

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081122\
 Data File : VX030571.D
 Acq On : 11 Aug 2022 14:19
 Operator : JC/MD
 Sample : N4076-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBUU0

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: VX030571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.118	3	5	11	rVB	12263	16484	0.76%	0.154%
2	1.301	29	35	43	rBV	87123	288347	13.29%	2.690%
3	1.368	43	46	53	rVB	116410	145214	6.70%	1.355%
4	1.666	92	95	106	rVB	98643	129602	5.98%	1.209%
5	2.306	195	200	209	rVB2	186534	296066	13.65%	2.762%
6	2.398	211	215	220	rVV2	4205	6850	0.32%	0.064%
7	2.526	229	236	238	rBV4	2776	5756	0.27%	0.054%
8	3.093	323	329	341	rVB	141403	273272	12.60%	2.549%
9	3.617	409	415	423	rVB2	8904	20380	0.94%	0.190%
10	3.678	423	425	428	rVB	591	437	0.02%	0.004%
11	3.721	428	432	434	rVB4	493	633	0.03%	0.006%
12	3.745	434	436	439	rBV2	455	525	0.02%	0.005%
13	4.056	485	487	489	rBV2	370	429	0.02%	0.004%
14	4.148	498	502	504	rVB2	435	508	0.02%	0.005%
15	4.184	504	508	510	rBV3	547	663	0.03%	0.006%
16	4.245	512	518	524	rBV7	1453	4306	0.20%	0.040%
17	4.495	546	559	579	rBV2	759483	2168895	100.00%	20.233%
18	4.757	600	602	604	rBV2	490	495	0.02%	0.005%
19	4.897	623	625	627	rVB2	649	520	0.02%	0.005%
