LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

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\82N033022W.M
Title : SW846 8260

Signal : TIC: VN071815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	61	rBV	341479	1401422	15.02%	2.586%
2	5.151	533	538	549	rVB3	32668	97232	1.04%	0.179%
3	5.622	605	618	630	rBV3	32863	112371	1.20%	0.207%
4	7.145	867	877	887	rBV3	65231	188107	2.02%	0.347%
5	8.022	1015	1026	1031	rBV	421542	1067867	11.45%	1.971%
6	8.086	1031	1037	1046	rVV	857996	1999910	21.44%	3.691%
7	8.175	1046	1052	1061	rVB5	55749	155814	1.67%	0.288%
8	8.298	1064	1073	1079	rBV2	46562	101719	1.09%	0.188%
9	8.433	1087	1096	1110	rBV	447369	1040371	11.15%	1.920%
10	8.575	1110	1120	1122	rVV3	42908	105330	1.13%	0.194%
11	8.622	1123	1128	1138	rVV4	70529	242416	2.60%	0.447%
12	8.963	1177	1186	1199	rBV	1279262	2716919	29.12%	5.014%
13	9.198	1219	1226	1230	rBV2	53645	111716	1.20%	0.206%
14	9.457	1256	1270	1277	rBV4	103336	305229	3.27%	0.563%
15	9.880	1336	1342	1351	rVB2	58802	115333	1.24%	0.213%
16	9.969	1351	1357	1360	rBV2	67363	126879	1.36%	0.234%
17	10.010	1360	1364	1372	rVB2	133677	270461	2.90%	0.499%
18	10.439	1429	1437	1443	rBV	1994111	3664582	39.28%	6.763%
19	10.504	1443	1448	1459	rVB	251733	472184	5.06%	0.871%
20	11.739	1650	1658	1668	rBV	1907473	3444989	36.93%	6.358%
21	11.839	1668	1675	1685	rVV	1929165	3289679	35.26%	6.071%
22	11.945	1685	1693	1706	rVB	5019372	9329646	100.00%	17.219%
23	12.274	1740	1749	1762	rBV	1118070	1902253	20.39%	3.511%
24	12.574	1793	1800	1808	rBV	1279720	2090972	22.41%	3.859%
25	12.727	1818	1826	1837	rBV	1472404	2527904	27.10%	4.665%
26	12.915	1851	1858	1863	rBV	550191	901567	9.66%	1.664%
27	12.980	1863	1869	1872	rVV	921980	1525361	16.35%	2.815%
28	13.010	1872	1874	1878	rVV	424020	628704	6.74%	1.160%
29	13.057	1878	1882	1890	rVB	684333	1066657	11.43%	1.969%
30	13.215	1902	1909	1920	rVB	454704	748374	8.02%	1.381%
31	13.363	1925	1934	1948	rVV	2922119	4677526	50.14%	8.633%
32	13.668	1979	1986	1989	rBV	1659388	2866726	30.73%	5.291%
33	13.833	2007	2014	2015	rBV	122194	150960	1.62%	0.279%
34	13.874	2015	2021	2037	rVB	1082855	2238188	23.99%	4.131%
35	14.062	2047	2053	2059	rBV2	94627	163963	1.76%	0.303%
36	14.127	2059	2064	2066	rVV	89918	144025	1.54%	0.266%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

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\82N033022W.M
Title : SW846 8260

37	14.157	2066	2069	2073	rVV2	81433	122714	1.32%	0.226%
38	14.215	2073	2079	2084	rVB	146821	232508	2.49%	0.429%
39	14.321	2092	2097	2105	rVB2	127505	219897	2.36%	0.406%
40	14.533	2126	2133	2136	rBV	165376	266159	2.85%	0.491%
41	14.574	2136	2140	2146	rVB	224785	349184	3.74%	0.644%
42	14.804	2174	2179	2185	rBV2	93246	154849	1.66%	0.286%
43	14.927	2191	2200	2206	rBV3	215730	433473	4.65%	0.800%
44	15.504	2290	2298	2309	rBV	211592	410905	4.40%	0.758%

