LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
Data File : VX035176.D
Acq On : 19 Apr 2023 17:47
Operator : JC/MD
Sample : 02333-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0MH0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_X\Method\SFAMXLM041823WMA.M
Title : VOC Analysis

Signal : TIC: VX035176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	43	rBV	141388	342336	24.41%	3.089%
2	1.367	43	46	58	rVB	158028	183608	13.09%	1.657%
3	1.672	92	96	107	rBV	113253	153256	10.93%	1.383%
4	2.306	193	200	211	rBV	301048	473155	33.74%	4.269%
5	2.514	232	234	238	rVB2	615	597	0.04%	0.005%
6	2.703	262	265	267	rVB2	433	393	0.03%	0.004%
7	2.788	275	279	284	rVB4	1180	1988	0.14%	0.018%
8	2.855	288	290	291	rBV2	245	258	0.02%	0.002%
9	2.886	293	295	298	rBV3	279	316	0.02%	0.003%
10	2.934	300	303	307	rVV3	513	784	0.06%	0.007%
11	3.038	318	320	323	rVB2	242	226	0.02%	0.002%
12	3.312	363	365	368	rBV	167	205	0.01%	0.002%
13	3.398	378	379	382	rBV2	344	263	0.02%	0.002%
14	3.513	395	398	399	rBV2	239	236	0.02%	0.002%
15	3.721	430	432	434	rBV	317	323	0.02%	0.003%
16	3.769	437	440	441	rVB2	194	200	0.01%	0.002%
17	3.867	454	456	457	rBV	213	176	0.01%	0.002%
18	3.983	472	475	476	rBV	243	225	0.02%	0.002%
19	4.038	482	484	487	rVB	363	419	0.03%	0.004%
20	4.306	526	528	530	rVV2	383	264	0.02%	0.002%
21	4.471	545	555	573	rBV2	75403	250411	17.86%	2.259%
22	4.958	633	635	638	rVB2	358	330	0.02%	0.003%
23	5.056	638	651	670	rBV2	168880	511686	36.49%	4.617%
24	5.342	697	698	700	rVB2	269	188	0.01%	0.002%
25	5.397	700	707	709	rBV3	478	848	0.06%	0.008%
26	5.464	717	718	721	rVB2	247	177	0.01%	0.002%
27	5.550	725	732	738	rBV5	1034	2803	0.20%	0.025%
28	5.678	750	753	756	rVV	238	220	0.02%	0.002%
29	5.830	775	778	780	rBV	271	286	0.02%	0.003%
30	5.970	787	801	828	rVV2	455738	1402359	100.00%	12.653%
31	6.269	848	850	852	rBV	332	263	0.02%	0.002%
32	6.354	860	864	867	rVB2	275	345	0.02%	0.003%
33	6.525	890	892	893	rBV	257	246	0.02%	0.002%
34	6.556	895	897	898	rVB	311	187	0.01%	0.002%
35	6.757	920	930	944	rBV	457171	1107816	79.00%	9.996%
36	7.074	980	982	985	rBV2	288	376	0.03%	0.003%

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MSVOA_X
ClientSampleId :
C0MH0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_X\Method\SFAMXLM041823WMA.M
Title : VOC Analysis

