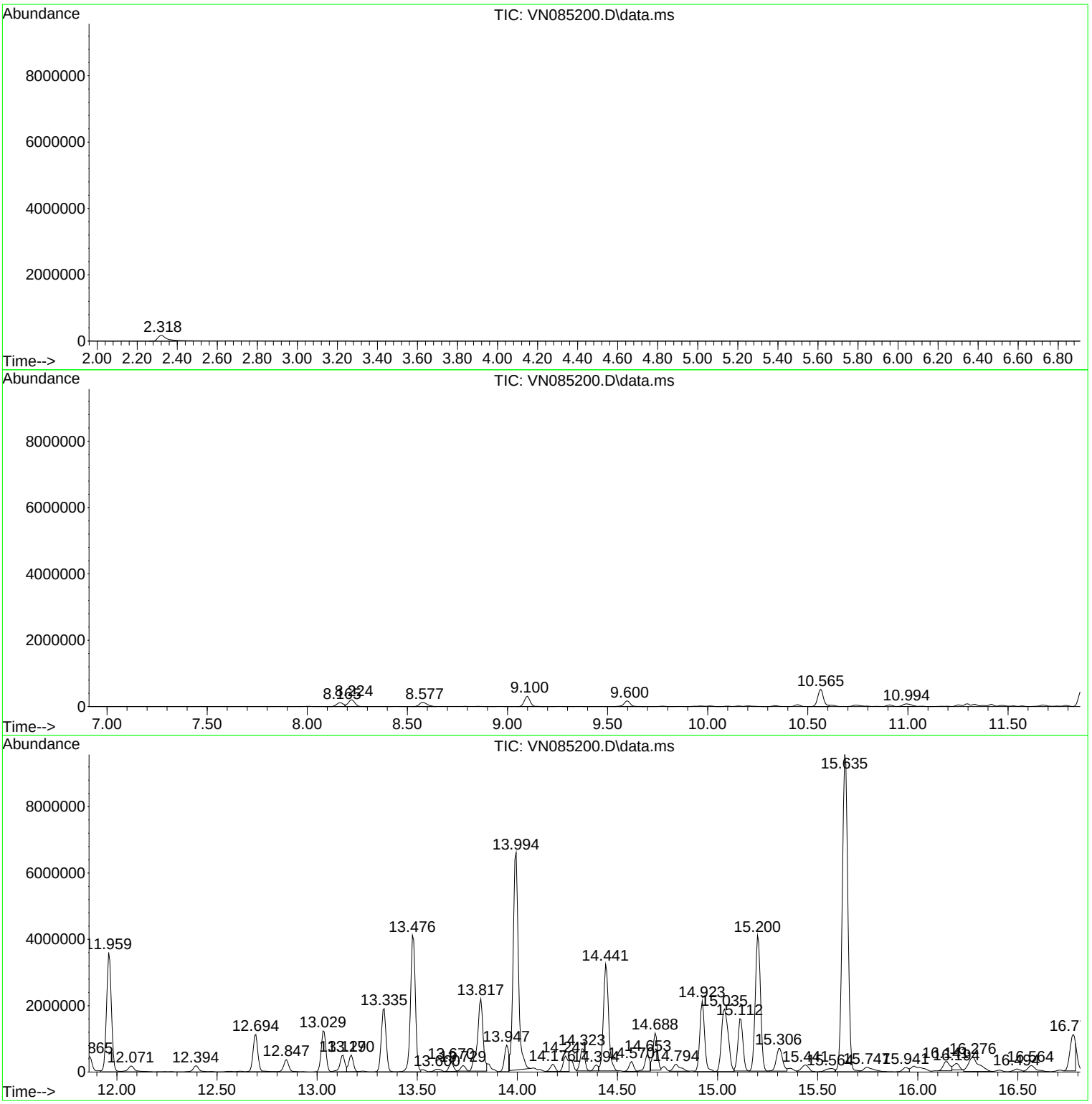
Sum of corrected areas: 103035946

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

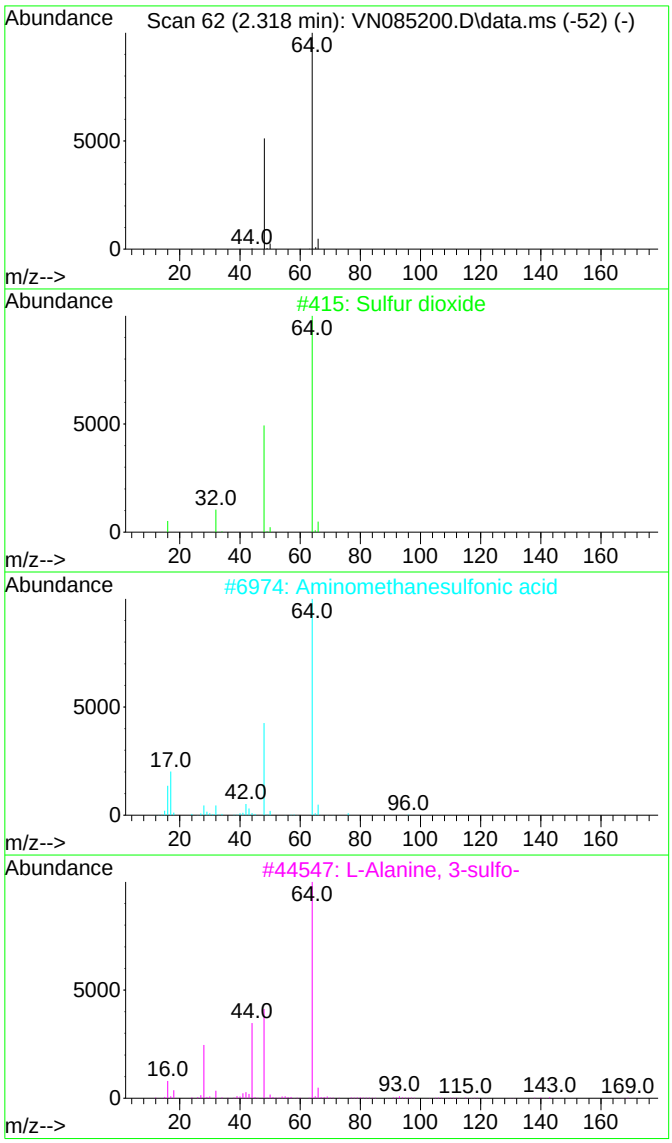
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

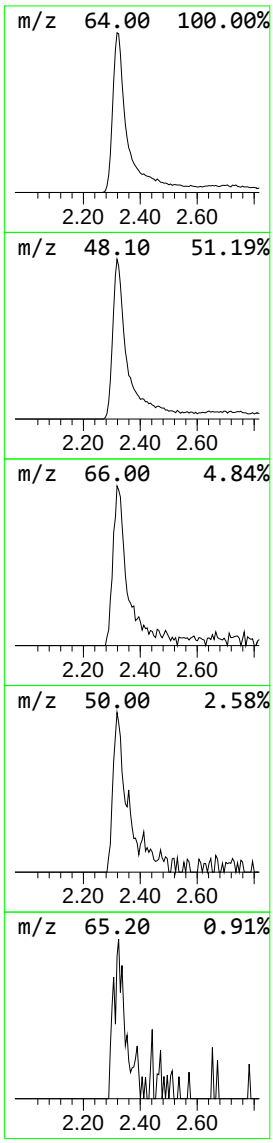
****

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.318	58.92 ug/l	548459	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

