

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042781.D
 Acq On : 31 Jul 2024 18:21
 Operator : JC/MD
 Sample : P3398-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08K8

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	33	rBV	13142	18715	4.13%	0.549%
2	1.367	43	46	55	rBV	39841	51321	11.33%	1.504%
3	1.648	89	92	99	rVB	28813	32995	7.29%	0.967%
4	2.294	192	198	211	rBV	90397	149024	32.91%	4.368%
5	2.562	240	242	243	rBV	498	359	0.08%	0.011%
6	2.739	269	271	275	rVB	278	338	0.07%	0.010%
7	2.788	275	279	284	rBV2	895	1649	0.36%	0.048%
8	2.946	298	305	314	rVB2	2495	5636	1.24%	0.165%
9	3.014	314	316	318	rBV	245	177	0.04%	0.005%
10	3.196	344	346	348	rBV2	184	178	0.04%	0.005%
11	3.337	367	369	371	rBV2	329	229	0.05%	0.007%
12	3.471	389	391	393	rBV2	219	173	0.04%	0.005%
13	3.538	399	402	404	rBB	254	222	0.05%	0.007%
14	3.617	413	415	418	rBV	181	229	0.05%	0.007%
15	3.843	450	452	457	rBB	107	197	0.04%	0.006%
16	3.952	468	470	473	rVB	220	206	0.05%	0.006%
17	4.074	487	490	491	rBV	180	165	0.04%	0.005%
18	4.111	494	496	498	rBV	145	184	0.04%	0.005%
19	4.208	510	512	514	rBV	192	189	0.04%	0.006%
20	4.471	546	555	570	rBV	32839	96470	21.31%	2.828%
21	4.733	596	598	600	rVB	373	248	0.05%	0.007%
22	4.897	620	625	628	rBV2	200	389	0.09%	0.011%