37	7.116	985	989	996	rVB4	1406	3215	0.23%	0.029%
38	7.312	1011	1021	1035	rBV	268297	601440	42.89%	5.427%
39	7.482	1043	1049	1050	rBV4	1014	1227	0.09%	0.011%
40	7.525	1054	1056	1059	rVB2	596	604	0.04%	0.005%
41	7.848	1106	1109	1110	rBV2	282	251	0.02%	0.002%
42	7.879	1110	1114	1118	rBV2	278	415	0.03%	0.004%
43	7.946	1122	1125	1127	rBV	432	481	0.03%	0.004%
44	8.208	1167	1168	1170	rBV	342	193	0.01%	0.002%
45	8.226	1170	1171	1178	rVB2	309	431	0.03%	0.004%
46	8.281	1178	1180	1181	rBV	244	188	0.01%	0.002%
47	8.324	1181	1187	1205	rVV	132234	220846	15.75%	1.993%
48	8.494	1213	1215	1217	rBV2	346	248	0.02%	0.002%
49	8.647	1233	1240	1261	rBV	686255	1098100	78.30%	9.908%
50	8.951	1285	1290	1303	rVB	90314	136093	9.70%	1.228%
51	9.098	1313	1314	1316	rBV	279	218	0.02%	0.002%
52	9.159	1322	1324	1325	rBV	361	285	0.02%	0.003%
53	9.177	1325	1327	1328	rVB	346	187	0.01%	0.002%
54	9.275	1341	1343	1348	rVB4	967	1360	0.10%	0.012%
55	9.384	1356	1361	1373	rBV	364428	536458	38.25%	4.840%
56	10.055	1465	1471	1489	rBV	912231	1340952	95.62%	12.099%
57	10.378	1522	1524	1526	rBV2	297	183	0.01%	0.002%
58	10.415	1528	1530	1533	rBV	349	305	0.02%	0.003%
59	10.591	1557	1559	1562	rBV	210	252	0.02%	0.002%
60	10.701	1574	1577	1579	rVB	285	284	0.02%	0.003%
61	10.726	1579	1581	1582	rBV	299	210	0.01%	0.002%
62	10.768	1586	1588	1593	rBV2	329	494	0.04%	0.004%
63	11.018	1628	1629	1633	rBV2	251	412	0.03%	0.004%
64	11.189	1652	1657	1666	rVV	433523	571047	40.72%	5.152%
65	11.305	1674	1676	1682	rVB3	593	738	0.05%	0.007%
66	11.561	1717	1718	1721	rBV2	260	292	0.02%	0.003%
67	11.689	1736	1739	1741	rBV3	326	313	0.02%	0.003%
68	11.847	1763	1765	1767	rBV	302	189	0.01%	0.002%
69	11.896	1772	1773	1776	rVB2	216	185	0.01%	0.002%
70	11.975	1781	1786	1788	rBV3	3092	4440	0.32%	0.040%
71	12.024	1788	1794	1811	rVB	883710	1175864	83.85%	10.610%
72	12.219	1823	1826	1836	rVB2	3503	5890	0.42%	0.053%
73	12.323	1837	1843	1856	rVB	652265	914616	65.22%	8.252%
74	12.634	1892	1894	1896	rVB2	391	239	0.02%	0.002%
75	12.695	1902	1904	1906	rBV	277	196	0.01%	0.002%
76	12.719	1906	1908	1910	rVB	388	251	0.02%	0.002%

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0MH0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_X\Method\SFAMXLM041823WMA.M
Title : VOC Analysis

77	12.768	1910	1916	1917	rBV3	477	886	0.06%	0.008%
78	12.811	1921	1923	1926	rBV2	222	184	0.01%	0.002%
79	12.896	1936	1937	1939	rBV	271	214	0.02%	0.002%
80	12.939	1942	1944	1946	rBV2	232	193	0.01%	0.002%
81	13.036	1959	1960	1963	rBV2	247	255	0.02%	0.002%
82	13.170	1980	1982	1984	rBV2	322	272	0.02%	0.002%
83	13.195	1984	1986	1989	rVB2	236	236	0.02%	0.002%
84	13.219	1989	1990	1993	rBV2	218	264	0.02%	0.002%
85	13.249	1993	1995	1997	rVB	272	172	0.01%	0.002%
86	13.591	2047	2051	2057	rBV	11378	14894	1.06%	0.134%
87	13.737	2073	2075	2077	rBV	298	272	0.02%	0.002%
88	13.908	2100	2103	2106	rVB3	355	461	0.03%	0.004%
89	13.963	2106	2112	2119	rBV5	1491	2536	0.18%	0.023%
90	14.158	2142	2144	2145	rVB	336	171	0.01%	0.002%
91	14.292	2165	2166	2168	rVB2	390	226	0.02%	0.002%
92	14.353	2174	2176	2178	rBV	438	430	0.03%	0.004%
93	14.390	2180	2182	2183	rBV	522	350	0.02%	0.003%
94	14.603	2215	2217	2218	rBV2	530	327	0.02%	0.003%
95	14.646	2223	2224	2227	rBV2	311	253	0.02%	0.002%
96	14.969	2275	2277	2278	rBV	542	436	0.03%	0.004%
97	15.139	2303	2305	2306	rBV	466	212	0.02%	0.002%
98	15.194	2312	2314	2317	rBV2	556	518	0.04%	0.005%
99	15.255	2321	2324	2327	rVB3	1443	1700	0.12%	0.015%
100	15.615	2382	2383	2384	rBV	539	203	0.01%	0.002%