20	4.965	632	636	639	rBV5	853	1321	0.06%	0.012%
21	5.068	641	653	666	rBV	150576	446761	20.60%	4.168%
22	5.312	691	693	695	rBV3	465	507	0.02%	0.005%
23	5.531	727	729	731	rBV2	672	603	0.03%	0.006%
24	5.702	755	757	760	rVB3	884	598	0.03%	0.006%
25	5.824	775	777	780	rVB3	677	672	0.03%	0.006%
26	5.873	780	785	790	rBV3	694	1717	0.08%	0.016%
27	5.977	790	802	822	rBV2	369242	1089849	50.25%	10.167%
28	6.379	864	868	870	rBV4	1328	1962	0.09%	0.018%
29	6.513	888	890	892	rBV2	648	481	0.02%	0.004%
30	6.769	922	932	947	rBV	248221	584916	26.97%	5.457%
31	7.117	982	989	999	rVB9	5192	15558	0.72%	0.145%
32	7.312	1012	1021	1035	rBV	233300	511588	23.59%	4.772%
33	7.604	1066	1069	1072	rBV3	348	467	0.02%	0.004%
34	7.708	1082	1086	1087	rBV	741	831	0.04%	0.008%
35	7.885	1112	1115	1117	rBV2	592	543	0.03%	0.005%
36	7.933	1121	1123	1125	rBV2	900	744	0.03%	0.007%

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37	8.116	1149	1153	1154	rBV2	630	739	0.03%	0.007%
38	8.244	1172	1174	1178	rBV3	515	748	0.03%	0.007%
39	8.330	1182	1188	1198	rVV	155692	257616	11.88%	2.403%
40	8.549	1223	1224	1228	rVB	669	599	0.03%	0.006%
41	8.653	1233	1241	1250	rBV	546062	800273	36.90%	7.466%
42	8.848	1271	1273	1276	rVB3	805	812	0.04%	0.008%
43	8.878	1276	1278	1280	rVB2	488	443	0.02%	0.004%