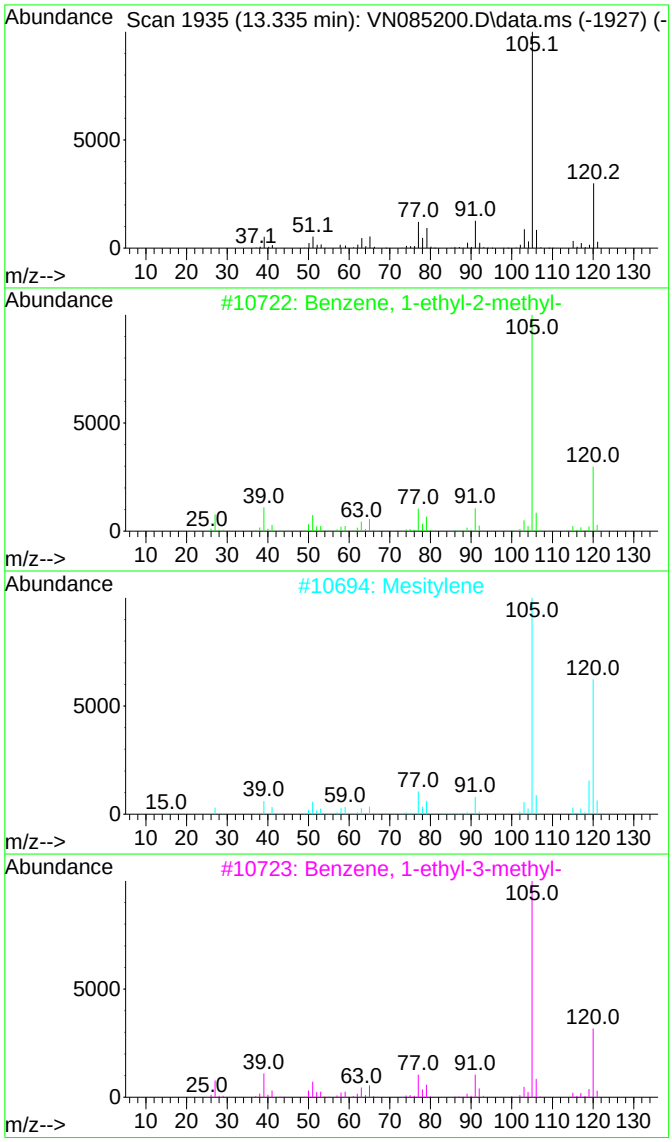
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

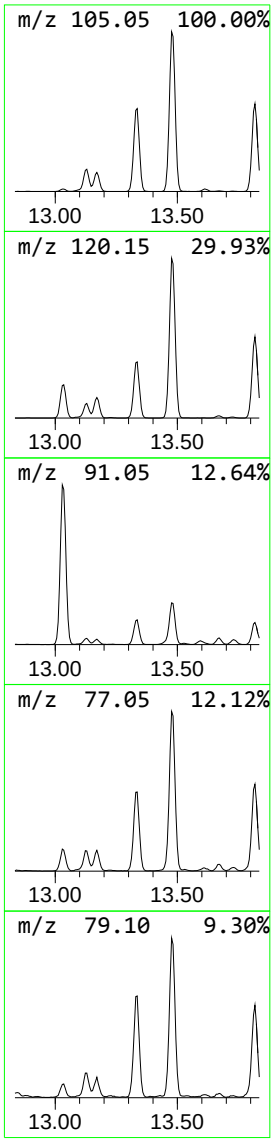
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	37.22 ug/l	3185360	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	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

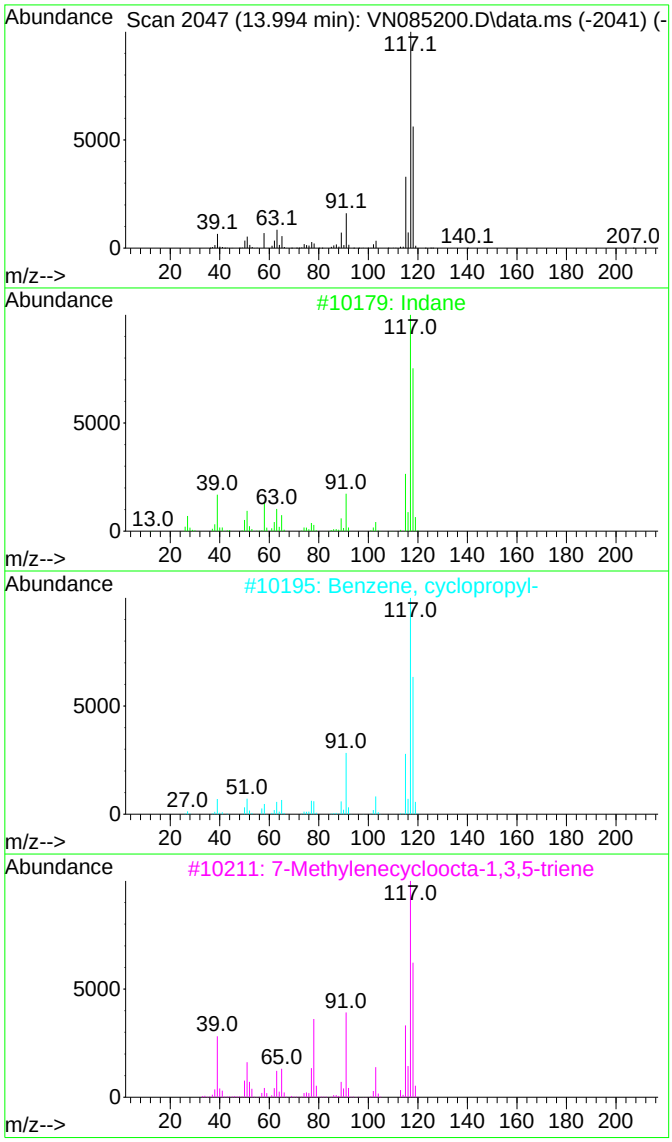
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