Sum of corrected areas: 11083026

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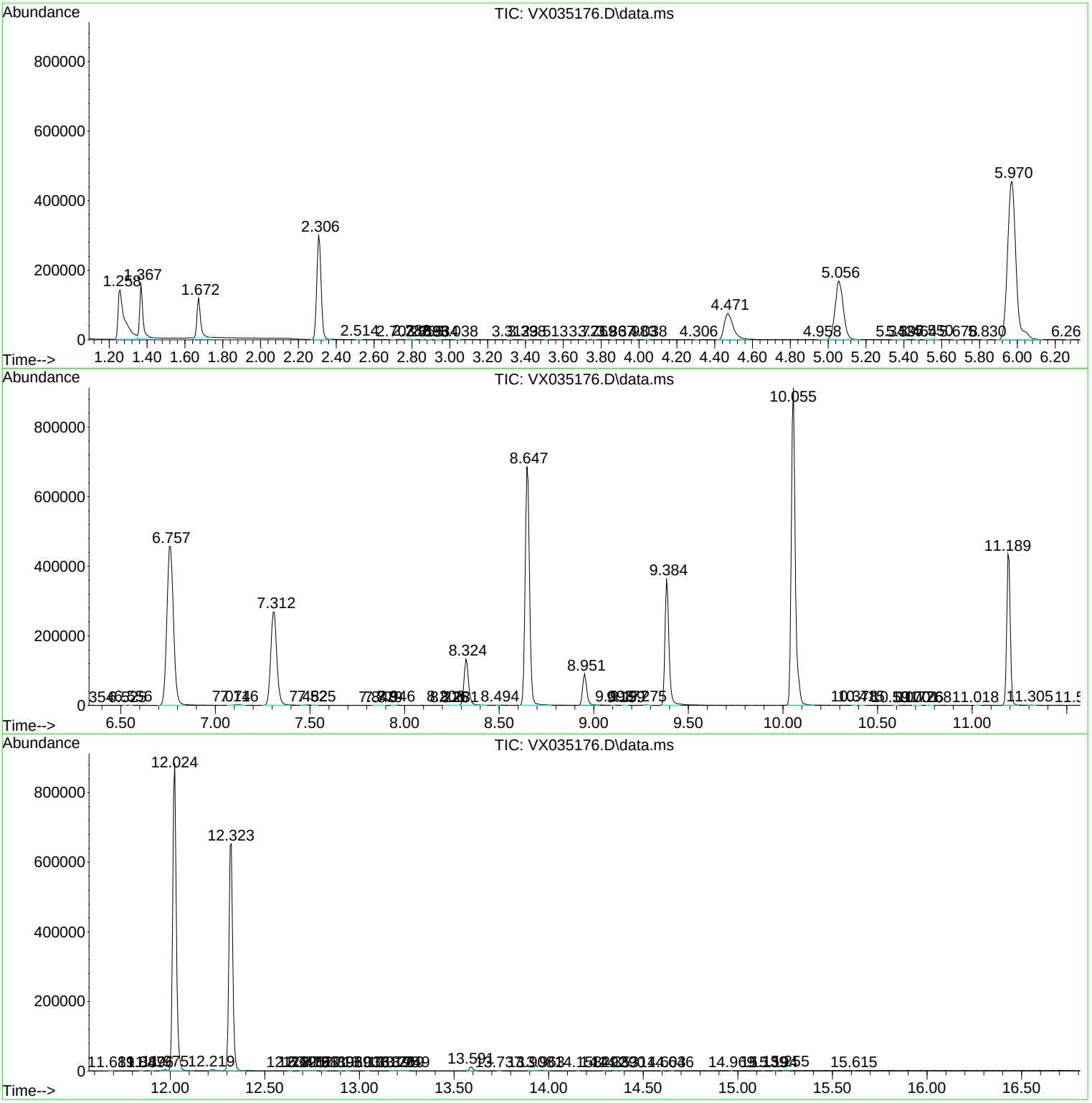
ClientSampleId :
C0MH0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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



