LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035133.D
Acq On : 18 Apr 2023 19:10
Operator : JC/MD
Sample : 02333-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0MG3

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: VX035133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	42	rBV	283178	520233	34.68%	4.245%
2	1.368	43	46	57	rVB	186983	208139	13.88%	1.699%
3	1.672	92	96	108	rVB	128288	169504	11.30%	1.383%
4	2.306	194	200	210	rBV	337830	530205	35.35%	4.327%
5	2.508	230	233	239	rVB3	1019	1763	0.12%	0.014%
6	2.709	265	266	269	rVB2	435	302	0.02%	0.002%
7	2.788	275	279	280	rBV3	1252	1608	0.11%	0.013%
8	2.855	289	290	292	rBV	236	175	0.01%	0.001%
9	2.886	294	295	298	rVB	292	169	0.01%	0.001%
10	2.922	299	301	302	rBV	367	237	0.02%	0.002%
11	2.995	311	313	315	rBV2	250	247	0.02%	0.002%
12	3.166	339	341	343	rBV	332	298	0.02%	0.002%
13	3.209	347	348	350	rBV2	269	167	0.01%	0.001%
14	3.337	367	369	371	rBV2	338	262	0.02%	0.002%
15	3.446	386	387	391	rBV	379	406	0.03%	0.003%
16	3.489	391	394	395	rBV2	260	268	0.02%	0.002%
17	3.568	406	407	409	rVB	301	170	0.01%	0.001%
18	3.745	432	436	438	rBV2	270	263	0.02%	0.002%
19	3.818	445	448	454	rBV3	252	680	0.05%	0.006%
20	3.904	460	462	466	rVB	372	401	0.03%	0.003%
21	4.154	502	503	506	rVB	438	306	0.02%	0.002%
22	4.184	506	508	512	rBV2	249	306	0.02%	0.002%
23	4.465	545	554	569	rBV	89080	278496	18.57%	2.273%
24	5.056	638	651	670	rVV	181641	568264	37.88%	4.637%
25	5.385	700	705	706	rBV3	705	1077	0.07%	0.009%
26	5.556	726	733	739	rBV5	2007	5115	0.34%	0.042%
27	5.629	742	745	746	rBV2	214	200	0.01%	0.002%
28	5.684	751	754	758	rVB2	318	436	0.03%	0.004%
29	5.879	783	786	789	rBV2	178	255	0.02%	0.002%
30	5.970	789	801	822	rBV2	501177	1499995	100.00%	12.241%
31	6.214	839	841	843	rBV	320	358	0.02%	0.003%
32	6.294	853	854	856	rVB	312	195	0.01%	0.002%
33	6.324	856	859	860	rBV	476	460	0.03%	0.004%
34	6.489	884	886	889	rVB2	204	235	0.02%	0.002%
35	6.519	889	891	893	rBV2	220	276	0.02%	0.002%
36	6.543	893	895	899	rVB2	440	497	0.03%	0.004%

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Instrument :
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ClientSampleId :
C0MG3

