

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081022\
 Data File : VX030557.D
 Acq On : 10 Aug 2022 17:08
 Operator : JC/MD
 Sample : N4076-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBUV0

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: VX030557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	32	rBV	167061	286491	22.34%	2.876%
2	1.368	43	46	53	rVB	151677	167162	13.03%	1.678%
3	1.666	92	95	105	rVB	120878	153746	11.99%	1.543%
4	2.306	194	200	210	rVB	248607	394384	30.75%	3.959%
5	2.514	230	234	235	rBV2	1160	1416	0.11%	0.014%
6	2.648	254	256	258	rBV3	651	419	0.03%	0.004%
7	2.782	276	278	280	rBV3	1494	1404	0.11%	0.014%
8	2.855	288	290	293	rBV4	664	780	0.06%	0.008%
9	3.093	323	329	339	rBV	46737	95203	7.42%	0.956%
10	3.221	349	350	354	rVB4	381	409	0.03%	0.004%
11	3.410	379	381	383	rBV2	397	331	0.03%	0.003%
12	3.501	394	396	397	rBV	634	360	0.03%	0.004%
13	3.544	399	403	404	rVV3	572	546	0.04%	0.005%
14	3.611	412	414	417	rVB2	699	708	0.06%	0.007%
15	3.678	422	425	428	rVB3	652	586	0.05%	0.006%
16	3.727	428	433	434	rBV3	444	684	0.05%	0.007%
17	3.830	449	450	452	rVV	513	326	0.03%	0.003%
18	3.867	452	456	457	rVV3	523	577	0.04%	0.006%
19	3.946	468	469	471	rVV2	492	346	0.03%	0.003%
20	4.087	489	492	496	rBV3	502	742	0.06%	0.007%
