

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081022\
 Data File : VX030560.D
 Acq On : 10 Aug 2022 18:19
 Operator : JC/MD
 Sample : N4114-05RE
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D74RE

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: VX030560.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.124	3	6	10	rBV	43469	58783	4.55%	0.593%
2	1.252	23	27	29	rBV	75857	105226	8.15%	1.062%
3	1.368	43	46	56	rVB	255061	296895	22.99%	2.996%
4	1.666	92	95	104	rVB	124672	152872	11.84%	1.543%
5	2.306	194	200	211	rVB	270812	404666	31.33%	4.084%
6	2.526	230	236	237	rBV2	2233	3500	0.27%	0.035%
7	3.093	324	329	339	rVB2	19698	36560	2.83%	0.369%
8	3.556	402	405	406	rBV2	456	379	0.03%	0.004%
9	3.696	426	428	429	rBV	554	362	0.03%	0.004%
10	3.800	443	445	448	rVB2	333	294	0.02%	0.003%
11	3.837	450	451	455	rBV2	568	617	0.05%	0.006%
12	3.904	459	462	467	rBV3	685	998	0.08%	0.010%
13	4.038	483	484	487	rVB2	420	339	0.03%	0.003%
14	4.087	490	492	495	rVB5	447	428	0.03%	0.004%
15	4.129	497	499	502	rBV3	580	793	0.06%	0.008%
16	4.160	502	504	505	rVV2	499	304	0.02%	0.003%
17	4.367	536	538	540	rBV	557	468	0.04%	0.005%
18	4.483	545	557	572	rBV3	189996	625469	48.43%	6.312%
19	5.068	639	653	669	rBV	176262	529365	40.99%	5.342%
20	5.220	676	678	679	rBV2	534	476	0.04%	0.005%
21	5.349	698	699	700	rBV	678	365	0.03%	0.004%
22	5.678	750	753	755	rVB2	535	491	0.04%	0.005%
23	5.763	763	767	769	rBV2	589	1010	0.08%	0.010%
24	5.976	790	802	818	rBV2	446052	1291589	100.00%	13.035%
25	6.196	835	838	840	rBV3	448	640	0.05%	0.006%
26	6.336	860	861	864	rBV3	572	661	0.05%	0.007%
27	6.470	880	883	886	rBV2	655	756	0.06%	0.008%
28	6.769	921	932	942	rBV	296005	683900	52.95%	6.902%
29	7.037	975	976	978	rBV	496	397	0.03%	0.004%
30	7.129	983	991	1000	rVB6	8965	23561	1.82%	0.238%
31	7.318	1013	1022	1036	rVB	277782	602045	46.61%	6.076%
32	7.604	1065	1069	1074	rBV4	719	1200	0.09%	0.012%
33	7.903	1116	1118	1119	rBV	671	426	0.03%	0.004%
34	7.940	1122	1124	1125	rBV2	723	659	0.05%	0.007%
35	8.019	1135	1137	1139	rBV2	778	671	0.05%	0.007%
36	8.043	1139	1141	1143	rVV3	600	508	0.04%	0.005%