Sum of corrected areas: 54183045

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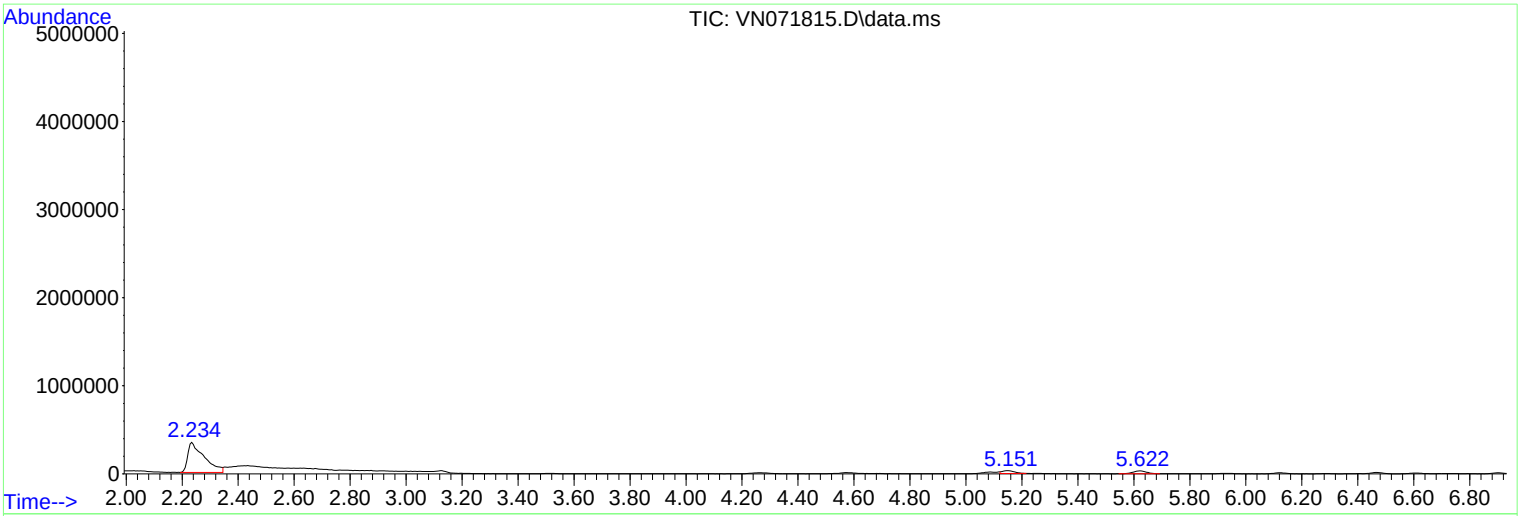
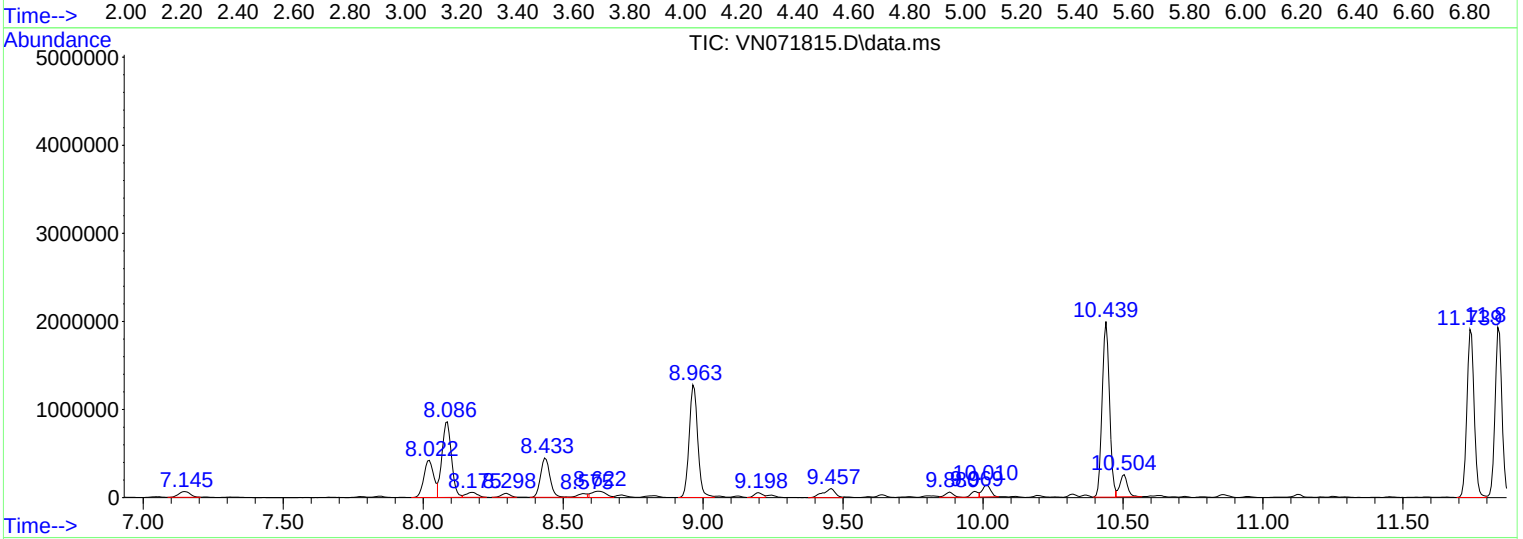
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

