

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042466.D
 Acq On : 23 Jul 2024 13:02
 Operator : JC/MD
 Sample : VX0724MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK690

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042466.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	22	25	37	rBV	59773	80891	8.03%	1.076%
2	1.368	42	46	58	rVV	98456	112724	11.19%	1.500%
3	1.660	90	94	108	rVB	66318	98214	9.75%	1.307%
4	2.300	193	199	209	rBV	183072	300024	29.79%	3.992%
5	2.514	229	234	238	rVB2	1007	1395	0.14%	0.019%
6	2.788	275	279	287	rVB3	1356	2662	0.26%	0.035%
7	2.861	289	291	293	rBV3	147	106	0.01%	0.001%
8	2.886	293	295	299	rBV3	149	147	0.01%	0.002%
9	3.087	325	328	329	rBV2	375	353	0.04%	0.005%
10	3.221	347	350	352	rBV3	174	209	0.02%	0.003%
11	3.270	355	358	359	rVV	168	113	0.01%	0.002%
12	3.361	371	373	377	rBV2	251	301	0.03%	0.004%
13	3.428	383	384	387	rBV2	104	102	0.01%	0.001%
14	3.654	417	421	422	rVV2	164	133	0.01%	0.002%
15	3.715	426	431	432	rBV2	136	143	0.01%	0.002%
16	3.745	435	436	439	rVB	131	104	0.01%	0.001%
17	3.898	457	461	462	rBV	146	162	0.02%	0.002%
18	3.965	469	472	474	rBV2	141	191	0.02%	0.003%
19	3.995	474	477	479	rVV2	130	151	0.01%	0.002%
20	4.178	505	507	508	rVB2	154	102	0.01%	0.001%
21	4.196	508	510	511	rBV	173	125	0.01%	0.002%
22	4.245	515	518	519	rBV	160	169	0.02%	0.002%
23	4.367	537	538	541	rVB	135	112	0.01%	0.001%
24	4.458	545	553	573	rBV	76916	231352	22.97%	3.078%
25	4.873	619	621	624	rVB2	132	103	0.01%	0.001%
26	5.056	639	651	667	rBV	128490	392444	38.96%	5.222%
27	5.196	672	674	676	rBV2	300	272	0.03%	0.004%
28	5.373	701	703	704	rBV	403	319	0.03%	0.004%
29	5.562	725	734	739	rBV2	1192	3147	0.31%	0.042%
30	5.666	748	751	754	rBV2	166	260	0.03%	0.003%
31	5.727	760	761	765	rVB2	114	112	0.01%	0.001%
32	5.769	765	768	769	rBV	141	134	0.01%	0.002%
33	5.849	777	781	782	rVB	195	165	0.02%	0.002%
34	5.964	788	800	821	rBV2	339385	1007206	100.00%	13.402%
35	6.342	860	862	863	rBV	151	111	0.01%	0.001%
36	6.391	869	870	872	rBV	178	157	0.02%	0.002%

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 Title : VOC Analysis

37	6.476	881	884	885	rBV2	180	199	0.02%	0.003%
38	6.550	894	896	898	rBV2	254	186	0.02%	0.002%
39	6.757	921	930	946	rBV	245677	597821	59.35%	7.955%
40	6.982	965	967	970	rBV2	179	229	0.02%	0.003%
41	7.117	983	989	997	rVB7	2258	5155	0.51%	0.069%
42	7.306	1011	1020	1038	rBV	201799	446975	44.38%	5.948%
43	7.470	1046	1047	1048	rBV	284	111	0.01%	0.001%
44	7.519	1054	1055	1059	rVB2	302	197	0.02%	0.003%
45	7.653	1075	1077	1078	rBV2	136	127	0.01%	0.002%
46	7.824	1100	1105	1106	rBV	179	262	0.03%	0.003%
47	7.952	1121	1126	1132	rBV4	644	1381	0.14%	0.018%
48	8.324	1181	1187	1205	rBV	127787	215008	21.35%	2.861%
49	8.500	1214	1216	1218	rBV	504	533	0.05%	0.007%
50	8.647	1234	1240	1260	rBV	535722	822148	81.63%	10.940%
51	8.952	1285	1290	1301	rBV	89099	134739	13.38%	1.793%
52	9.226	1333	1335	1338	rBV2	119	156	0.02%	0.002%
53	9.275	1338	1343	1349	rVV2	4790	7292	0.72%	0.097%
54	9.384	1356	1361	1385	rBV	341140	500474	49.69%	6.659%
55	9.762	1421	1423	1425	rVB2	158	109	0.01%	0.001%
56	9.854	1435	1438	1441	rBV	123	137	0.01%	0.002%
57	10.055	1465	1471	1488	rBV	500556	686300	68.14%	9.132%
58	10.195	1492	1494	1500	rVB3	700	1017	0.10%	0.014%
59	10.305	1508	1512	1518	rBV3	815	1426	0.14%	0.019%
60	10.354	1518	1520	1524	rBV2	136	199	0.02%	0.003%
61	10.476	1537	1540	1542	rBV	152	117	0.01%	0.002%
62	10.653	1564	1569	1570	rBV3	511	701	0.07%	0.009%
63	10.902	1609	1610	1614	rBV2	117	164	0.02%	0.002%
64	10.963	1617	1620	1625	rVV2	606	975	0.10%	0.013%
65	11.110	1639	1644	1646	rVB4	373	540	0.05%	0.007%
66	11.189	1652	1657	1673	rBV	386518	504595	50.10%	6.714%
67	11.317	1677	1678	1679	rVV	232	111	0.01%	0.001%
68	11.335	1679	1681	1686	rVB2	283	292	0.03%	0.004%
69	11.378	1686	1688	1690	rBV	198	140	0.01%	0.002%
70	11.457	1697	1701	1706	rVB3	518	819	0.08%	0.011%
71	11.494	1706	1707	1712	rBV	167	177	0.02%	0.002%
72	11.537	1712	1714	1715	rBV	144	106	0.01%	0.001%
73	11.671	1734	1736	1739	rVV2	87	121	0.01%	0.002%
74	11.713	1741	1743	1745	rVV	379	280	0.03%	0.004%
75	11.762	1747	1751	1754	rVB2	819	1090	0.11%	0.015%
76	11.866	1766	1768	1770	rBV2	127	118	0.01%	0.002%