23	5.062	640	652	668	rBV2	61757	190530	42.08%	5.585%
24	5.281	686	688	691	rBV	211	271	0.06%	0.008%
25	5.653	746	749	751	rVB2	212	230	0.05%	0.007%
26	5.824	774	777	780	rBB2	257	281	0.06%	0.008%
27	5.970	788	801	818	rBV3	155760	452802	100.00%	13.272%
28	6.409	870	873	874	rBV	167	187	0.04%	0.005%
29	6.556	894	897	900	rBV	214	221	0.05%	0.006%
30	6.623	907	908	911	rBV	223	193	0.04%	0.006%
31	6.684	916	918	921	rBV	293	341	0.08%	0.010%
32	6.763	922	931	941	rBV2	120692	284878	62.91%	8.350%
33	7.013	970	972	975	rBV	218	230	0.05%	0.007%
34	7.068	979	981	982	rBV	278	203	0.04%	0.006%
35	7.220	1004	1006	1009	rBV	284	247	0.05%	0.007%
36	7.312	1012	1021	1036	rVV	86692	200956	44.38%	5.890%

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 Title : VOC Analysis

37	7.555	1059	1061	1063	rBV	205	191	0.04%	0.006%
38	7.671	1076	1080	1082	rBV	248	225	0.05%	0.007%
39	7.836	1101	1107	1111	rVB4	2145	4036	0.89%	0.118%
40	7.872	1111	1113	1117	rVB2	211	179	0.04%	0.005%
41	8.025	1137	1138	1140	rBV2	293	181	0.04%	0.005%
42	8.116	1150	1153	1155	rBV	209	286	0.06%	0.008%
43	8.171	1160	1162	1163	rBV	198	171	0.04%	0.005%
44	8.287	1179	1181	1182	rBV	236	224	0.05%	0.007%
45	8.330	1182	1188	1200	rVV	53112	92643	20.46%	2.716%
46	8.592	1229	1231	1233	rBV	286	285	0.06%	0.008%