44	8.952	1284	1290	1301	rBV	117415	177022	8.16%	1.651%
45	9.171	1321	1326	1332	rBV6	1860	3837	0.18%	0.036%
46	9.244	1333	1338	1350	rVB	15022	25360	1.17%	0.237%
47	9.336	1350	1353	1356	rBV3	561	842	0.04%	0.008%
48	9.391	1356	1362	1380	rBV	458301	668548	30.82%	6.237%
49	9.616	1397	1399	1402	rBV2	653	822	0.04%	0.008%
50	9.817	1430	1432	1433	rBV2	672	464	0.02%	0.004%
51	10.012	1461	1464	1465	rVV2	959	1071	0.05%	0.010%
52	10.055	1466	1471	1486	rVB	538238	719532	33.18%	6.712%
53	10.201	1493	1495	1497	rBV2	1027	805	0.04%	0.008%
54	10.244	1501	1502	1505	rVB	907	446	0.02%	0.004%
55	10.378	1519	1524	1532	rVB2	24038	33477	1.54%	0.312%
56	10.451	1534	1536	1539	rVB3	473	594	0.03%	0.006%
57	10.488	1539	1542	1544	rBV2	584	627	0.03%	0.006%
58	10.756	1584	1586	1588	rBV3	560	411	0.02%	0.004%
59	10.835	1596	1599	1600	rBV2	631	465	0.02%	0.004%
60	10.933	1614	1615	1618	rVB2	462	421	0.02%	0.004%
61	10.963	1618	1620	1623	rBV2	935	1013	0.05%	0.009%
62	11.195	1652	1658	1667	rVB	446009	556468	25.66%	5.191%
63	11.341	1679	1682	1684	rBV4	638	810	0.04%	0.008%
64	11.378	1686	1688	1692	rVB2	758	531	0.02%	0.005%
65	11.457	1699	1701	1703	rBV	1099	893	0.04%	0.008%
66	11.573	1715	1720	1725	rVB4	1256	2080	0.10%	0.019%
67	11.646	1730	1732	1736	rVB2	771	750	0.03%	0.007%