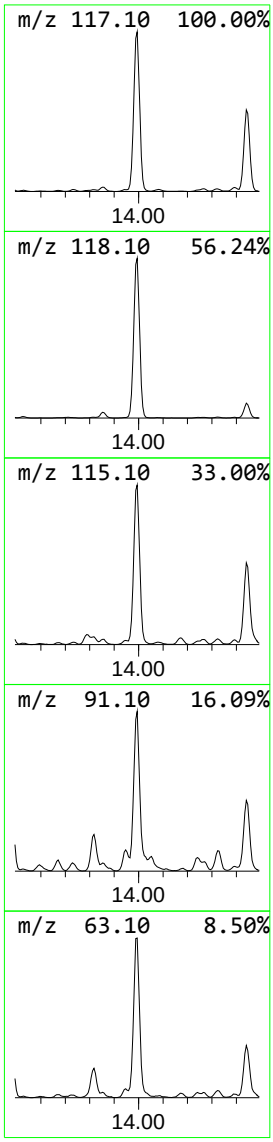
****

Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	138.88 ug/l	11886100	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
3	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	59
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

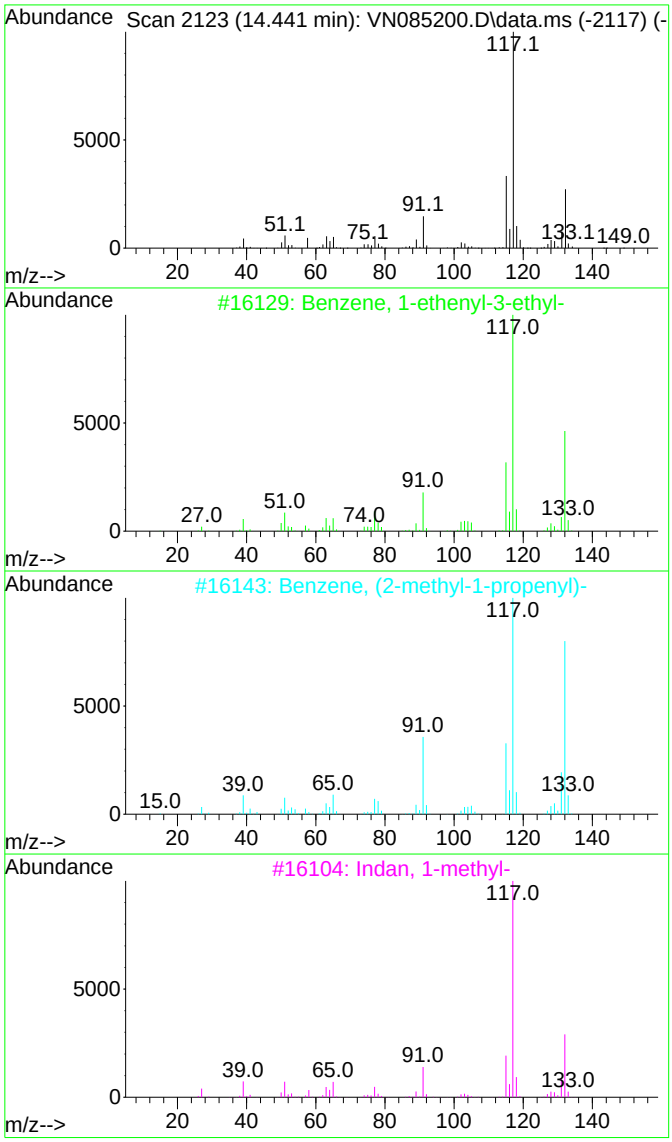
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