21	4.141	498	501	503	rBV2	502	469	0.04%	0.005%
22	4.196	505	510	511	rBV3	669	1083	0.08%	0.011%
23	4.483	547	557	573	rBV3	166441	548636	42.78%	5.508%
24	4.873	619	621	623	rBV2	636	539	0.04%	0.005%
25	5.068	641	653	669	rBV	166539	523240	40.80%	5.253%
26	5.976	789	802	819	rBV2	437506	1282600	100.00%	12.876%
27	6.348	862	863	864	rBV	621	425	0.03%	0.004%
28	6.464	880	882	885	rBV2	470	320	0.02%	0.003%
29	6.653	909	913	915	rBV3	727	796	0.06%	0.008%
30	6.671	915	916	919	rVB	691	545	0.04%	0.005%
31	6.696	919	920	923	rBV2	613	714	0.06%	0.007%
32	6.769	923	932	946	rVV	281732	671695	52.37%	6.743%
33	6.946	958	961	963	rBV3	325	369	0.03%	0.004%
34	7.013	968	972	977	rBV4	720	1282	0.10%	0.013%
35	7.116	985	989	999	rVB9	5839	13859	1.08%	0.139%
36	7.312	1012	1021	1034	rVV	276675	604949	47.17%	6.073%

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 Title : VOC Analysis

37	7.641	1074	1075	1077	rBV	586	410	0.03%	0.004%
38	8.000	1133	1134	1136	rVB2	602	324	0.03%	0.003%
39	8.128	1154	1155	1157	rBV2	357	346	0.03%	0.003%
40	8.330	1180	1188	1196	rBV	180525	290901	22.68%	2.920%
41	8.452	1206	1208	1210	rBV3	530	359	0.03%	0.004%
42	8.494	1213	1215	1217	rBV2	629	495	0.04%	0.005%
43	8.592	1228	1231	1234	rBV4	498	703	0.05%	0.007%