68	11.701	1736	1741	1747	rBV6	2211	3720	0.17%	0.035%
69	11.774	1747	1753	1756	rBV5	838	1452	0.07%	0.014%
70	11.829	1758	1762	1763	rVB2	609	735	0.03%	0.007%
71	11.890	1765	1772	1782	rVB5	4889	7741	0.36%	0.072%
72	11.975	1782	1786	1789	rBV3	1297	1609	0.07%	0.015%
73	12.024	1789	1794	1803	rBV	543272	651777	30.05%	6.080%
74	12.323	1837	1843	1852	rBV	629848	755452	34.83%	7.047%
75	12.518	1871	1875	1878	rBV5	1116	1566	0.07%	0.015%
76	12.786	1917	1919	1923	rVB2	606	696	0.03%	0.006%

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 Title : VOC Analysis

77	13.048	1958	1962	1964	rVV2	716	771	0.04%	0.007%
78	13.115	1966	1973	1978	rBV3	1377	3049	0.14%	0.028%
79	13.317	2004	2006	2010	rVV4	700	805	0.04%	0.008%
80	13.347	2010	2011	2015	rVV2	524	539	0.02%	0.005%
81	13.390	2015	2018	2020	rVV	771	841	0.04%	0.008%
82	13.451	2024	2028	2029	rBV	651	778	0.04%	0.007%
83	13.475	2029	2032	2034	rBV	454	570	0.03%	0.005%
84	13.731	2072	2074	2077	rBV3	447	434	0.02%	0.004%
85	13.786	2080	2083	2086	rBV2	599	801	0.04%	0.007%
86	14.024	2118	2122	2123	rBV3	522	540	0.02%	0.005%
87	14.152	2142	2143	2146	rBV2	361	420	0.02%	0.004%
88	14.298	2166	2167	2170	rVB2	483	402	0.02%	0.004%
89	14.323	2170	2171	2173	rBV2	664	516	0.02%	0.005%
90	14.359	2175	2177	2179	rVB	691	406	0.02%	0.004%
