LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042411.D
Acq On : 19 Jul 2024 18:52
Operator : JC/MD
Sample : P3238-09MERE
Misc : 5.41g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF4MERE

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\SFAMXLM070324WMA.M
Title : VOC Analysis

Signal : TIC: VX042411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	27	rBV	41905	46190	8.19%	1.345%
2	1.374	43	47	64	rVB	16643	45153	8.01%	1.315%
3	1.630	86	89	90	rBV	11787	12219	2.17%	0.356%
4	2.282	189	196	209	rBV	50920	96679	17.15%	2.816%
5	2.544	237	239	241	rVB2	238	158	0.03%	0.005%
6	2.721	262	268	274	rBV	10983	22202	3.94%	0.647%
7	2.947	298	305	316	rVB	7120	17431	3.09%	0.508%
8	3.178	341	343	348	rBV2	83	149	0.03%	0.004%
9	3.337	367	369	371	rVV2	250	220	0.04%	0.006%
10	3.416	379	382	387	rBV2	162	321	0.06%	0.009%
11	3.520	396	399	401	rVV2	201	256	0.05%	0.007%
12	3.593	407	411	413	rVV2	202	259	0.05%	0.008%
13	3.623	413	416	418	rVB	133	139	0.02%	0.004%
14	3.776	439	441	445	rVB2	104	140	0.02%	0.004%
15	3.965	469	472	473	rBV2	231	205	0.04%	0.006%
16	4.294	522	526	528	rBV2	106	148	0.03%	0.004%
17	4.495	551	559	578	rBV	16751	61548	10.92%	1.793%
18	5.056	640	651	668	rBV2	38880	121739	21.60%	3.546%
19	5.342	696	698	700	rBV	236	230	0.04%	0.007%
20	5.373	700	703	704	rBV2	193	215	0.04%	0.006%
21	5.544	727	731	732	rBV2	357	502	0.09%	0.015%
22	5.855	778	782	785	rVB2	148	196	0.03%	0.006%
23	5.891	785	788	789	rBV	136	149	0.03%	0.004%
24	5.964	789	800	818	rBV2	112707	323730	57.43%	9.429%
25	6.178	833	835	839	rBV3	170	272	0.05%	0.008%
26	6.245	843	846	848	rBV2	194	183	0.03%	0.005%
27	6.379	866	868	870	rBV2	340	244	0.04%	0.007%
28	6.665	906	915	921	rBV3	880	2215	0.39%	0.065%
29	6.757	921	930	950	rVV	201283	487722	86.53%	14.206%
30	6.995	966	969	970	rBV2	196	199	0.04%	0.006%
31	7.062	978	980	982	rBV2	263	242	0.04%	0.007%
32	7.226	1001	1007	1012	rVV2	769	1394	0.25%	0.041%
33	7.306	1012	1020	1036	rVV	61798	140655	24.95%	4.097%
34	7.495	1050	1051	1055	rBV2	161	172	0.03%	0.005%
35	7.555	1059	1061	1063	rBV	164	152	0.03%	0.004%
36	7.598	1067	1068	1071	rBV	183	191	0.03%	0.006%

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Instrument :
MSVOA_X
ClientSampleId :
A4BF4MERE

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\SFAMXLM070324WMA.M
Title : VOC Analysis