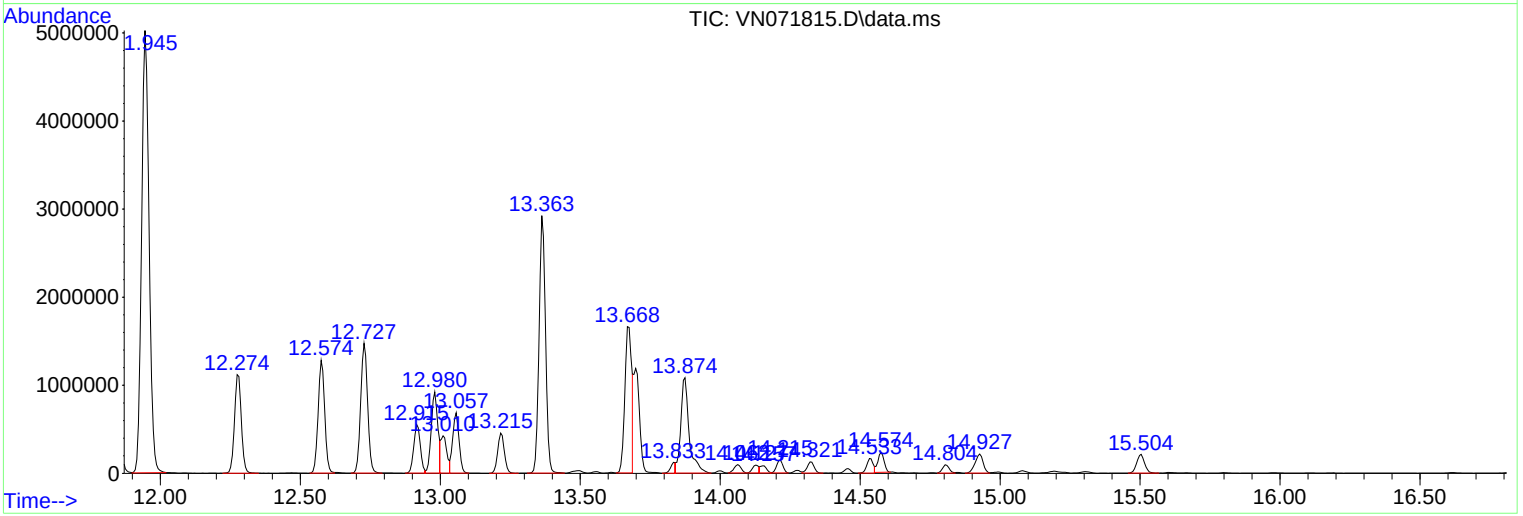
Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