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 Title : VOC Analysis

37	8.074	1143	1146	1148	rVV2	393	497	0.04%	0.005%
38	8.171	1161	1162	1164	rBV	578	500	0.04%	0.005%
39	8.275	1178	1179	1182	rBV	556	460	0.04%	0.005%
40	8.330	1182	1188	1198	rBV	72779	119267	9.23%	1.204%
41	8.494	1213	1215	1218	rBV4	425	403	0.03%	0.004%
42	8.592	1230	1231	1232	rBV	794	486	0.04%	0.005%
43	8.653	1234	1241	1251	rVV	642865	985436	76.30%	9.945%
44	8.958	1285	1291	1299	rBV	87221	132187	10.23%	1.334%
45	9.275	1340	1343	1350	rVB4	1855	2787	0.22%	0.028%
46	9.390	1356	1362	1371	rBV	540870	771942	59.77%	7.790%
47	9.555	1386	1389	1393	rBV6	931	1351	0.10%	0.014%
48	9.628	1399	1401	1404	rBV3	701	808	0.06%	0.008%
49	9.921	1446	1449	1450	rBV2	436	410	0.03%	0.004%
50	10.055	1466	1471	1482	rBV	575803	775826	60.07%	7.830%
51	10.159	1486	1488	1489	rBV2	419	323	0.03%	0.003%
52	10.238	1500	1501	1503	rBV2	879	550	0.04%	0.006%
53	10.274	1505	1507	1508	rBV	930	592	0.05%	0.006%
54	10.384	1522	1525	1526	rBV3	366	388	0.03%	0.004%
55	10.445	1533	1535	1539	rBV2	518	753	0.06%	0.008%
56	10.543	1547	1551	1553	rBV3	670	999	0.08%	0.010%
57	10.634	1564	1566	1569	rBV3	797	1049	0.08%	0.011%
58	10.750	1583	1585	1589	rVB3	442	335	0.03%	0.003%
59	10.780	1589	1590	1594	rVB	388	316	0.02%	0.003%
60	10.976	1620	1622	1625	rBV2	391	323	0.03%	0.003%
61	11.073	1637	1638	1640	rBV2	413	351	0.03%	0.004%
62	11.195	1653	1658	1669	rVB	492423	619526	47.97%	6.252%
63	11.518	1709	1711	1714	rBV3	616	638	0.05%	0.006%
64	11.585	1721	1722	1725	rBV2	750	513	0.04%	0.005%
65	11.610	1725	1726	1728	rVV	465	397	0.03%	0.004%
66	11.652	1730	1733	1737	rVV5	1392	2260	0.17%	0.023%
67	11.719	1740	1744	1747	rVB3	574	943	0.07%	0.010%
68	11.866	1766	1768	1770	rVB2	555	465	0.04%	0.005%
69	11.951	1781	1782	1785	rBV2	376	313	0.02%	0.003%
70	12.024	1788	1794	1805	rBV	636108	746948	57.83%	7.538%
71	12.183	1818	1820	1821	rVB2	630	379	0.03%	0.004%
72	12.225	1824	1827	1828	rBV2	874	647	0.05%	0.007%
73	12.323	1837	1843	1853	rBV	721147	892858	69.13%	9.011%
74	12.597	1887	1888	1890	rBV2	468	386	0.03%	0.004%
75	12.731	1909	1910	1913	rVB2	428	317	0.02%	0.003%
76	12.841	1925	1928	1932	rBV4	447	667	0.05%	0.007%

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Integrator: RTE

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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	12.884	1932	1935	1936	rBV2	722	605	0.05%	0.006%
78	12.902	1936	1938	1939	rVV	645	408	0.03%	0.004%
79	13.048	1960	1962	1967	rBV2	496	941	0.07%	0.009%
80	13.170	1980	1982	1985	rBV4	304	311	0.02%	0.003%
81	13.280	1997	2000	2004	rVB3	834	1178	0.09%	0.012%
82	13.384	2015	2017	2019	rBV2	486	362	0.03%	0.004%
83	13.402	2019	2020	2022	rVV2	574	324	0.03%	0.003%
84	13.420	2022	2023	2025	rBV	482	306	0.02%	0.003%
85	13.469	2030	2031	2036	rVB2	874	704	0.05%	0.007%
86	13.829	2088	2090	2091	rVB2	552	351	0.03%	0.004%
87	13.847	2091	2093	2096	rBV3	506	606	0.05%	0.006%
88	13.877	2096	2098	2100	rVV3	614	553	0.04%	0.006%
89	13.902	2100	2102	2104	rVV2	410	361	0.03%	0.004%
90	14.219	2152	2154	2156	rVB2	1199	737	0.06%	0.007%
91	14.268	2160	2162	2164	rVB2	834	574	0.04%	0.006%
92	14.365	2176	2178	2180	rBV2	394	409	0.03%	0.004%
93	14.560	2207	2210	2212	rBV3	923	962	0.07%	0.010%
94	14.749	2235	2241	2244	rBV4	879	1471	0.11%	0.015%
95	15.456	2355	2357	2358	rBV2	575	317	0.02%	0.003%
96	15.517	2365	2367	2369	rBV3	632	481	0.04%	0.005%
97	15.792	2410	2412	2417	rVB5	764	1158	0.09%	0.012%
98	15.987	2442	2444	2445	rBV2	787	734	0.06%	0.007%
99	16.450	2518	2520	2525	rBV4	897	1165	0.09%	0.012%
100	16.584	2540	2542	2544	rVB2	667	478	0.04%	0.005%