47	8.647	1234	1240	1259	rVV	219908	360422	79.60%	10.565%
48	8.915	1281	1284	1285	rBV	151	164	0.04%	0.005%
49	8.951	1285	1290	1302	rVV	37748	59051	13.04%	1.731%
50	9.086	1310	1312	1315	rBV2	180	188	0.04%	0.006%
51	9.165	1323	1325	1328	rVB	238	221	0.05%	0.006%
52	9.275	1338	1343	1348	rVB3	2593	4228	0.93%	0.124%
53	9.311	1348	1349	1351	rBV3	183	160	0.04%	0.005%
54	9.390	1357	1362	1371	rBV	132526	203751	45.00%	5.972%
55	9.640	1398	1403	1404	rBV2	314	514	0.11%	0.015%
56	9.671	1404	1408	1409	rVV	211	226	0.05%	0.007%
57	9.756	1419	1422	1425	rBV	384	395	0.09%	0.012%
58	9.787	1425	1427	1430	rVV2	204	185	0.04%	0.005%
59	9.915	1446	1448	1451	rBV2	146	191	0.04%	0.006%
60	10.055	1465	1471	1484	rBV	239995	335615	74.12%	9.837%
61	10.189	1491	1493	1498	rVB3	380	507	0.11%	0.015%
62	10.701	1573	1577	1579	rBB	274	376	0.08%	0.011%
63	10.805	1590	1594	1599	rBV3	1941	3000	0.66%	0.088%
64	10.884	1604	1607	1611	rBV	261	260	0.06%	0.008%
65	11.146	1646	1650	1652	rBV	206	317	0.07%	0.009%
66	11.189	1652	1657	1665	rBV	171374	233544	51.58%	6.846%
67	11.311	1671	1677	1682	rBV2	2623	3802	0.84%	0.111%
68	11.500	1706	1708	1711	rBV	165	215	0.05%	0.006%
69	11.549	1714	1716	1719	rBV2	173	211	0.05%	0.006%
70	11.634	1728	1730	1733	rVB	182	215	0.05%	0.006%