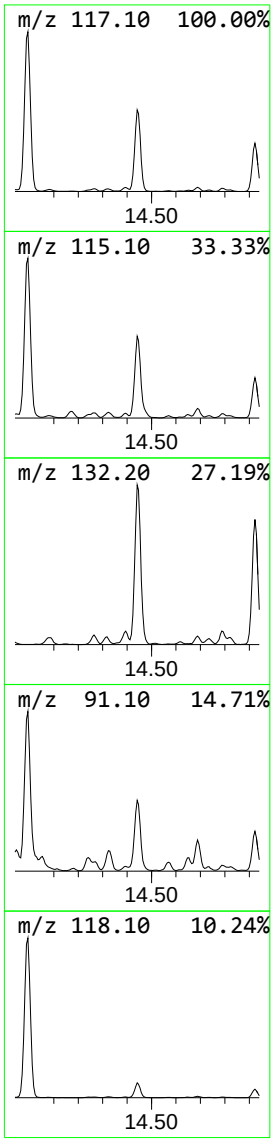
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.441	66.89 ug/l	5724870	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

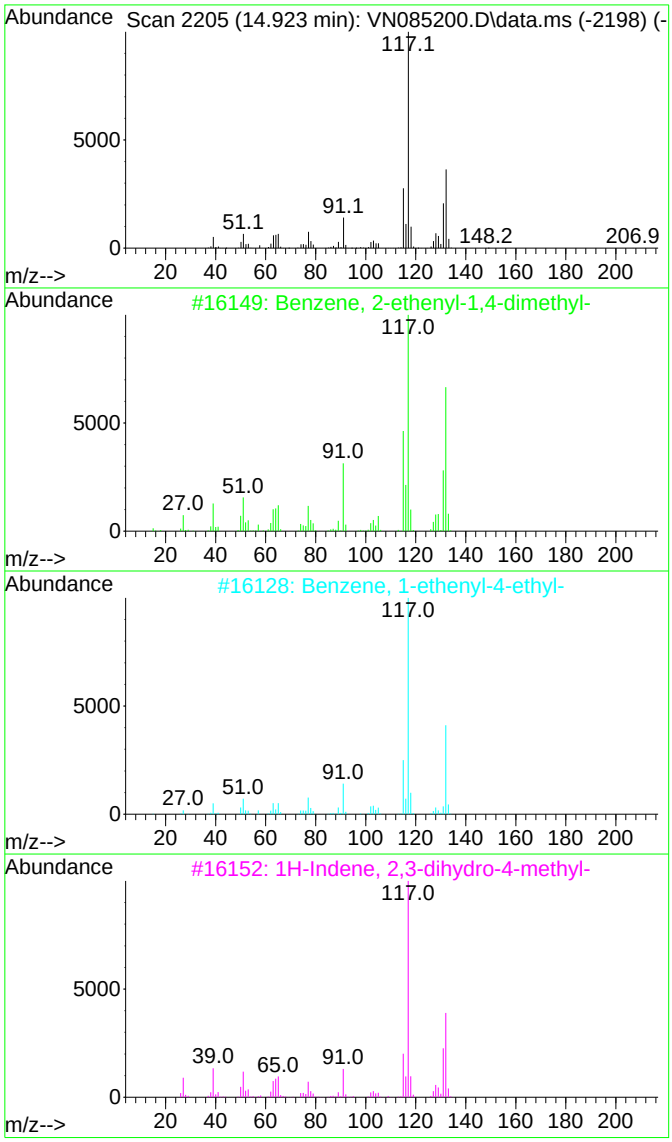
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

