

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081122\
 Data File : VX030578.D
 Acq On : 11 Aug 2022 17:04
 Operator : JC/MD
 Sample : N4008-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK002

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\SFAMXML080422WMA.M

Title : VOC Analysis

Signal : TIC: VX030578.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	24	28	42	rBV	44054	100056	8.80%	1.138%
2	1.368	42	46	56	rVB	116138	125128	11.00%	1.423%
3	1.666	91	95	109	rVB	103707	129076	11.35%	1.468%
4	2.306	194	200	211	rVB	233391	346953	30.50%	3.946%
5	2.508	231	233	237	rBV3	757	844	0.07%	0.010%
6	2.788	274	279	286	rVB2	3326	5198	0.46%	0.059%
7	2.953	298	306	316	rVB	14851	35874	3.15%	0.408%
8	3.044	318	321	323	rBV2	321	355	0.03%	0.004%
9	3.148	336	338	340	rVB2	352	360	0.03%	0.004%
10	3.227	349	351	353	rBV2	394	419	0.04%	0.005%
11	3.325	364	367	371	rBV2	348	397	0.03%	0.005%
12	3.416	379	382	383	rVB	668	380	0.03%	0.004%
13	3.440	383	386	388	rBV2	350	460	0.04%	0.005%
14	3.623	414	416	423	rVB2	652	936	0.08%	0.011%
15	3.678	423	425	427	rBB	435	362	0.03%	0.004%
16	3.715	427	431	436	rBV2	469	768	0.07%	0.009%
17	3.800	440	445	447	rBV2	512	751	0.07%	0.009%
18	4.178	504	507	508	rBV	557	394	0.03%	0.004%
19	4.202	508	511	514	rBV2	671	1060	0.09%	0.012%
20	4.233	514	516	518	rVB2	633	528	0.05%	0.006%
21	4.288	523	525	529	rVV4	459	428	0.04%	0.005%
22	4.477	547	556	571	rBV	102034	311536	27.38%	3.543%
23	4.776	604	605	607	rBV2	541	377	0.03%	0.004%
24	4.873	619	621	622	rBV2	500	370	0.03%	0.004%
25	4.897	623	625	627	rVB	655	377	0.03%	0.004%
26	4.916	627	628	630	rBV2	840	518	0.05%	0.006%
27	5.062	642	652	670	rVB	154460	470138	41.33%	5.347%
28	5.330	693	696	699	rBV2	782	1100	0.10%	0.013%
29	5.556	729	733	742	rVB6	2163	4987	0.44%	0.057%
30	5.647	746	748	752	rVB	744	875	0.08%	0.010%
31	5.977	788	802	820	rBV2	391048	1137624	100.00%	12.939%
32	6.208	838	840	842	rVB2	555	368	0.03%	0.004%
33	6.318	854	858	859	rBV2	456	542	0.05%	0.006%
34	6.440	876	878	879	rBV	499	462	0.04%	0.005%
35	6.604	904	905	909	rVB2	766	658	0.06%	0.007%
36	6.641	909	911	912	rBV	485	385	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