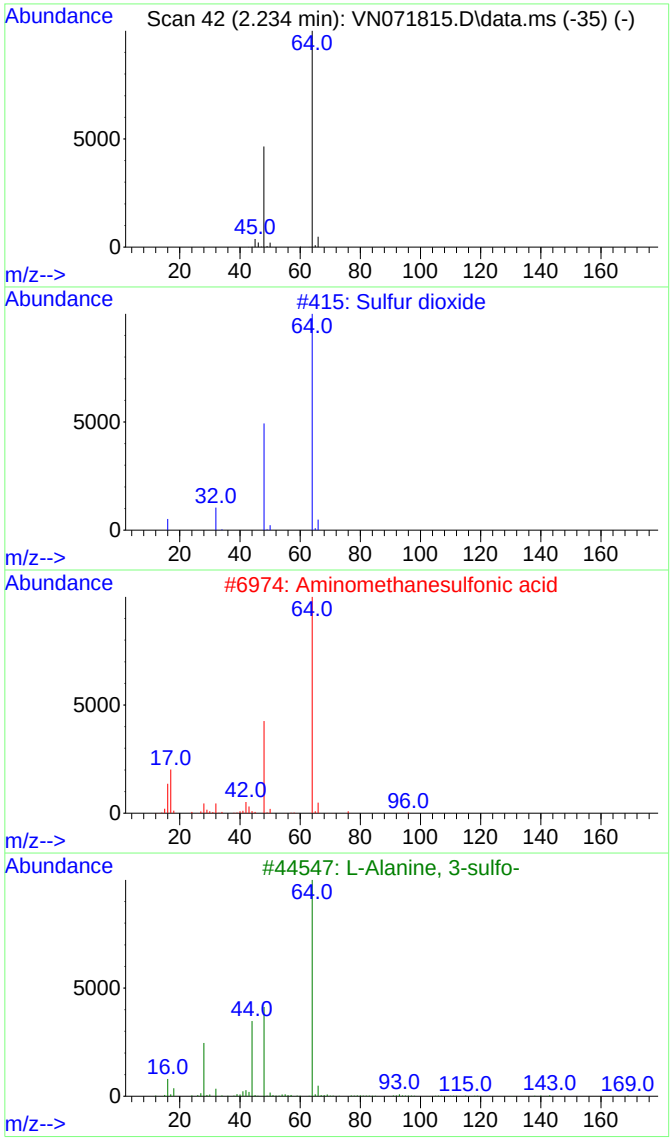
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

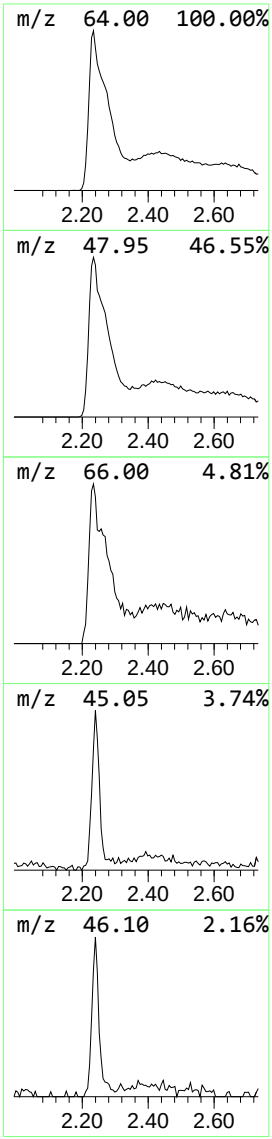
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	35.04 ug/l	1401420	Pentafluorobenzene	8.086

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	7
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071815.D
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Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

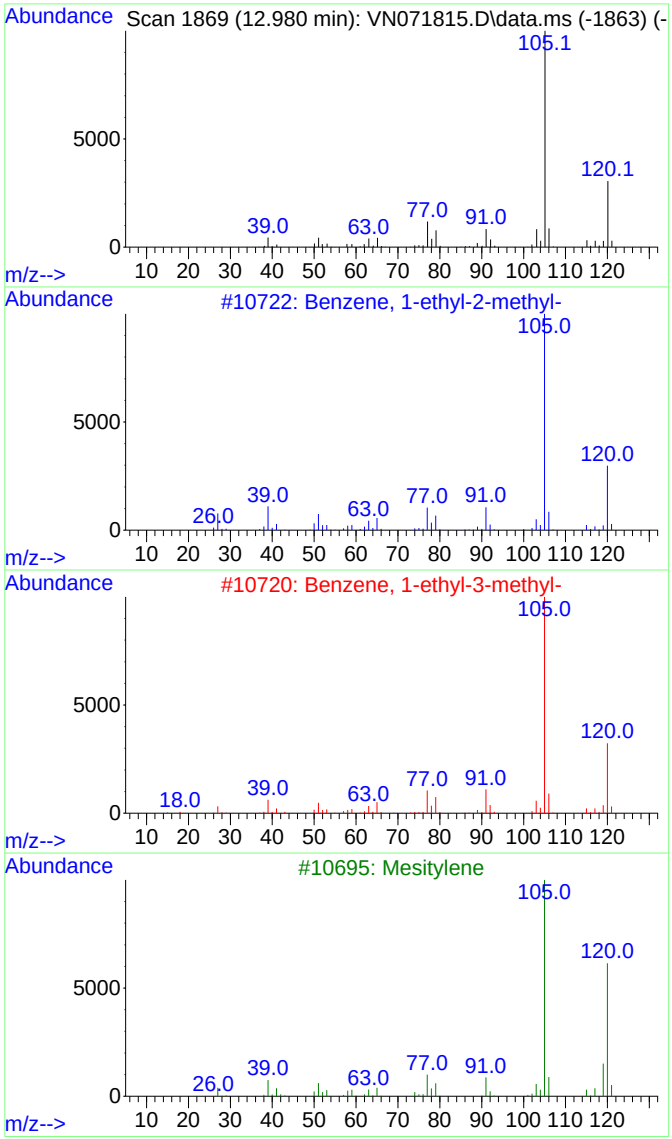
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