37	7.647	1073	1076	1079	rBV2	155	214	0.04%	0.006%
38	7.799	1097	1101	1105	rBV2	211	381	0.07%	0.011%
39	7.976	1127	1130	1132	rBV3	463	652	0.12%	0.019%
40	8.330	1179	1188	1205	rBV	31694	58076	10.30%	1.692%
41	8.476	1210	1212	1214	rVB2	191	156	0.03%	0.005%
42	8.500	1214	1216	1219	rBV	213	278	0.05%	0.008%
43	8.647	1227	1240	1250	rBV	163418	261922	46.47%	7.629%
44	8.909	1282	1283	1285	rBV	178	142	0.03%	0.004%
45	8.952	1285	1290	1304	rBV	22425	36827	6.53%	1.073%
46	9.104	1312	1315	1319	rVB2	271	389	0.07%	0.011%
47	9.134	1319	1320	1323	rBV2	197	214	0.04%	0.006%
48	9.275	1339	1343	1347	rVB4	472	631	0.11%	0.018%
49	9.397	1358	1363	1382	rBV	65895	137742	24.44%	4.012%
50	9.708	1410	1414	1422	rBV5	1370	3231	0.57%	0.094%
51	9.817	1430	1432	1434	rBV2	231	191	0.03%	0.006%
52	9.836	1434	1435	1439	rVV2	189	144	0.03%	0.004%
53	10.055	1465	1471	1483	rBV	405861	563646	100.00%	16.417%
54	10.305	1509	1512	1521	rVB3	754	1421	0.25%	0.041%
55	10.366	1521	1522	1526	rBV2	147	192	0.03%	0.006%
56	10.427	1531	1532	1536	rVB2	123	153	0.03%	0.004%
57	10.470	1536	1539	1540	rBV	146	181	0.03%	0.005%
58	10.646	1563	1568	1569	rBV3	383	468	0.08%	0.014%
59	10.823	1594	1597	1598	rBV2	131	154	0.03%	0.004%
60	10.970	1616	1621	1625	rBV2	2572	3738	0.66%	0.109%
61	11.098	1639	1642	1643	rBV2	306	280	0.05%	0.008%
62	11.195	1652	1658	1668	rBV	120458	158780	28.17%	4.625%
63	11.317	1674	1678	1682	rVB4	498	773	0.14%	0.023%
64	11.390	1687	1690	1692	rVB2	172	177	0.03%	0.005%
65	11.439	1695	1698	1699	rVB3	326	220	0.04%	0.006%
66	11.457	1699	1701	1704	rBV3	396	526	0.09%	0.015%
67	11.622	1726	1728	1731	rVV3	226	252	0.04%	0.007%
68	11.707	1737	1742	1746	rVV2	379	541	0.10%	0.016%
69	11.768	1746	1752	1755	rVV4	1427	2693	0.48%	0.078%
70	11.817	1758	1760	1763	rBV2	205	154	0.03%	0.004%
71	11.939	1777	1780	1783	rBV2	258	238	0.04%	0.007%
72	11.982	1783	1787	1789	rBV2	2203	2638	0.47%	0.077%
73	12.024	1789	1794	1807	rVB	414749	536684	95.22%	15.632%
74	12.225	1823	1827	1837	rVB4	1101	1961	0.35%	0.057%
75	12.323	1837	1843	1852	rBV	172726	237017	42.05%	6.904%
76	12.518	1873	1875	1877	rBV2	220	197	0.03%	0.006%

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A4BF4MERE

Integration Parameters: LSCINT.P
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

77	12.609	1886	1890	1892	rBV2	182	196	0.03%	0.006%
78	12.664	1898	1899	1903	rBV	180	265	0.05%	0.008%
79	12.762	1911	1915	1921	rVB3	993	1635	0.29%	0.048%
80	12.872	1929	1933	1940	rBV	5906	8267	1.47%	0.241%
81	13.036	1959	1960	1962	rBV	172	161	0.03%	0.005%
82	13.103	1969	1971	1972	rBV	297	162	0.03%	0.005%
83	13.164	1977	1981	1983	rBV3	243	346	0.06%	0.010%
84	13.292	1998	2002	2006	rBV3	231	404	0.07%	0.012%
85	13.408	2016	2021	2025	rBV4	4978	8625	1.53%	0.251%
86	13.591	2050	2051	2055	rVB2	317	394	0.07%	0.011%
87	13.682	2063	2066	2071	rVB2	1473	2110	0.37%	0.061%
88	13.731	2071	2074	2077	rBV	166	186	0.03%	0.005%
89	13.780	2079	2082	2086	rBV2	1023	1367	0.24%	0.040%
90	13.884	2097	2099	2101	rBV	161	166	0.03%	0.005%
91	13.969	2111	2113	2116	rVB3	386	341	0.06%	0.010%
92	14.060	2126	2128	2129	rVB	292	151	0.03%	0.004%
93	14.127	2136	2139	2144	rVV2	928	1288	0.23%	0.038%
94	14.262	2157	2161	2166	rBV3	217	410	0.07%	0.012%
95	14.432	2185	2189	2192	rBV2	1535	1671	0.30%	0.049%
96	14.640	2221	2223	2224	rBV2	458	404	0.07%	0.012%
97	14.792	2243	2248	2251	rBV3	558	790	0.14%	0.023%
98	14.822	2251	2253	2256	rVB2	342	261	0.05%	0.008%
99	14.883	2260	2263	2271	rVB4	1570	2711	0.48%	0.079%
100	15.956	2436	2439	2445	rVB4	1953	2843	0.50%	0.083%