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

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Peak separation: 5

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

37	6.659	912	914	917	rBV2	150	201	0.01%	0.002%
38	6.763	921	931	952	rBV	504025	1213932	80.93%	9.907%
39	7.123	984	990	997	rVB4	1109	2597	0.17%	0.021%
40	7.306	1012	1020	1036	rBV	301404	670523	44.70%	5.472%
41	7.549	1058	1060	1062	rVB2	283	228	0.02%	0.002%
42	7.598	1067	1068	1069	rBV	340	209	0.01%	0.002%
43	7.805	1101	1102	1106	rBV2	184	212	0.01%	0.002%
44	7.860	1109	1111	1113	rBV2	205	207	0.01%	0.002%
45	7.946	1120	1125	1131	rBV3	544	1245	0.08%	0.010%
46	8.086	1145	1148	1149	rBV2	214	188	0.01%	0.002%
47	8.324	1181	1187	1197	rBV	169919	274339	18.29%	2.239%
48	8.458	1207	1209	1211	rBV2	289	316	0.02%	0.003%
49	8.574	1227	1228	1230	rBV	234	192	0.01%	0.002%
50	8.647	1233	1240	1258	rVV	775812	1235039	82.34%	10.079%
51	8.952	1284	1290	1304	rBV	113898	174694	11.65%	1.426%
52	9.275	1339	1343	1348	rVB2	2040	2665	0.18%	0.022%
53	9.330	1351	1352	1355	rBV	189	171	0.01%	0.001%
54	9.384	1355	1361	1378	rBV	438133	615302	41.02%	5.021%
55	9.604	1395	1397	1399	rBV2	429	270	0.02%	0.002%
56	9.860	1437	1439	1440	rBV2	225	189	0.01%	0.002%
57	10.055	1465	1471	1489	rVV	989639	1367952	91.20%	11.164%
58	10.238	1499	1501	1502	rBV2	359	189	0.01%	0.002%
59	10.335	1515	1517	1519	rBV2	368	380	0.03%	0.003%
60	10.427	1528	1532	1534	rBV	510	559	0.04%	0.005%
61	10.470	1537	1539	1541	rBV2	351	293	0.02%	0.002%
62	10.500	1542	1544	1546	rVB	272	204	0.01%	0.002%
63	10.518	1546	1547	1552	rBV	337	359	0.02%	0.003%
64	10.573	1552	1556	1558	rVB2	250	329	0.02%	0.003%
65	10.622	1562	1564	1565	rBV	281	191	0.01%	0.002%
66	10.677	1572	1573	1576	rVB2	260	233	0.02%	0.002%
67	10.701	1576	1577	1580	rBV2	397	249	0.02%	0.002%
68	10.909	1609	1611	1614	rVB2	210	218	0.01%	0.002%
69	10.963	1618	1620	1624	rVB	443	455	0.03%	0.004%
70	11.091	1640	1641	1643	rVB	352	197	0.01%	0.002%
71	11.189	1652	1657	1669	rBV	480645	647866	43.19%	5.287%
72	11.311	1674	1677	1683	rVB3	1535	1950	0.13%	0.016%
73	11.408	1691	1693	1695	rVB2	350	231	0.02%	0.002%
74	11.445	1697	1699	1701	rBV	332	271	0.02%	0.002%
75	11.549	1714	1716	1719	rVB	360	273	0.02%	0.002%
76	11.585	1719	1722	1724	rBV	261	309	0.02%	0.003%

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0MG3

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	11.695	1738	1740	1741	rBV	226	204	0.01%	0.002%
78	11.707	1741	1742	1746	rVB2	990	766	0.05%	0.006%
79	11.756	1746	1750	1754	rBV2	599	821	0.05%	0.007%
80	11.793	1754	1756	1757	rBV	326	188	0.01%	0.002%
81	11.878	1767	1770	1773	rBV2	245	321	0.02%	0.003%
82	11.975	1782	1786	1788	rVB3	609	822	0.05%	0.007%
83	12.024	1788	1794	1807	rBV	940791	1244414	82.96%	10.155%
84	12.219	1822	1826	1837	rVB2	4156	6825	0.46%	0.056%
85	12.317	1837	1842	1857	rBV	744687	987385	65.83%	8.058%
86	12.542	1877	1879	1881	rVB2	474	407	0.03%	0.003%
87	12.616	1889	1891	1893	rVB2	262	232	0.02%	0.002%
88	12.756	1911	1914	1915	rBV2	558	526	0.04%	0.004%
89	12.829	1924	1926	1929	rVB2	244	251	0.02%	0.002%
90	12.884	1933	1935	1936	rBV	189	176	0.01%	0.001%
91	12.926	1941	1942	1944	rBV	249	187	0.01%	0.002%
92	12.987	1950	1952	1953	rBV2	264	203	0.01%	0.002%
93	13.420	2021	2023	2024	rVB	382	169	0.01%	0.001%
94	13.548	2042	2044	2048	rBV2	285	358	0.02%	0.003%
95	13.591	2049	2051	2053	rBV2	681	508	0.03%	0.004%
96	13.682	2064	2066	2069	rBV	217	180	0.01%	0.001%
97	13.902	2099	2102	2103	rBV2	429	400	0.03%	0.003%
98	14.030	2121	2123	2125	rBV2	379	371	0.02%	0.003%
99	14.591	2213	2215	2216	rVB	471	189	0.01%	0.002%
100	14.749	2239	2241	2244	rVB3	544	476	0.03%	0.004%