44	8.653	1234	1241	1255	rBV	650326	996569	77.70%	10.005%
45	8.872	1273	1277	1280	rVB4	569	813	0.06%	0.008%
46	8.952	1284	1290	1300	rBV	133003	193966	15.12%	1.947%
47	9.086	1310	1312	1316	rVB3	1086	1187	0.09%	0.012%
48	9.165	1323	1325	1329	rVB3	651	694	0.05%	0.007%
49	9.195	1329	1330	1333	rBV3	467	362	0.03%	0.004%
50	9.250	1335	1339	1341	rBV3	481	633	0.05%	0.006%
51	9.342	1353	1354	1356	rBV2	631	539	0.04%	0.005%
52	9.390	1356	1362	1374	rVV	500478	714468	55.70%	7.173%
53	9.805	1429	1430	1431	rBV	539	358	0.03%	0.004%
54	9.939	1450	1452	1456	rBV2	653	655	0.05%	0.007%
55	10.000	1461	1462	1465	rBV2	532	587	0.05%	0.006%
56	10.055	1466	1471	1483	rVB	547527	763430	59.52%	7.664%
57	10.378	1520	1524	1528	rVB3	2954	4354	0.34%	0.044%
58	10.518	1546	1547	1550	rVB2	430	339	0.03%	0.003%
59	10.805	1593	1594	1598	rBV2	394	560	0.04%	0.006%
60	10.884	1606	1607	1610	rBV2	622	391	0.03%	0.004%
61	10.945	1615	1617	1619	rBV3	448	540	0.04%	0.005%
62	11.037	1629	1632	1634	rBV2	636	502	0.04%	0.005%
63	11.067	1636	1637	1638	rBV	507	330	0.03%	0.003%
64	11.195	1652	1658	1668	rBV	486181	609612	47.53%	6.120%
65	11.335	1678	1681	1682	rVB3	524	476	0.04%	0.005%
66	11.445	1698	1699	1701	rBV2	582	344	0.03%	0.003%
67	11.536	1713	1714	1718	rVB2	633	497	0.04%	0.005%
68	11.579	1718	1721	1722	rBV2	456	463	0.04%	0.005%