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77	11.921	1775	1777	1779	rBV	169	166	0.02%	0.002%
78	11.975	1782	1786	1788	rBV2	1351	1810	0.18%	0.024%
79	12.024	1788	1794	1803	rBV	481598	622657	61.82%	8.285%
80	12.317	1837	1842	1855	rBV	549848	702899	69.79%	9.353%
81	12.762	1912	1915	1916	rBV2	387	445	0.04%	0.006%
82	12.792	1918	1920	1922	rBV2	168	132	0.01%	0.002%
83	12.859	1930	1931	1935	rBV	156	168	0.02%	0.002%
84	13.006	1953	1955	1956	rBV2	156	130	0.01%	0.002%
85	13.024	1956	1958	1959	rVB	272	156	0.02%	0.002%
86	13.042	1959	1961	1962	rBV	164	105	0.01%	0.001%
87	13.073	1962	1966	1968	rVV2	164	222	0.02%	0.003%
88	13.115	1968	1973	1982	rVB3	1442	2379	0.24%	0.032%
89	13.189	1982	1985	1986	rBV2	172	204	0.02%	0.003%
90	13.372	2013	2015	2018	rBV	205	197	0.02%	0.003%
91	13.469	2029	2031	2032	rBV2	168	124	0.01%	0.002%
92	13.542	2042	2043	2046	rBV	116	127	0.01%	0.002%
93	13.591	2047	2051	2057	rVB2	2596	3292	0.33%	0.044%
94	13.780	2077	2082	2086	rBV	4434	5901	0.59%	0.079%
95	13.963	2106	2112	2119	rBV2	2696	4072	0.40%	0.054%
96	14.091	2131	2133	2136	rBV	193	274	0.03%	0.004%
97	14.128	2136	2139	2143	rVB2	1610	2151	0.21%	0.029%
98	14.225	2153	2155	2159	rBV2	284	429	0.04%	0.006%
99	14.280	2163	2164	2166	rVV2	210	127	0.01%	0.002%
100	14.847	2256	2257	2258	rBV	349	156	0.02%	0.002%