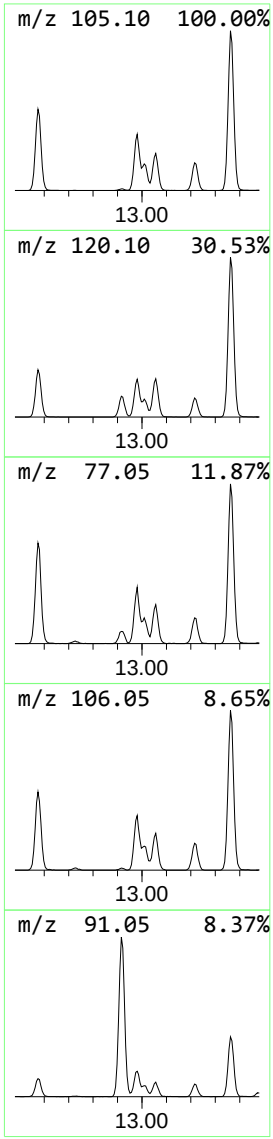
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	26.60 ug/l	1525360	1,4-Dichlorobenzene-d4	13.668

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	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040222\
Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

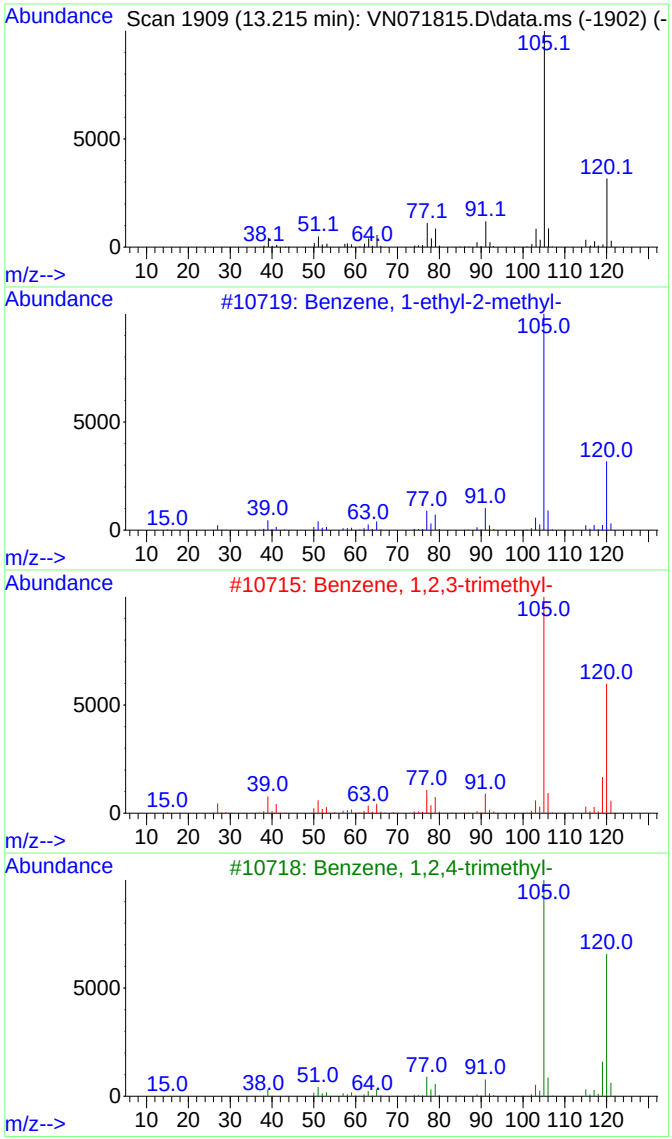
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