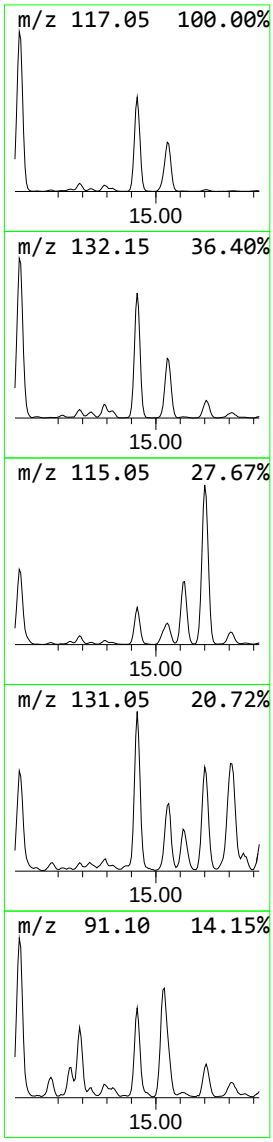
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.923	41.32 ug/l	3536100	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	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

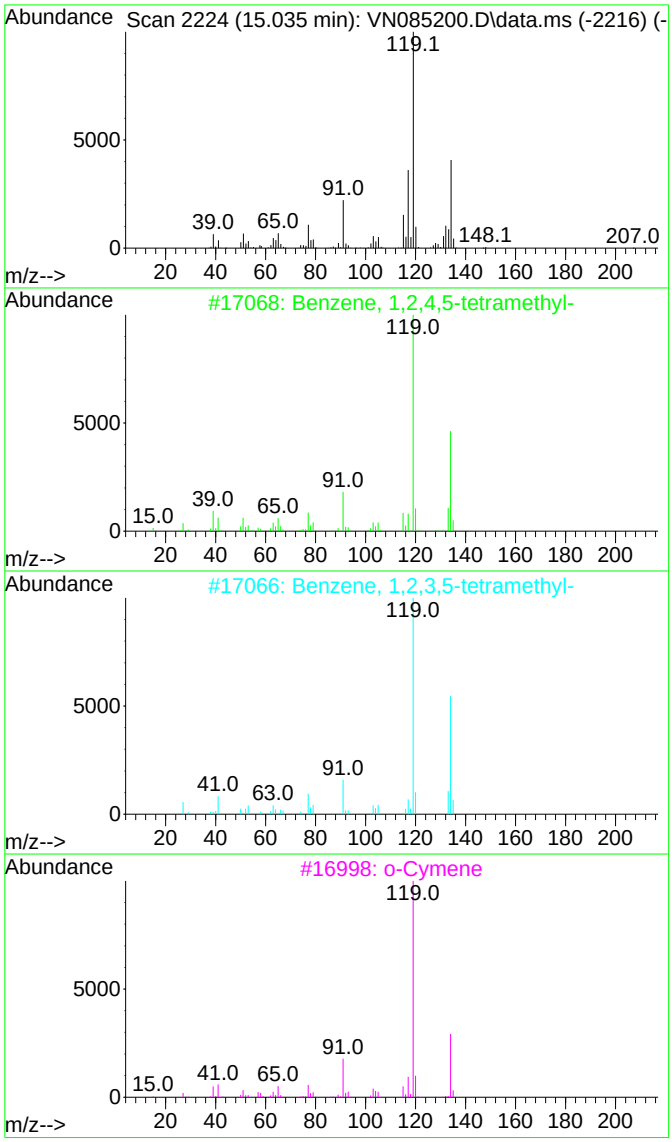
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

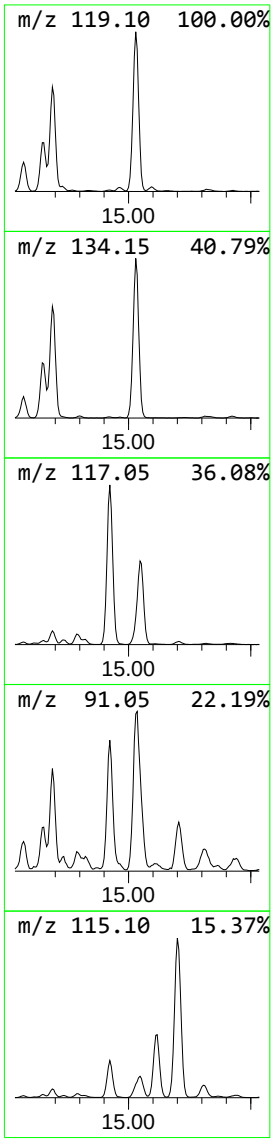
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	51.95 ug/l	4446080	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	90
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
3	o-Cymene	134	C10H14	000527-84-4	81
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	81
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