69	12.024	1789	1794	1802	rBV	590207	716587	55.87%	7.194%
70	12.128	1809	1811	1812	rVB	817	449	0.04%	0.005%
71	12.152	1812	1815	1819	rVB2	773	934	0.07%	0.009%
72	12.189	1819	1821	1822	rVB2	594	419	0.03%	0.004%
73	12.201	1822	1823	1825	rBV2	373	393	0.03%	0.004%
74	12.219	1825	1826	1827	rBV	910	452	0.04%	0.005%
75	12.323	1837	1843	1854	rBV	719442	880990	68.69%	8.844%
76	12.597	1885	1888	1890	rBV2	566	600	0.05%	0.006%

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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

77	13.012	1955	1956	1959	rVV2	429	399	0.03%	0.004%
78	13.085	1967	1968	1972	rVB2	818	897	0.07%	0.009%
79	13.128	1974	1975	1977	rVB	900	445	0.03%	0.004%
80	13.164	1977	1981	1984	rBV4	509	729	0.06%	0.007%
81	13.530	2039	2041	2043	rBV	626	520	0.04%	0.005%
82	13.670	2062	2064	2065	rBV	446	331	0.03%	0.003%
83	13.810	2085	2087	2089	rVB2	764	613	0.05%	0.006%
84	13.835	2089	2091	2093	rBV2	884	851	0.07%	0.009%
85	13.957	2107	2111	2112	rBV	762	1131	0.09%	0.011%
86	14.018	2120	2121	2123	rBV2	703	653	0.05%	0.007%
87	14.140	2138	2141	2143	rBV2	435	382	0.03%	0.004%
88	14.408	2182	2185	2187	rVB3	776	862	0.07%	0.009%
89	14.432	2187	2189	2190	rBV	761	528	0.04%	0.005%
90	14.585	2213	2214	2216	rBV	579	470	0.04%	0.005%