37	6.696	919	920	922	rBV	882	665	0.06%	0.008%
38	6.769	922	932	945	rVV	287634	680838	59.85%	7.744%
39	7.117	982	989	997	rBV4	9466	19551	1.72%	0.222%
40	7.202	1000	1003	1005	rBV3	703	677	0.06%	0.008%
41	7.312	1012	1021	1035	rBV	237561	529511	46.55%	6.022%
42	7.616	1069	1071	1072	rBV2	468	380	0.03%	0.004%
43	7.641	1073	1075	1078	rVB2	525	431	0.04%	0.005%
44	7.671	1078	1080	1082	rBV2	477	363	0.03%	0.004%
45	7.775	1093	1097	1103	rBV	625	1100	0.10%	0.013%
46	7.940	1119	1124	1126	rBV3	1684	2164	0.19%	0.025%
47	7.982	1129	1131	1134	rVV3	648	672	0.06%	0.008%
48	8.080	1145	1147	1149	rVV2	387	351	0.03%	0.004%
49	8.257	1174	1176	1180	rBV3	288	354	0.03%	0.004%
50	8.330	1180	1188	1196	rBV	158233	264267	23.23%	3.006%
51	8.464	1207	1210	1211	rBV2	509	469	0.04%	0.005%
52	8.653	1234	1241	1253	rBV	556159	865346	76.07%	9.842%
53	8.842	1270	1272	1274	rVB2	789	486	0.04%	0.006%
54	8.958	1284	1291	1301	rBV	112988	174894	15.37%	1.989%
55	9.189	1325	1329	1330	rBV2	427	429	0.04%	0.005%
56	9.263	1339	1341	1342	rBV2	457	375	0.03%	0.004%
57	9.275	1342	1343	1345	rBV	738	557	0.05%	0.006%
58	9.391	1356	1362	1372	rBV	487491	686183	60.32%	7.804%
59	9.701	1409	1413	1421	rVB3	4247	6356	0.56%	0.072%
60	9.756	1421	1422	1424	rBV2	685	576	0.05%	0.007%
61	10.055	1465	1471	1481	rBV	605928	795098	69.89%	9.043%
62	10.207	1494	1496	1497	rBV	757	468	0.04%	0.005%
63	10.524	1546	1548	1550	rVB	578	436	0.04%	0.005%
64	10.653	1565	1569	1572	rBV	564	779	0.07%	0.009%
65	10.695	1575	1576	1578	rBV	532	422	0.04%	0.005%
66	10.774	1587	1589	1592	rBV2	416	442	0.04%	0.005%
67	10.854	1597	1602	1604	rBV3	558	818	0.07%	0.009%
68	10.976	1620	1622	1628	rVB4	374	599	0.05%	0.007%
69	11.128	1646	1647	1649	rBV2	580	409	0.04%	0.005%
70	11.195	1653	1658	1669	rVB	452797	549158	48.27%	6.246%
71	11.433	1695	1697	1700	rVB3	489	530	0.05%	0.006%
72	11.463	1700	1702	1703	rBV	464	398	0.03%	0.005%
73	11.683	1735	1738	1743	rBV3	628	1175	0.10%	0.013%
74	11.835	1761	1763	1766	rBV2	440	519	0.05%	0.006%
75	11.896	1771	1773	1776	rVB2	469	376	0.03%	0.004%
76	11.969	1782	1785	1788	rBV3	526	675	0.06%	0.008%

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

77	12.024	1788	1794	1811	rVV	611788	737008	64.78%	8.382%
78	12.323	1837	1843	1851	rBV	621666	772615	67.91%	8.787%
79	12.853	1928	1930	1931	rBV	565	392	0.03%	0.004%
80	13.359	2010	2013	2014	rBV2	413	388	0.03%	0.004%
81	13.439	2023	2026	2029	rBV3	614	911	0.08%	0.010%
82	13.487	2032	2034	2037	rBV3	354	495	0.04%	0.006%
83	13.652	2059	2061	2063	rBV2	397	366	0.03%	0.004%
84	13.670	2063	2064	2067	rVV2	541	471	0.04%	0.005%
85	13.713	2069	2071	2074	rVB2	485	395	0.03%	0.004%
86	13.786	2081	2083	2086	rVB3	965	687	0.06%	0.008%
87	13.896	2099	2101	2105	rBV2	374	455	0.04%	0.005%
88	13.932	2105	2107	2109	rVB2	511	408	0.04%	0.005%
89	13.951	2109	2110	2113	rVB	575	483	0.04%	0.005%
90	13.975	2113	2114	2117	rBV3	608	697	0.06%	0.008%
91	14.030	2119	2123	2126	rBV3	901	888	0.08%	0.010%
92	14.060	2126	2128	2130	rBV	360	409	0.04%	0.005%
93	14.201	2146	2151	2153	rBV3	603	785	0.07%	0.009%
94	14.286	2163	2165	2166	rVB	588	380	0.03%	0.004%
95	14.310	2166	2169	2171	rBV3	261	373	0.03%	0.004%
96	14.438	2187	2190	2194	rBV2	421	852	0.07%	0.010%
97	14.591	2214	2215	2219	rBV3	358	409	0.04%	0.005%
98	14.926	2267	2270	2273	rBV4	599	871	0.08%	0.010%
99	14.981	2277	2279	2280	rBV	553	380	0.03%	0.004%
100	15.329	2332	2336	2337	rBV2	864	878	0.08%	0.010%