71	11.658	1733	1734	1737	rBV	235	222	0.05%	0.007%
72	11.756	1748	1750	1755	rVB2	355	466	0.10%	0.014%
73	11.835	1761	1763	1768	rBB2	222	330	0.07%	0.010%
74	11.884	1769	1771	1774	rVB	226	192	0.04%	0.006%
75	11.933	1774	1779	1783	rBV3	1171	1855	0.41%	0.054%
76	12.024	1789	1794	1801	rBV	224147	289211	63.87%	8.477%

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 Title : VOC Analysis

77	12.219	1824	1826	1834	rVB3	901	1486	0.33%	0.044%
78	12.323	1837	1843	1851	rBV	224618	302931	66.90%	8.879%
79	12.487	1868	1870	1876	rBB	209	362	0.08%	0.011%
80	12.530	1876	1877	1880	rBV	239	243	0.05%	0.007%
81	12.756	1912	1914	1920	rVB3	778	1127	0.25%	0.033%
82	12.859	1929	1931	1934	rVB2	1769	1821	0.40%	0.053%
83	12.993	1950	1953	1954	rBB2	225	170	0.04%	0.005%
84	13.152	1976	1979	1981	rBV	160	194	0.04%	0.006%
85	13.189	1981	1985	1986	rVV	235	257	0.06%	0.008%
86	13.237	1990	1993	1995	rVB	189	183	0.04%	0.005%
87	13.268	1995	1998	2000	rBB	258	253	0.06%	0.007%
88	13.298	2000	2003	2004	rBV2	299	317	0.07%	0.009%
89	13.396	2016	2019	2021	rBV	215	277	0.06%	0.008%
90	13.487	2031	2034	2037	rBV	217	356	0.08%	0.010%
91	13.780	2077	2082	2088	rBV	5501	7578	1.67%	0.222%
92	13.859	2093	2095	2097	rBV	189	206	0.05%	0.006%
93	14.127	2136	2139	2144	rVB2	1215	1654	0.37%	0.048%