Sum of corrected areas: 3433247

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Instrument :
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ClientSampleId :
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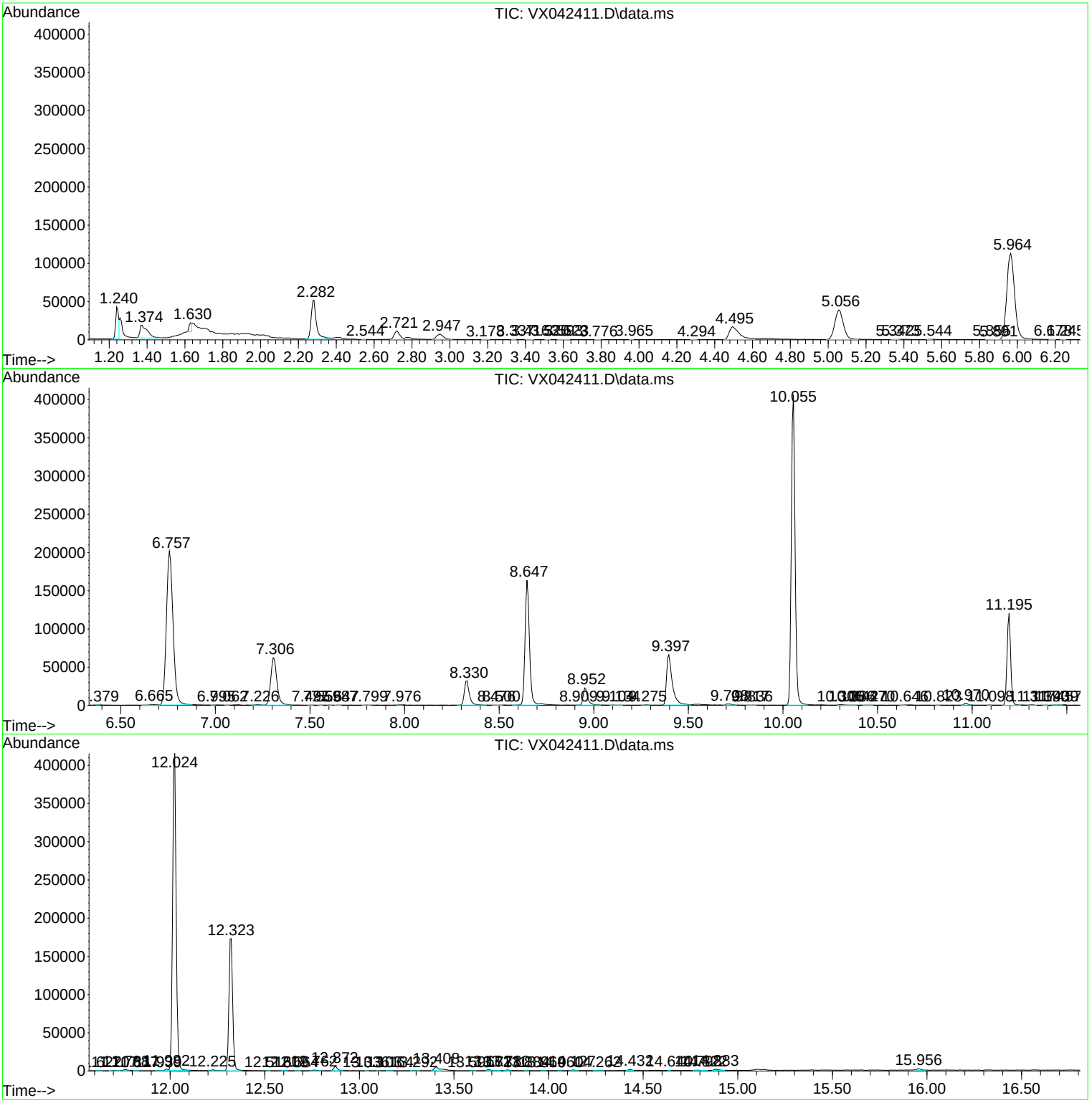
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
A4BF4MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