Sum of corrected areas: 12253774

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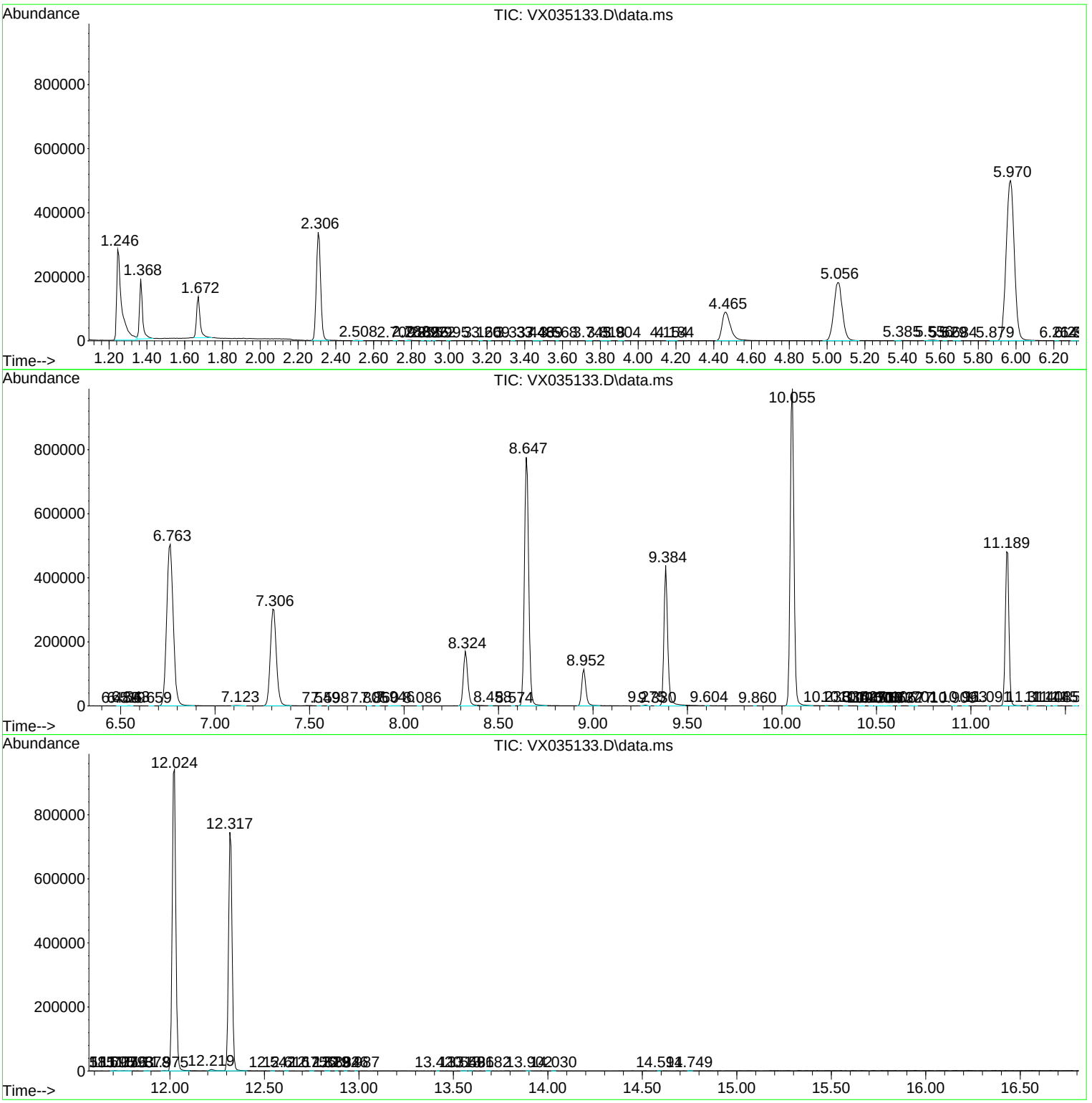
C0MG3