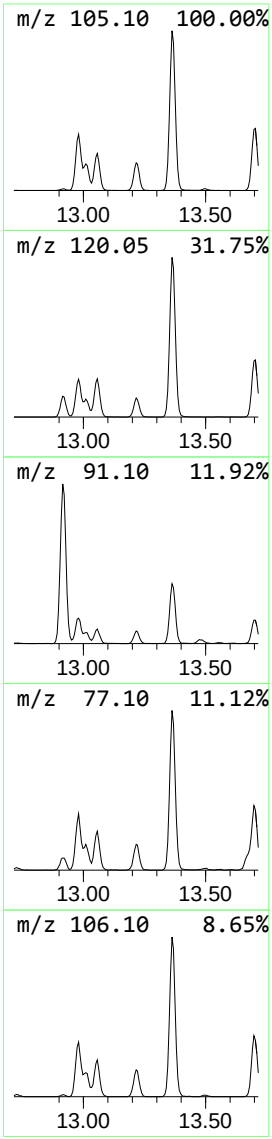
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	13.05 ug/l	748374	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
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\VN040222\
Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

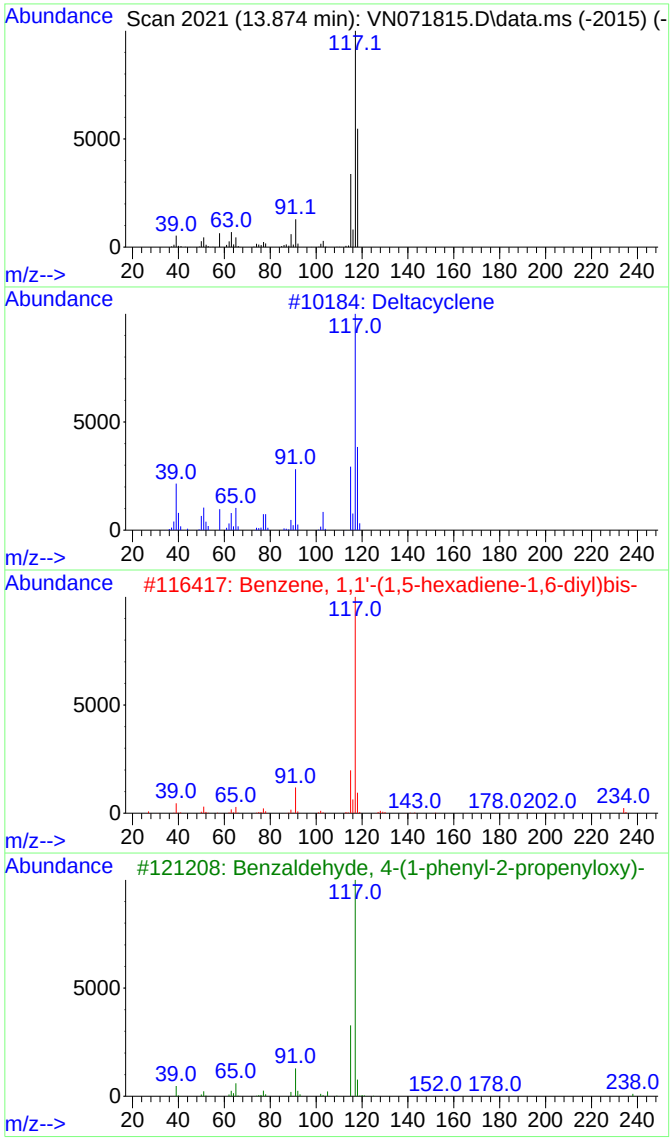
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