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MSVOA_X
ClientSampleId :
C0MH0

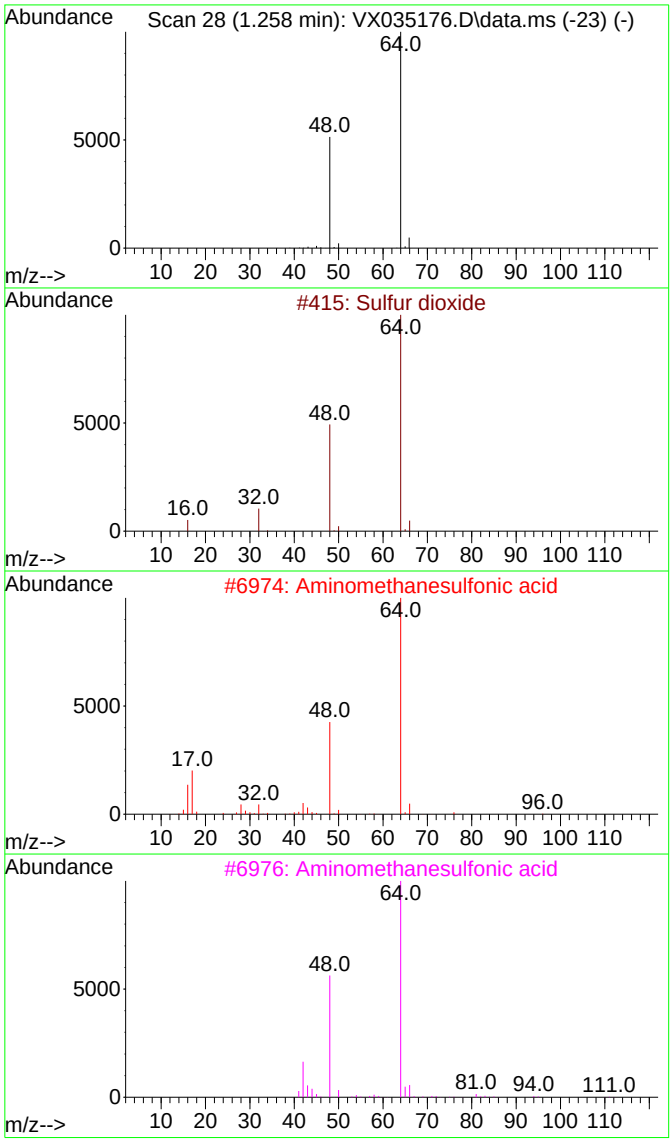
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

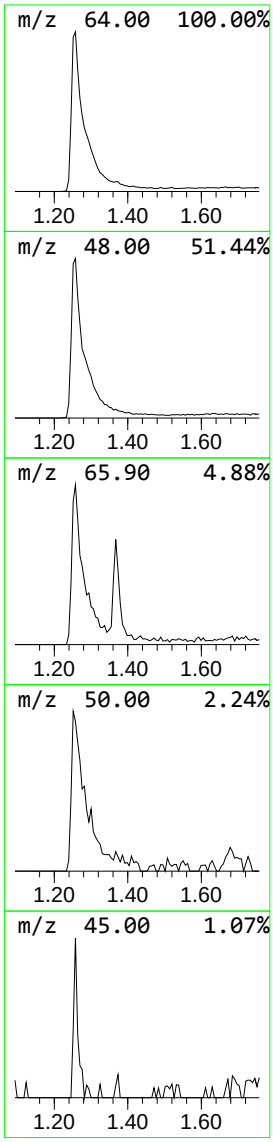
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	15.45 ug/L	342336	1,4-Difluorobenzene	6.757

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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	1.258	15.4	ug/L	342336	1	6.757	1107820	50.0