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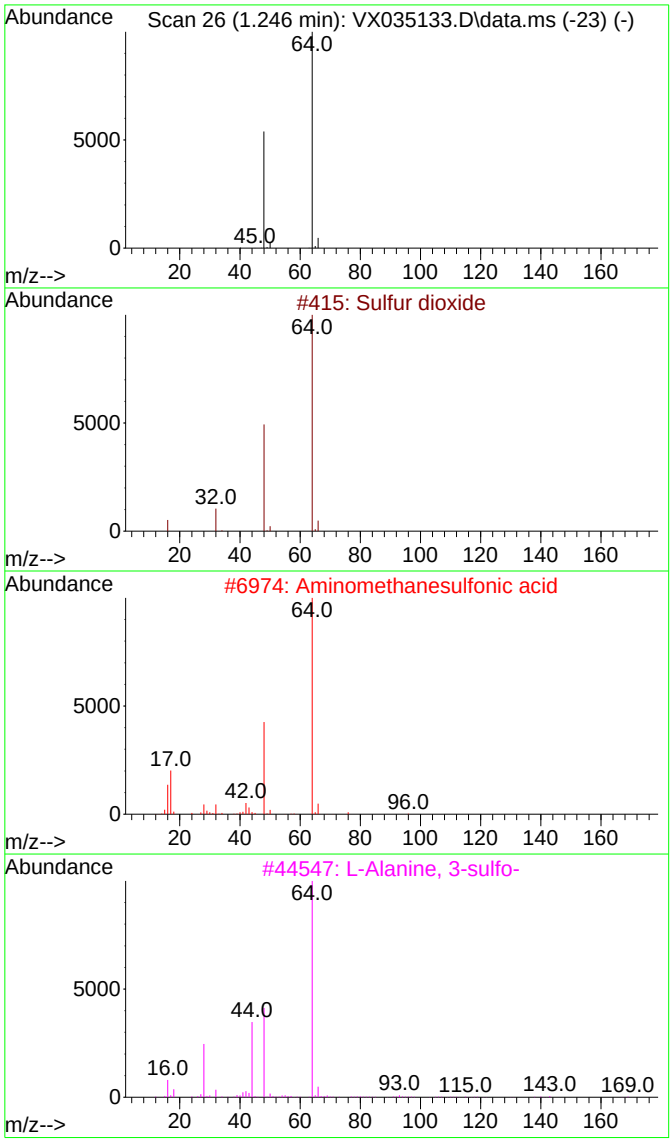
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

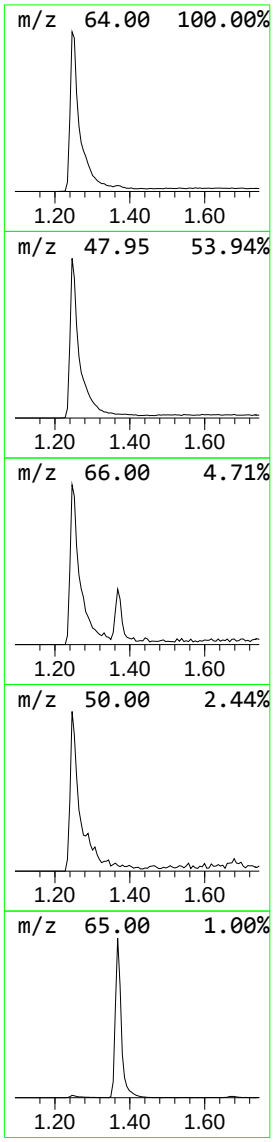
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	21.43 ug/L	520233	1,4-Difluorobenzene	6.763

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





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	1.246	21.4	ug/L	520233	1	6.763	1213930	50.0