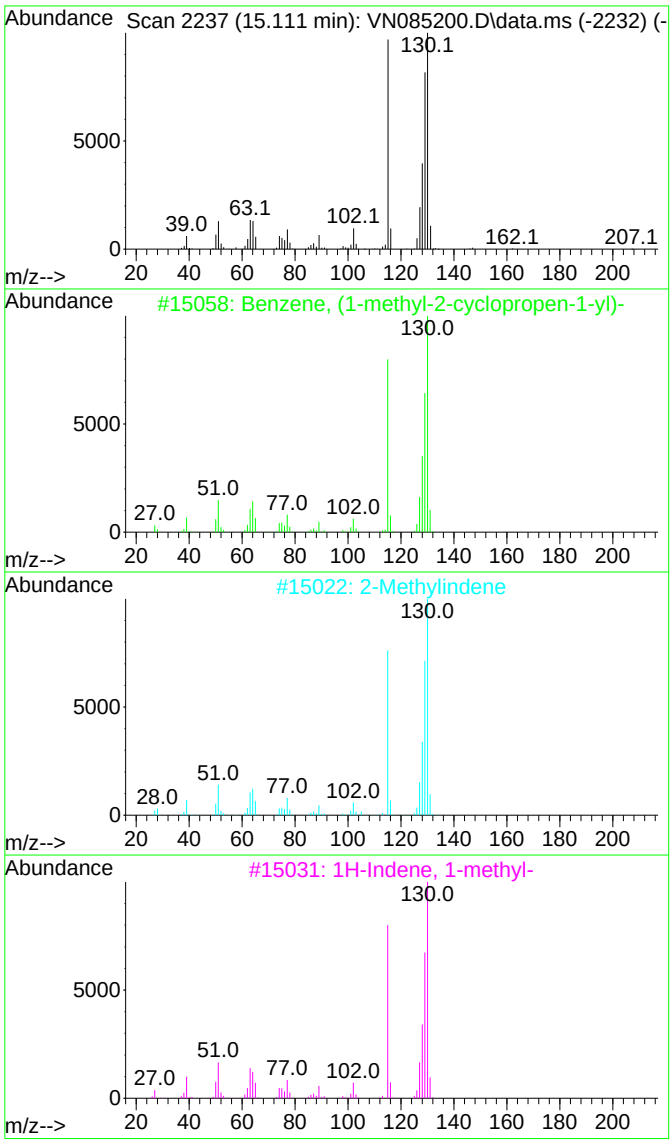
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

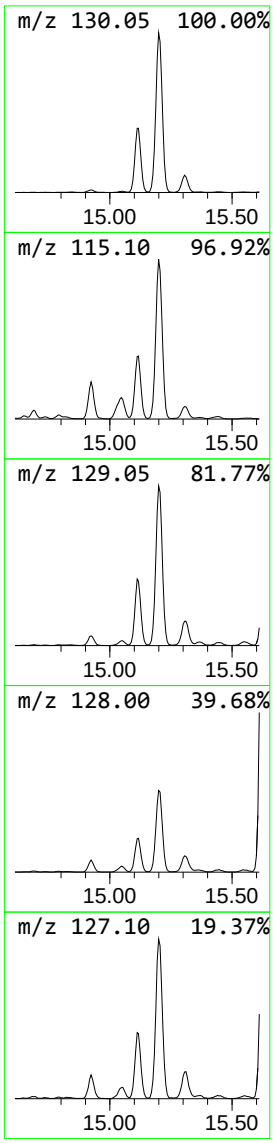
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (1-methyl-2-cyclop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.111	32.03 ug/l	2741540	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	97
2	2-Methylindene	130	C10H10	002177-47-1	97
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