94	14.390	2180	2182	2183	rBV	319	211	0.05%	0.006%
95	14.566	2210	2211	2214	rBV2	311	334	0.07%	0.010%
96	14.609	2216	2218	2220	rBV	217	169	0.04%	0.005%
97	14.652	2220	2225	2230	rVB2	644	1023	0.23%	0.030%
98	14.725	2235	2237	2239	rBV2	191	182	0.04%	0.005%
99	16.334	2498	2501	2504	rBV2	642	714	0.16%	0.021%
100	16.517	2529	2531	2532	rBV	371	263	0.06%	0.008%

Sum of corrected areas: 3411629

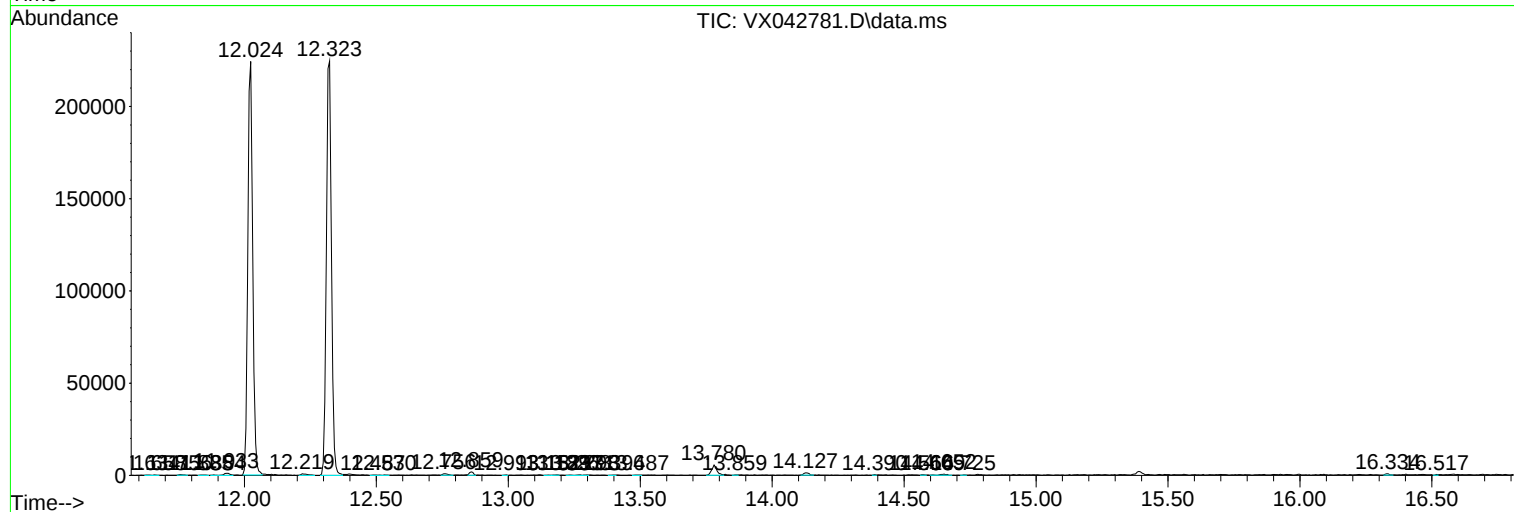
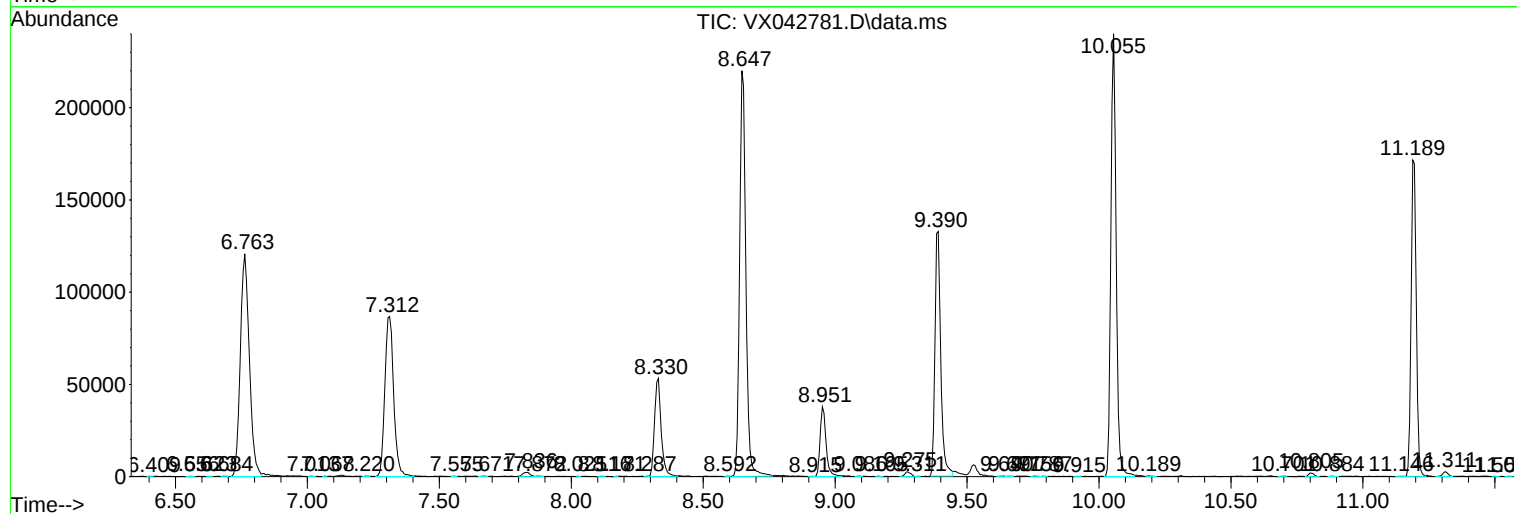
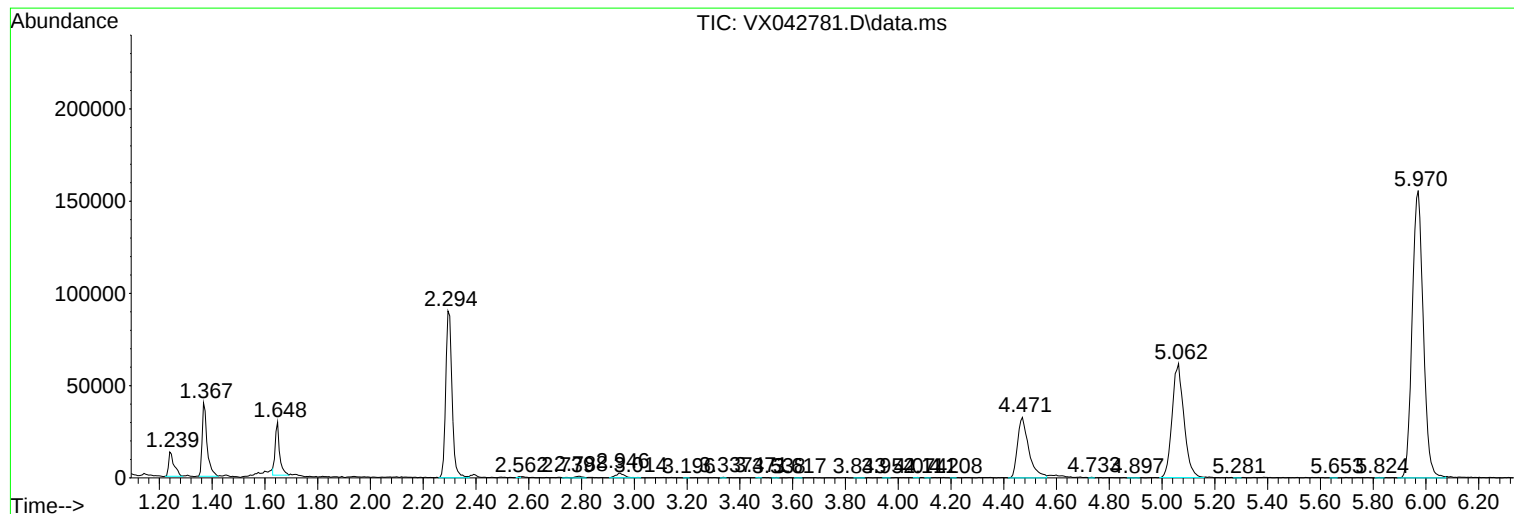
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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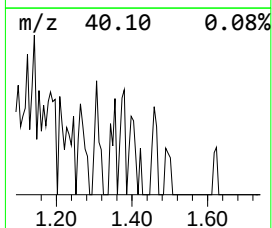
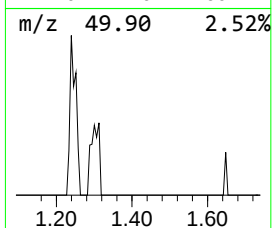
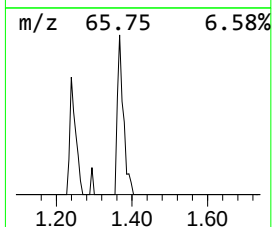
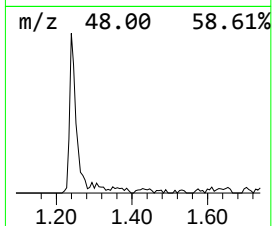
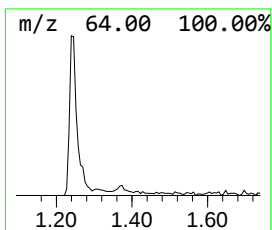
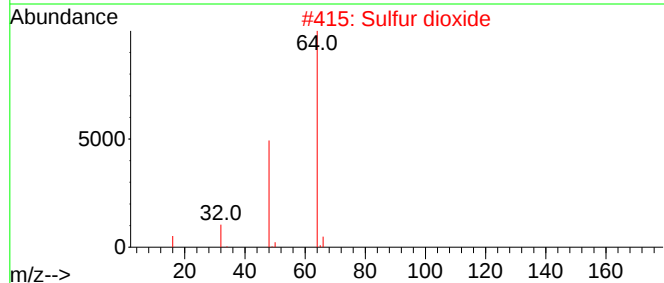
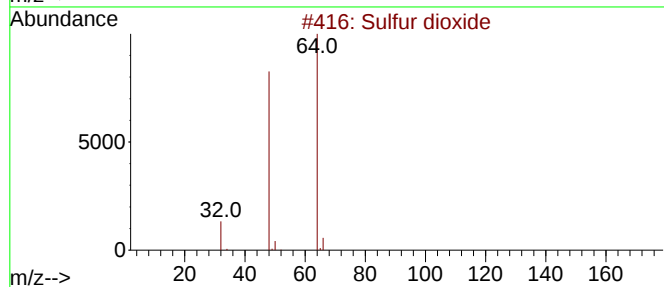
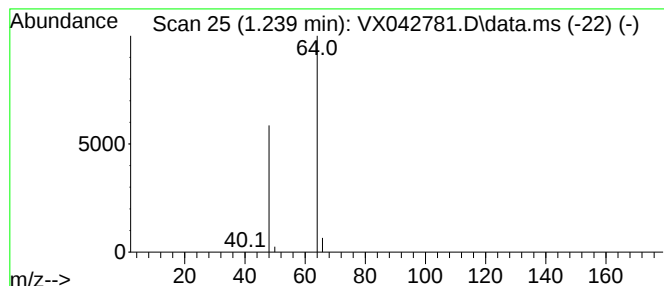
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.239	3.28 ug/L	18715	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Sulfur dioxide	64	O2S	007446-09-5	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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	3.3	ug/L	18715	1	6.763	284878	50.0