91	14.566	2208	2211	2212	rBV2	431	439	0.02%	0.004%
92	14.694	2230	2232	2233	rBV	617	513	0.02%	0.005%
93	14.762	2239	2243	2246	rBV3	653	1228	0.06%	0.011%
94	15.127	2300	2303	2304	rBV2	541	666	0.03%	0.006%
95	15.792	2410	2412	2413	rBV	1123	702	0.03%	0.007%
96	15.835	2417	2419	2422	rBV2	864	875	0.04%	0.008%
97	16.139	2467	2469	2472	rVB3	792	644	0.03%	0.006%
98	16.694	2558	2560	2561	rBV	874	442	0.02%	0.004%
99	16.749	2567	2569	2572	rBV4	704	657	0.03%	0.006%
100	16.779	2572	2574	2575	rBV2	690	699	0.03%	0.007%

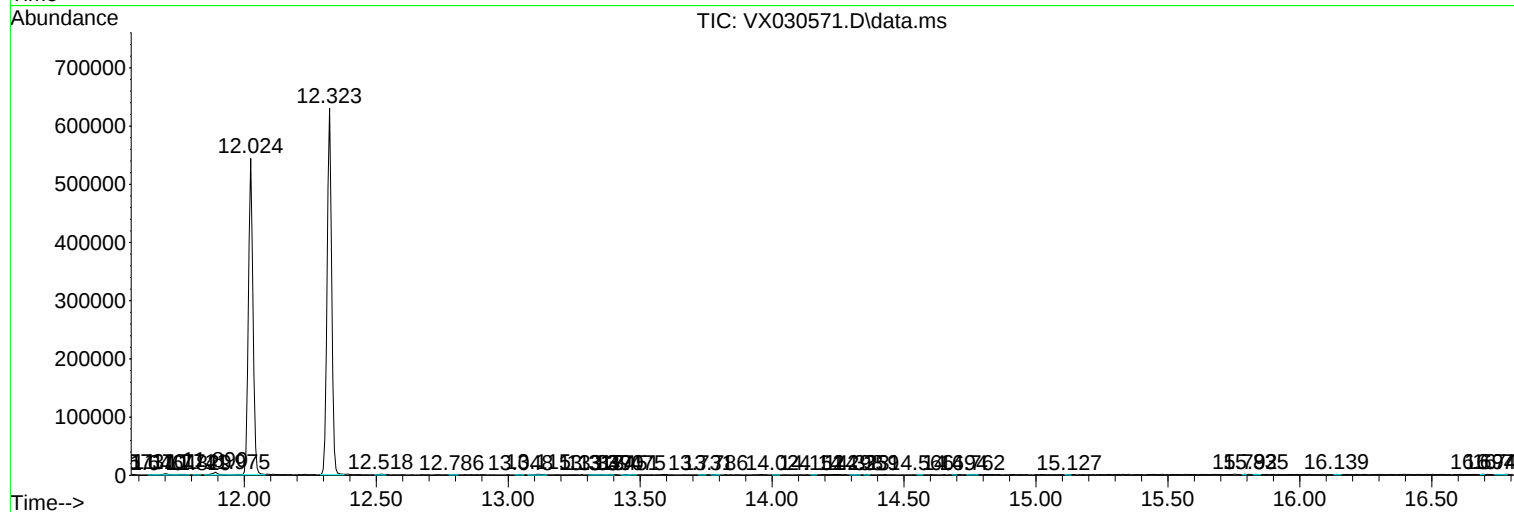
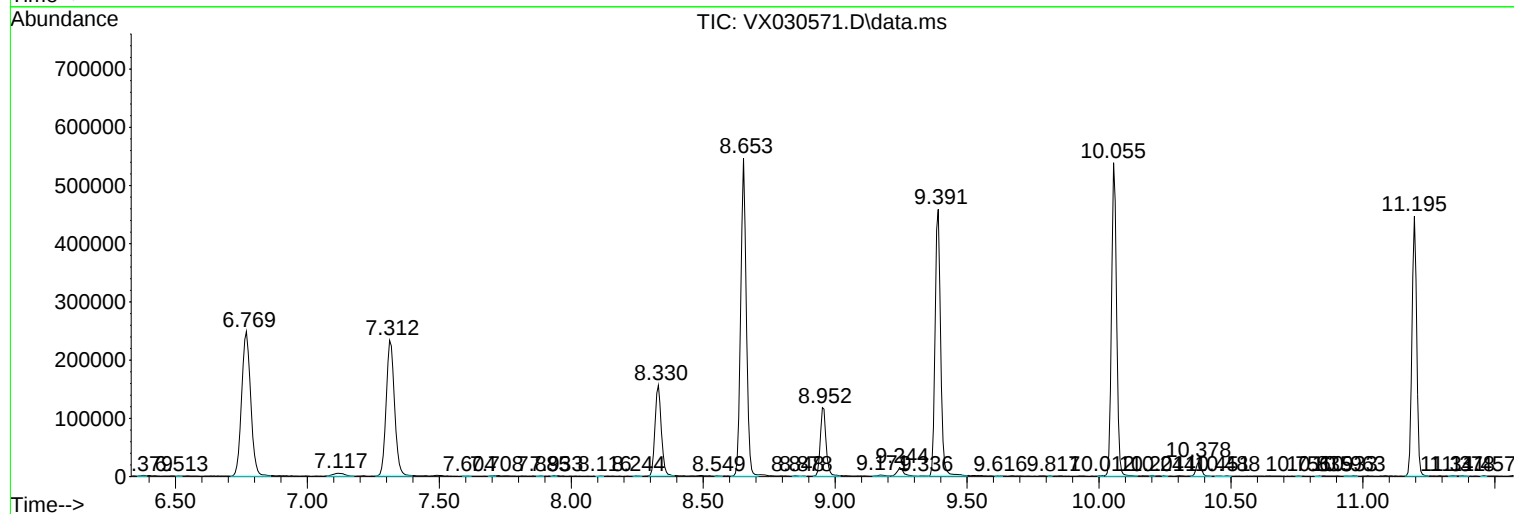
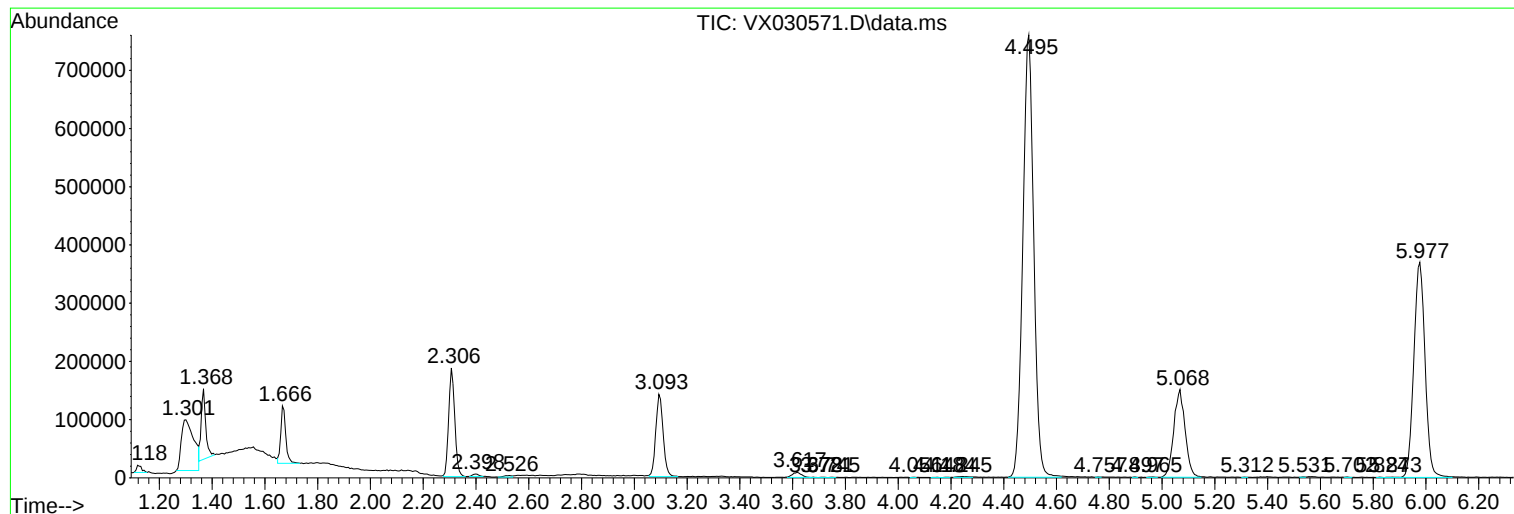
Sum of corrected areas: 10719504

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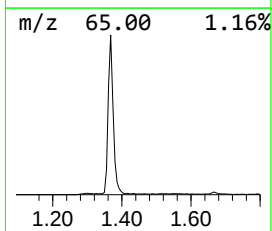
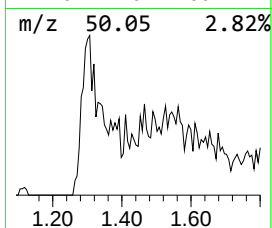
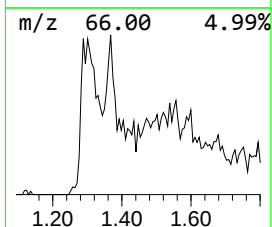
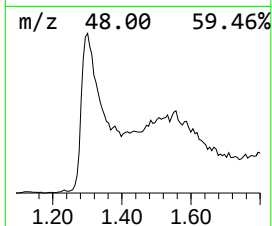
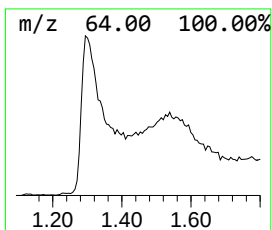
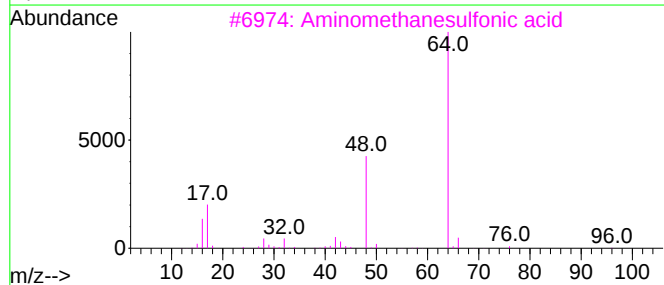
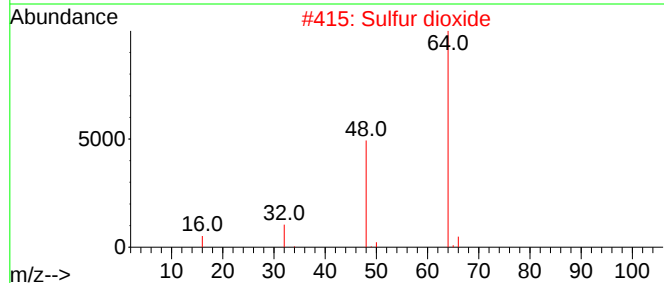
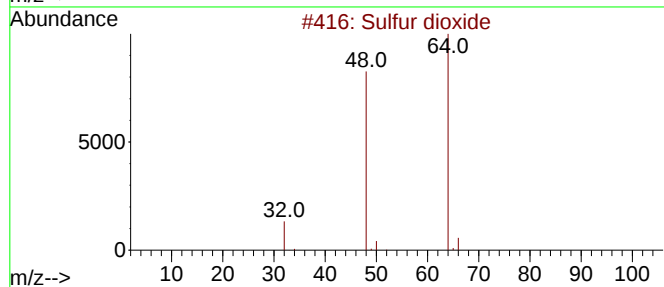
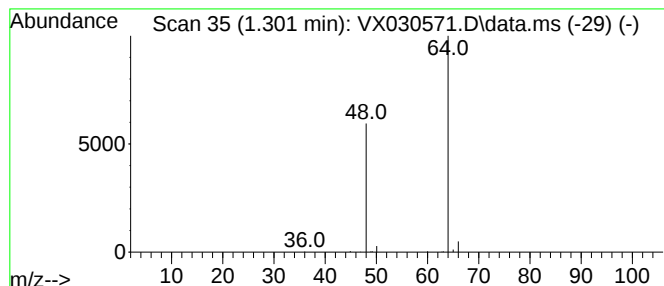
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
1.301	24.65 ug/L	288347	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.301	24.6	ug/L	288347	1	6.769	584916	50.0