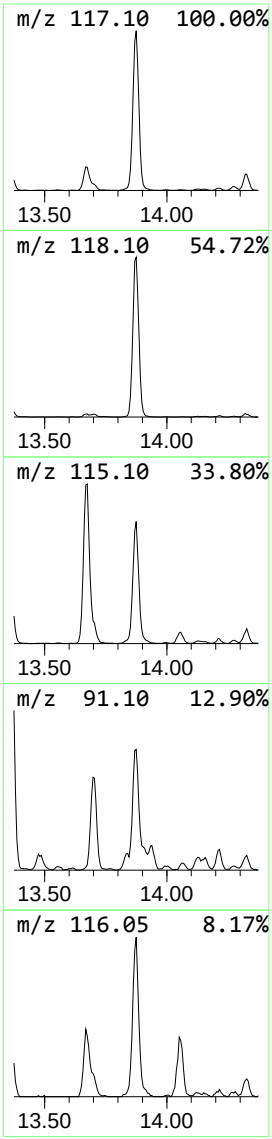
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	39.04 ug/l	2238190	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
4	Indole	117	C8H7N	000120-72-9	46
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45





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Data File : VN071815.D
Acq On : 02 Apr 2022 22:11
Operator : JC\MD
Sample : N2244-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

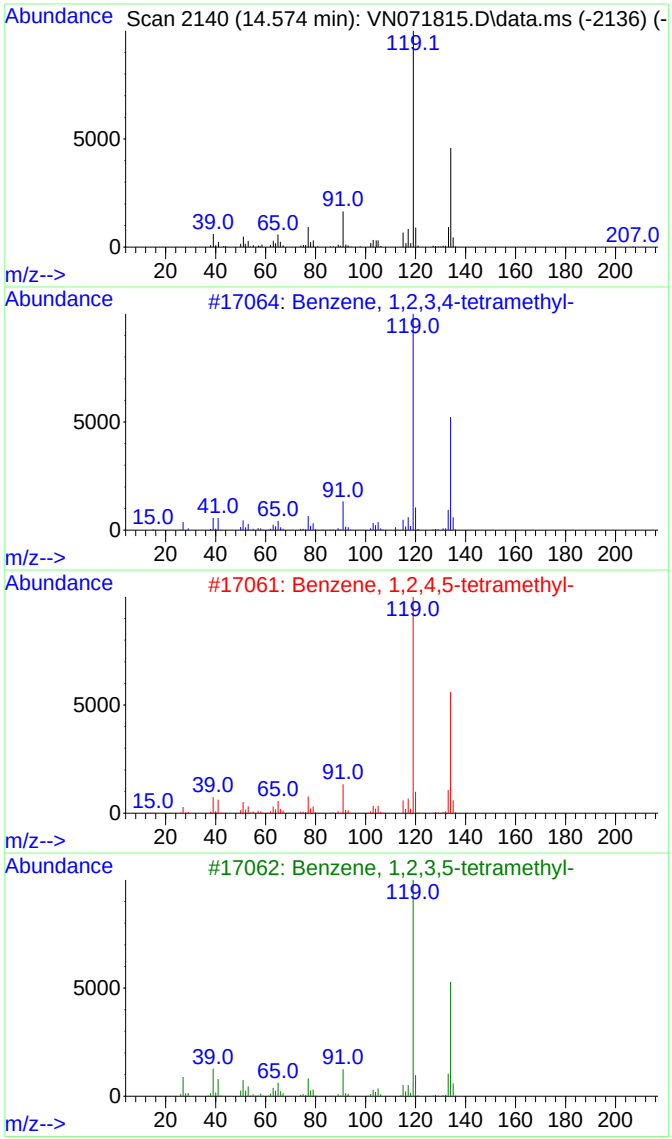
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

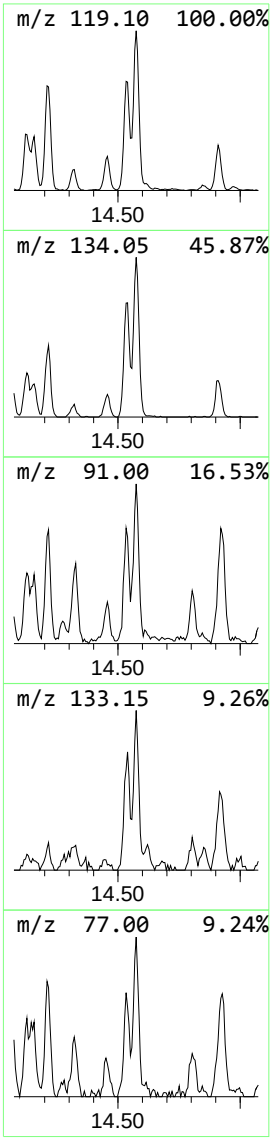
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	6.09 ug/l	349184	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