91	14.700	2231	2233	2234	rBV2	696	380	0.03%	0.004%
92	15.066	2291	2293	2296	rVB3	558	430	0.03%	0.004%
93	15.097	2296	2298	2299	rBV2	767	529	0.04%	0.005%
94	15.267	2324	2326	2327	rVB	1037	550	0.04%	0.006%
95	16.060	2454	2456	2457	rVB2	764	359	0.03%	0.004%
96	16.084	2457	2460	2464	rBV4	882	1793	0.14%	0.018%
97	16.359	2503	2505	2506	rBV2	779	678	0.05%	0.007%
98	16.407	2511	2513	2517	rVV4	875	1039	0.08%	0.010%
99	16.560	2536	2538	2542	rVB4	944	849	0.07%	0.009%
100	16.596	2542	2544	2545	rBV2	637	339	0.03%	0.003%

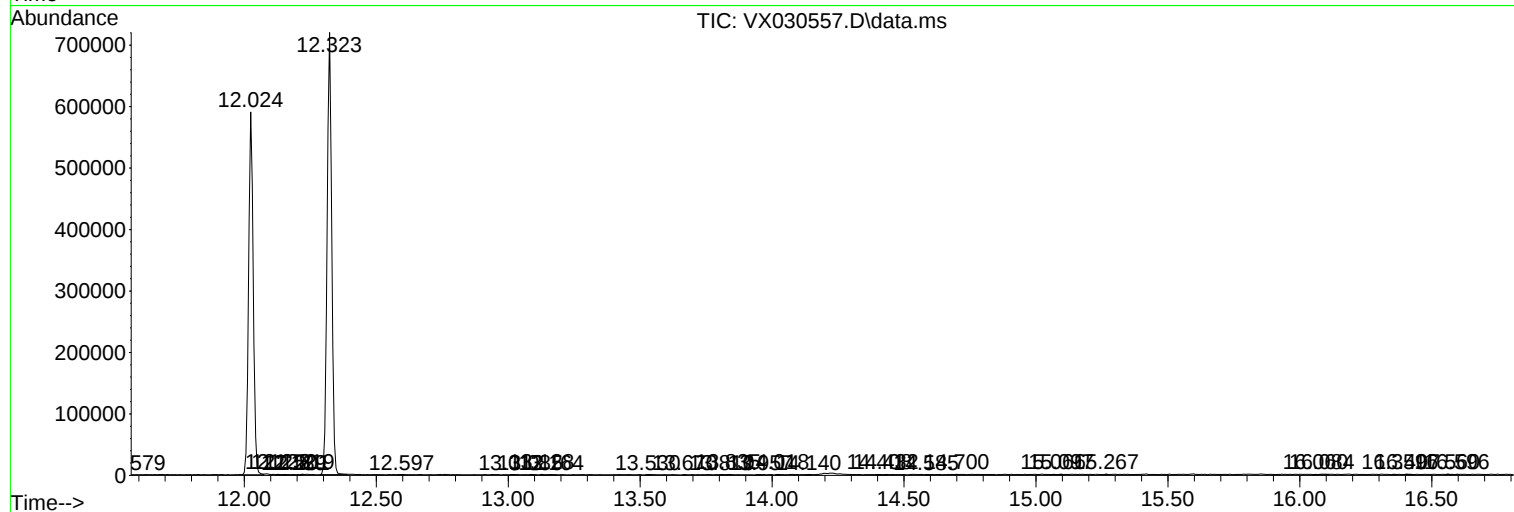
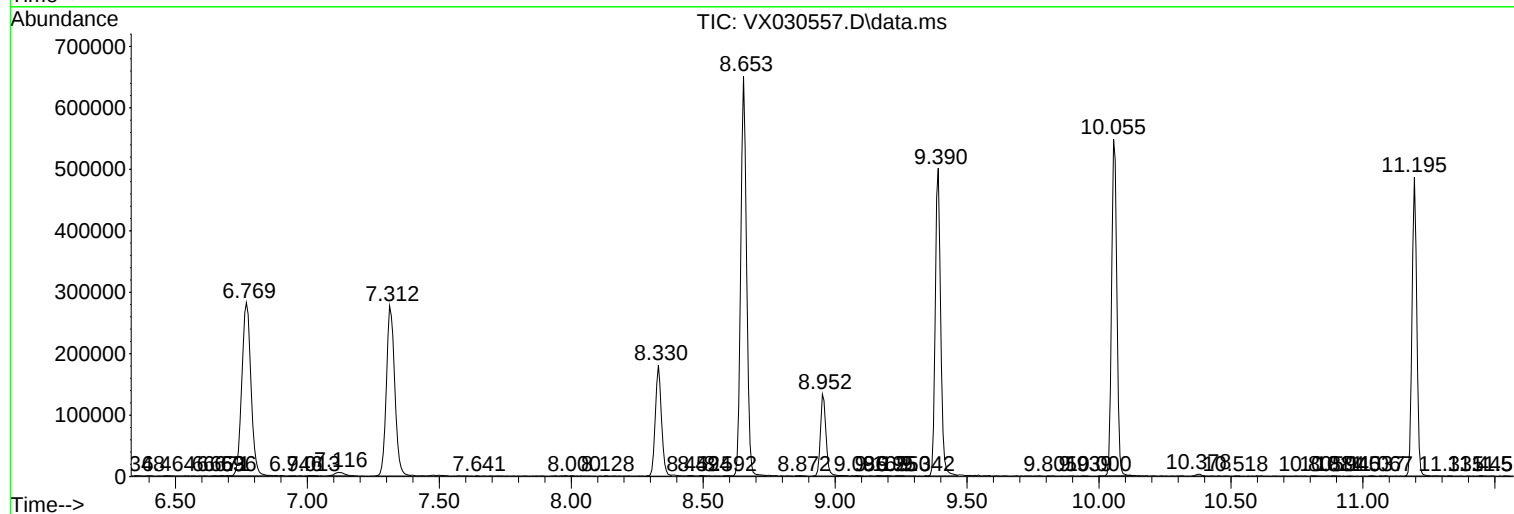
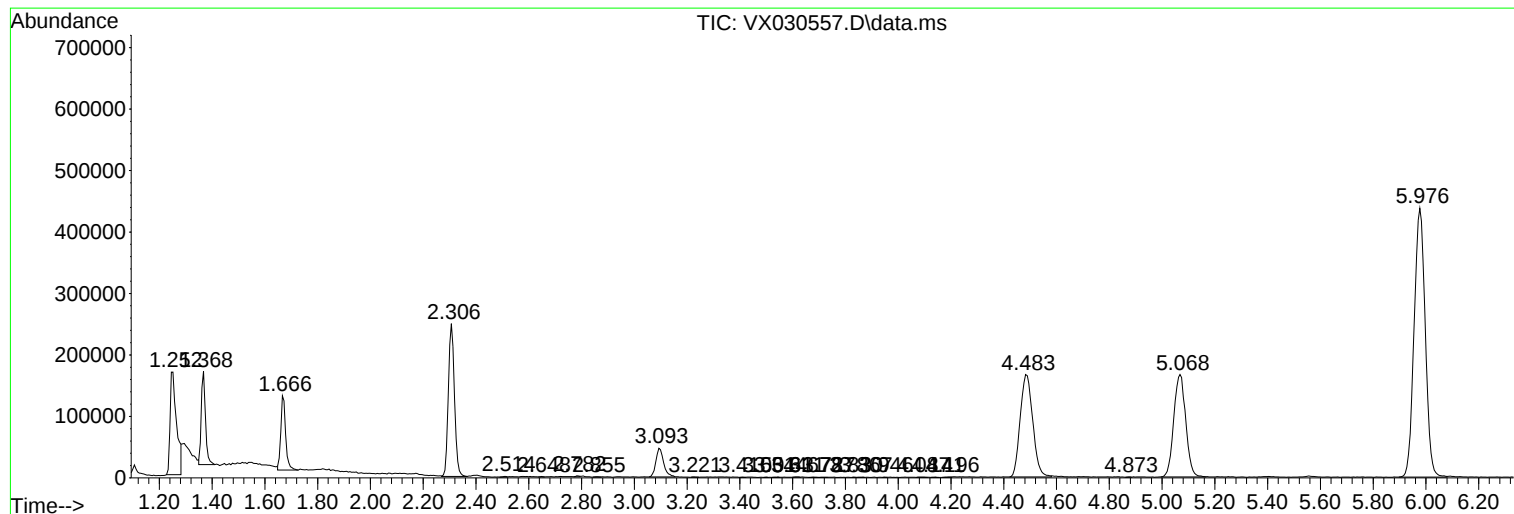
Sum of corrected areas: 9960929

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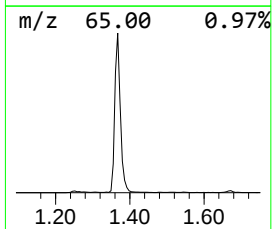
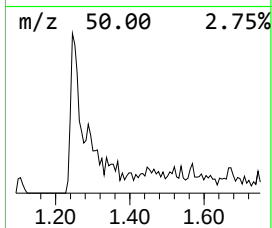
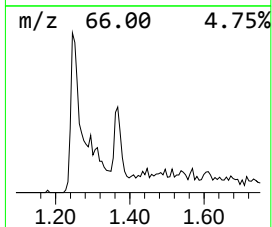
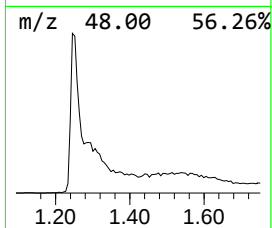
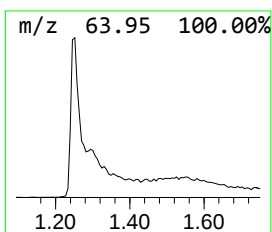
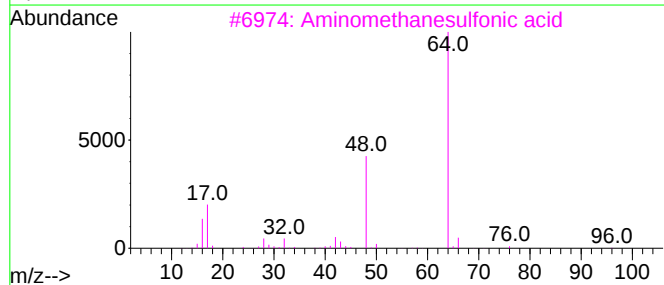
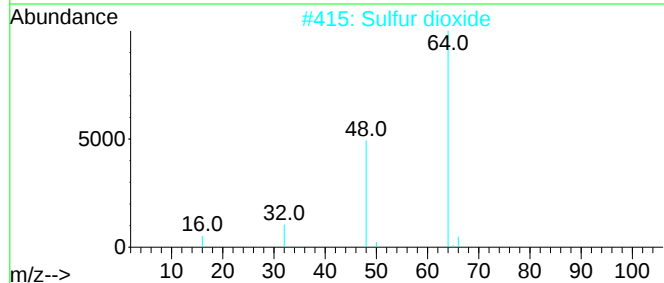
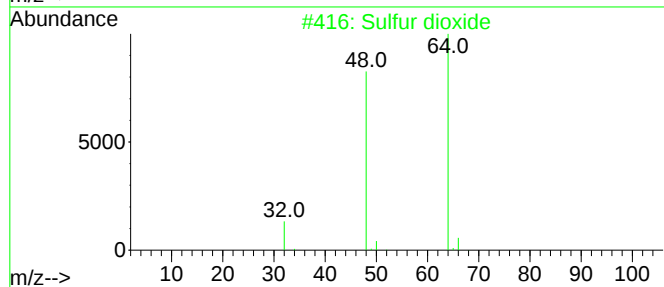
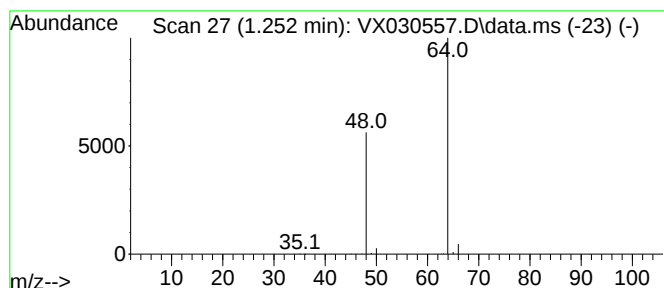
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	21.33 ug/L	286491	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	1.252	21.3	ug/L	286491	1	6.769	671695	50.0