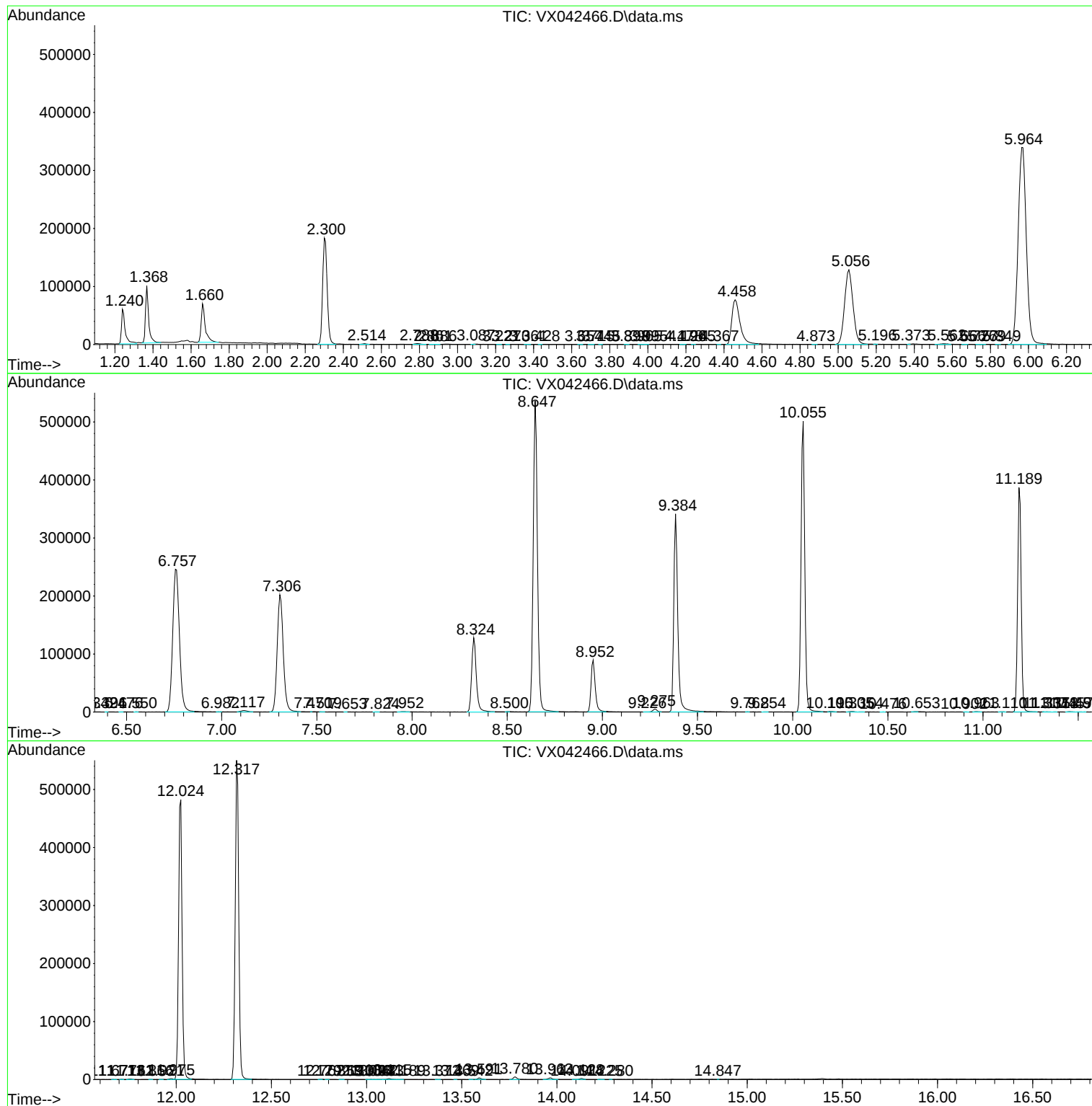
Sum of corrected areas: 7515265

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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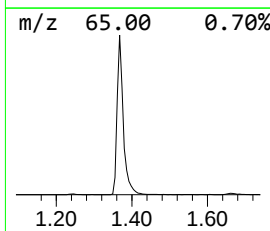
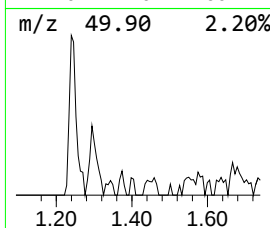
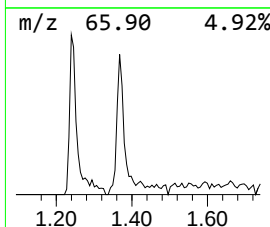
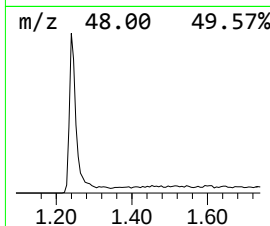
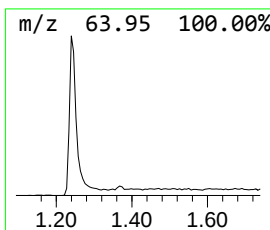
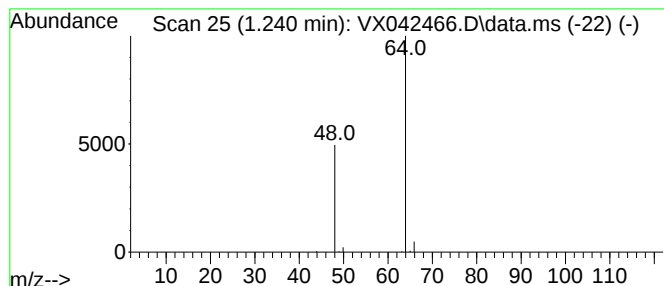
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	6.77 ug/L	80891	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	6.8	ug/L	80891	1	6.763	597821	50.0