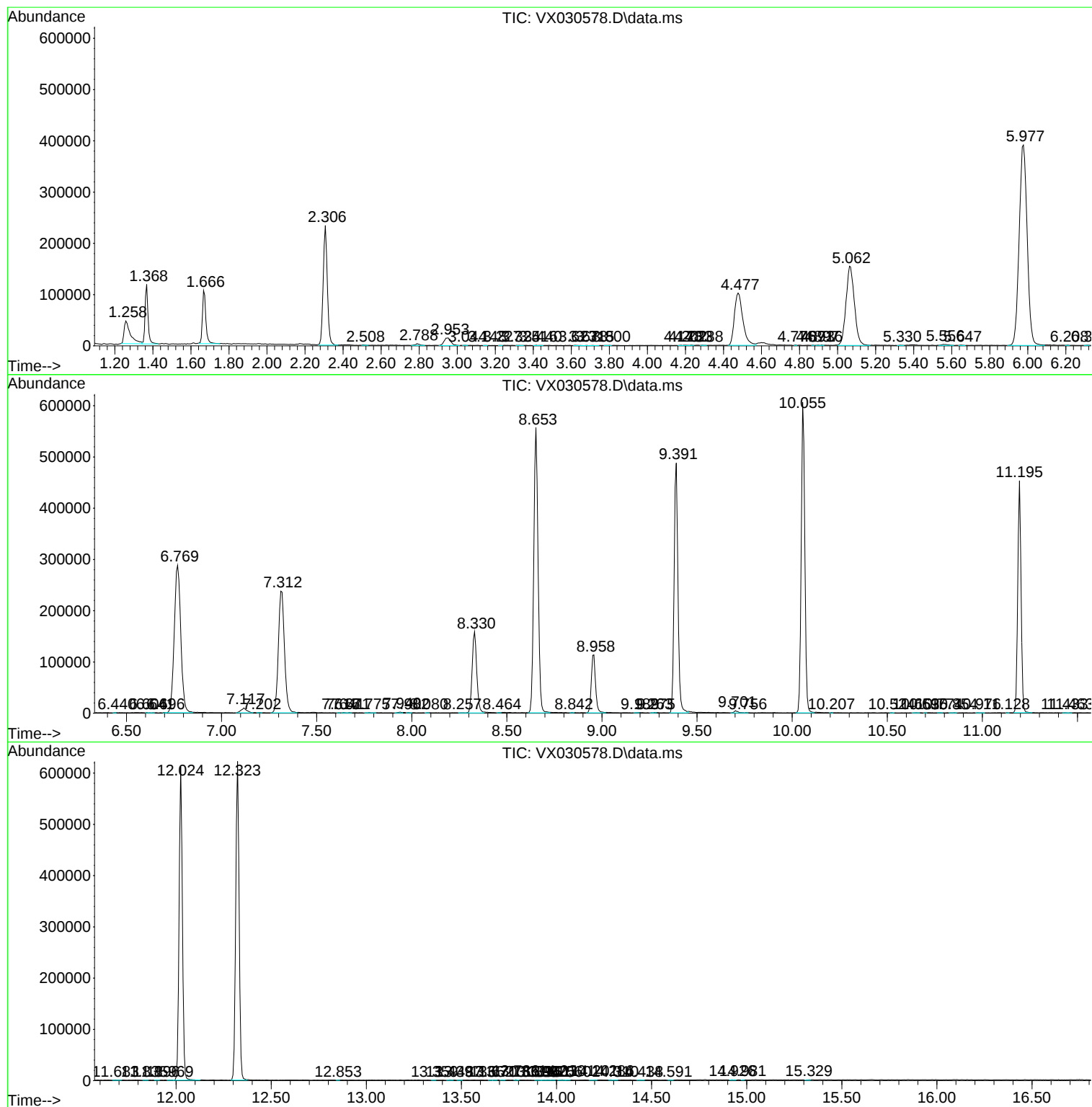
Sum of corrected areas: 8792337

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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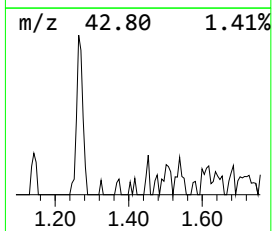
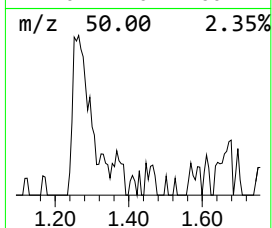
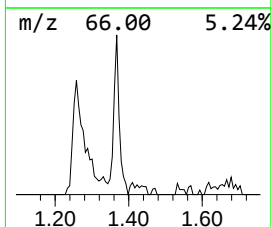
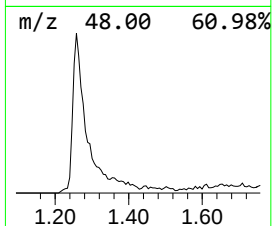
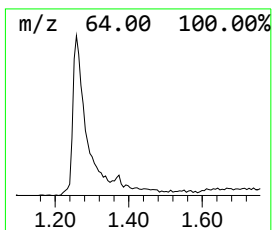
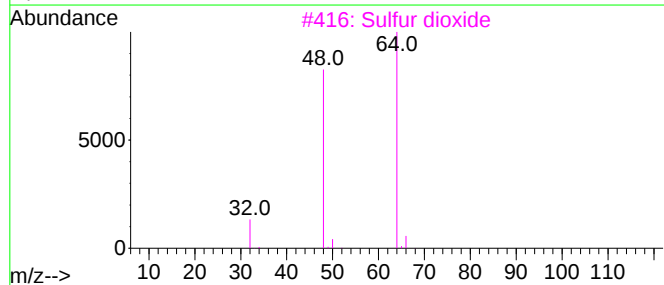
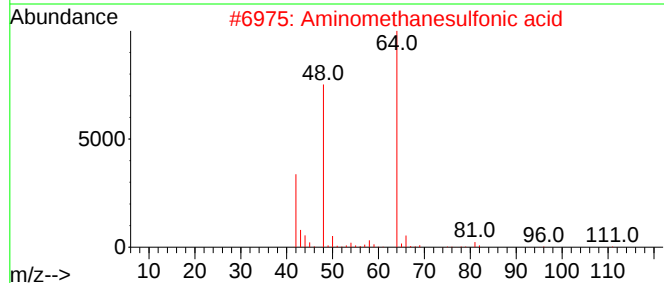