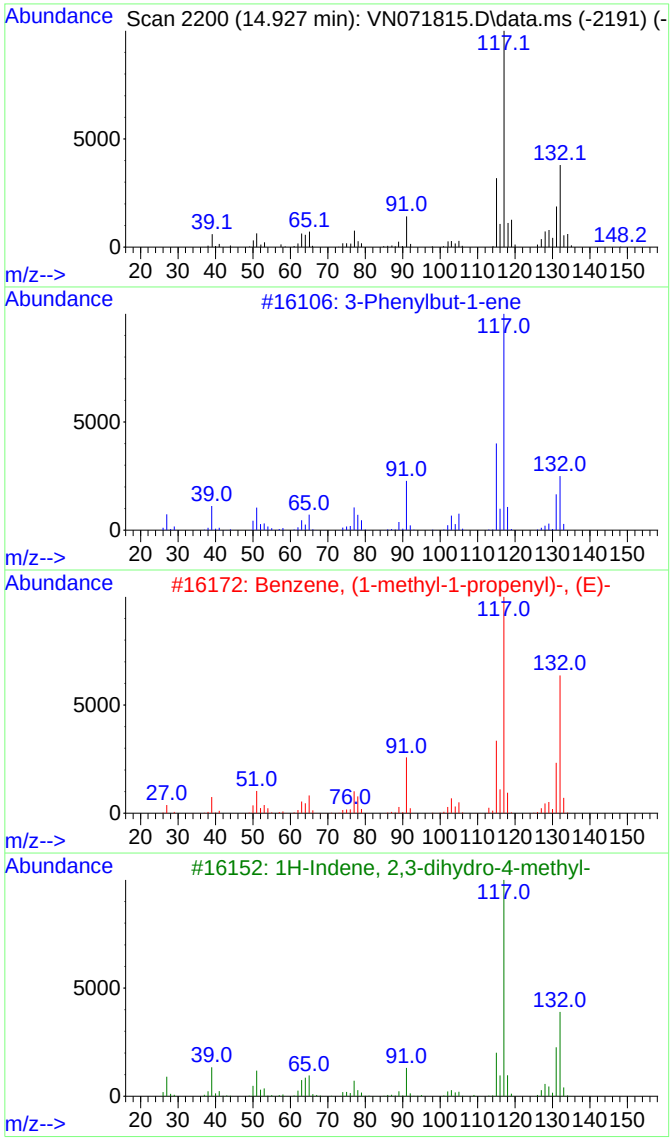
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

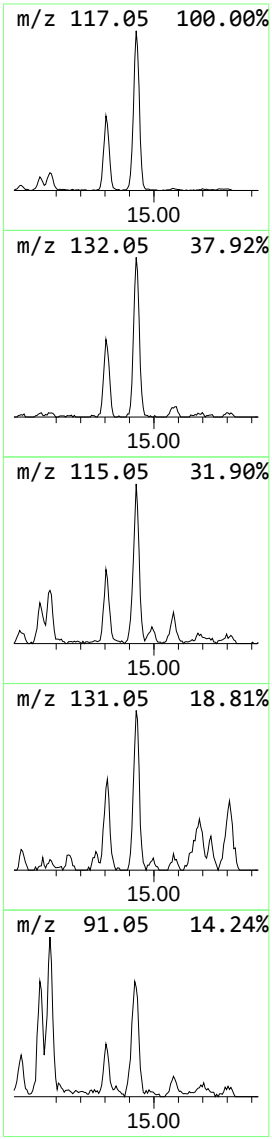
****

Peak Number 6 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	7.56 ug/l	433473	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	86





Tentatively Identified Compound (LSC) summary

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Data File : VN071815.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-BD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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	2.234	35.0	ug/l	1401420	1	8.086	1999910	50.0
Benzene, 1-ethy...	12.980	26.6	ug/l	1525360	4	13.668	2866730	50.0
Benzene, 1,2,3-...	13.216	13.1	ug/l	748374	4	13.668	2866730	50.0
Benzene, 1,1'-(...	13.874	39.0	ug/l	2238190	4	13.668	2866730	50.0
Benzene, 1,2,3,...	14.574	6.1	ug/l	349184	4	13.668	2866730	50.0
3-Phenylbut-1-ene	14.927	7.6	ug/l	433473	4	13.668	2866730	50.0