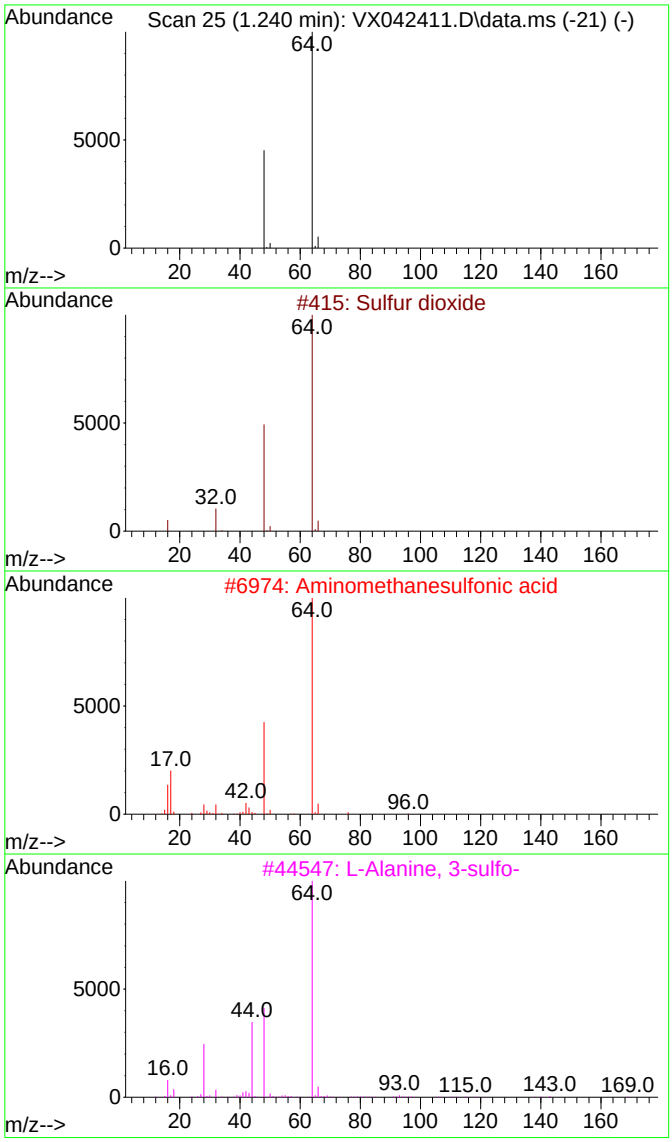
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

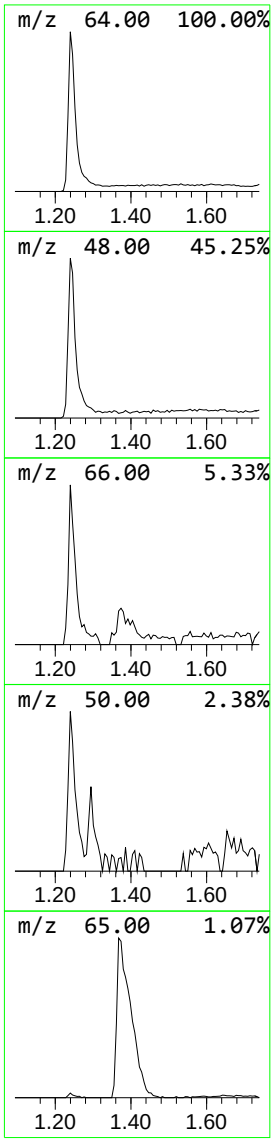
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.74 ug/L	46190	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	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5





Tentatively Identified Compound (LSC) summary

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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	1.240	4.7	ug/L	46190	1	6.757	487722	50.0