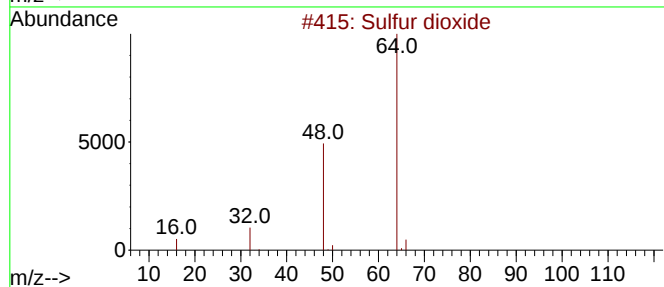
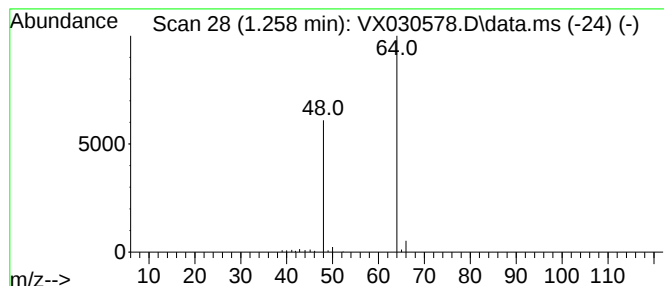
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM080422WMA.M
Quant Title : VOC Analysis

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.
1.258	7.35 ug/L	100056	1,4-Difluorobenzene	6.769

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	83
3			Sulfur dioxide	64	O2S	007446-09-5	83
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	7.3	ug/L	100056	1	6.769	680838	50.0