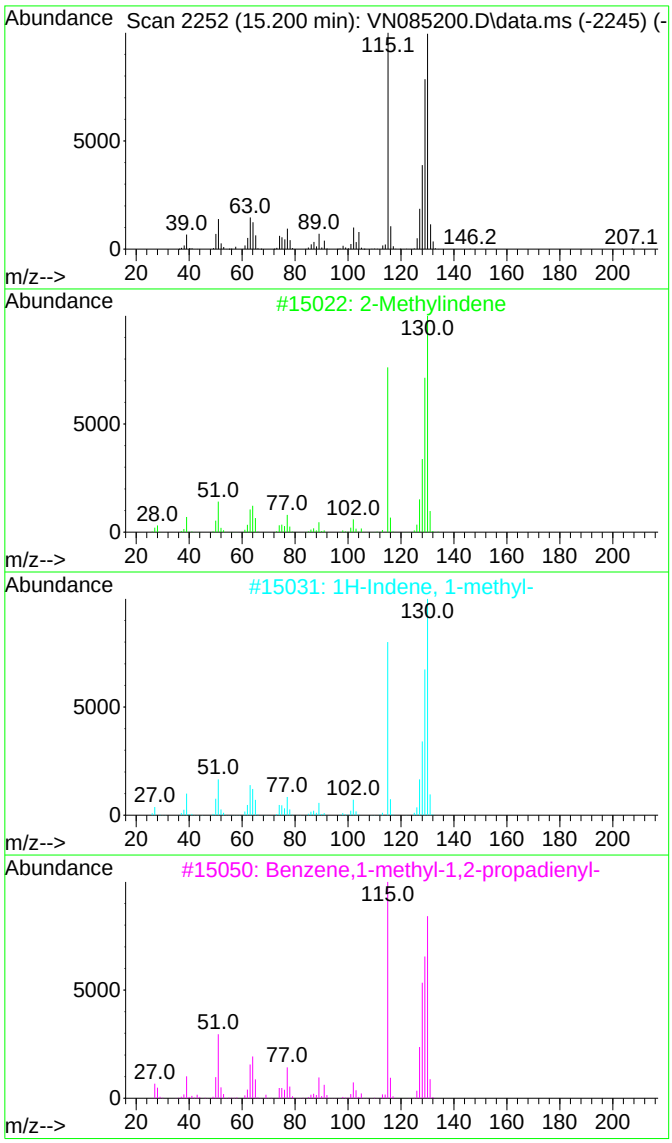
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

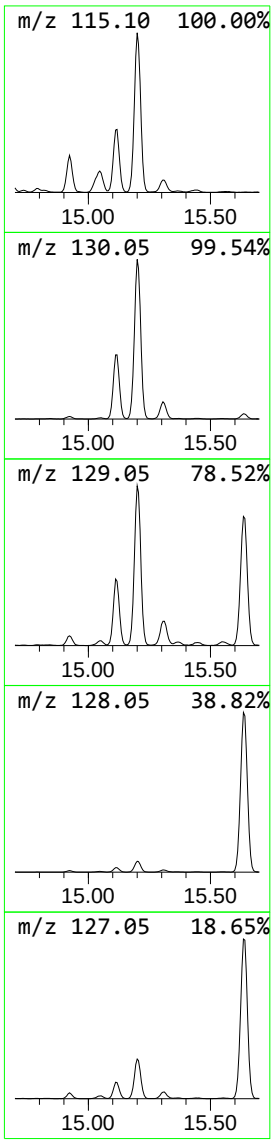
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Methylindene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.200	87.18 ug/l	7461110	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	97
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
4	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	95
5	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121324\
Data File : VN085200.D
Acq On : 13 Dec 2024 16:39
Operator : JC\MD
Sample : P5270-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW12-20241212

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.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
Sulfur dioxide	2.318	58.9	ug/l	548459	1	8.224	465421	50.0
Benzene, 1-ethy...	13.335	37.2	ug/l	3185360	4	13.788	4279150	50.0
Indane	13.994	138.9	ug/l	11886100	4	13.788	4279150	50.0
Benzene, 1-ethe...	14.441	66.9	ug/l	5724870	4	13.788	4279150	50.0
Benzene, 2-ethe...	14.923	41.3	ug/l	3536100	4	13.788	4279150	50.0
Benzene, 1,2,4,...	15.035	52.0	ug/l	4446080	4	13.788	4279150	50.0
Benzene, (1-met...	15.111	32.0	ug/l	2741540	4	13.788	4279150	50.0
2-Methylindene	15.200	87.2	ug/l	7461110	4	13.788	4279150	50.0