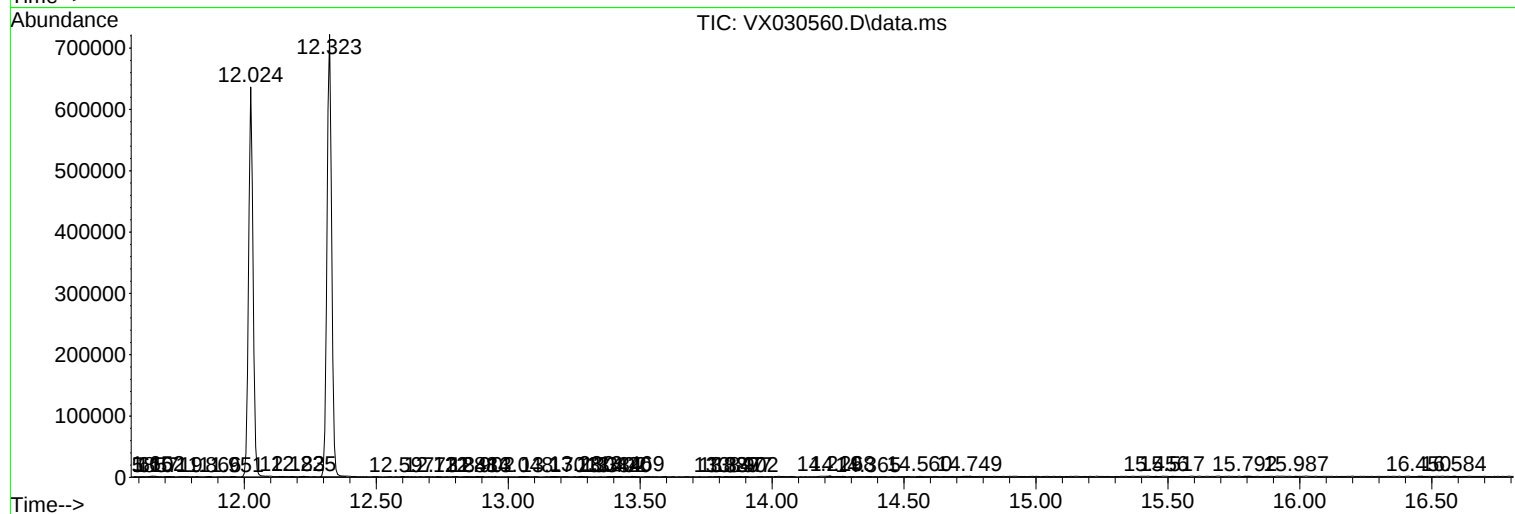
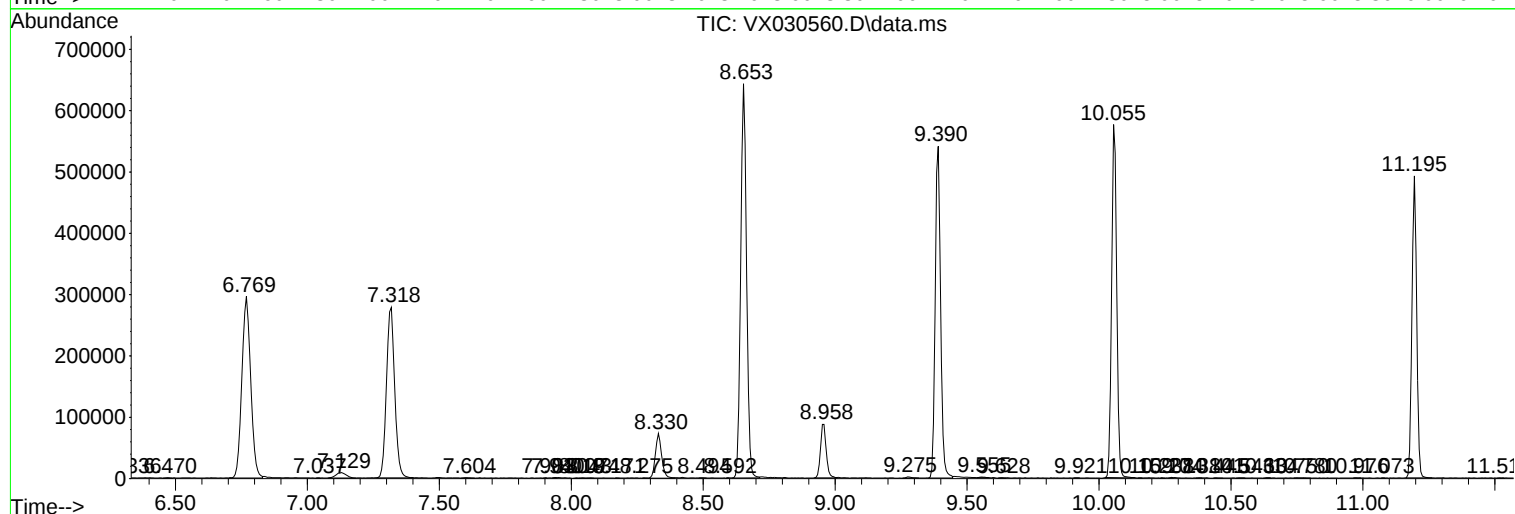
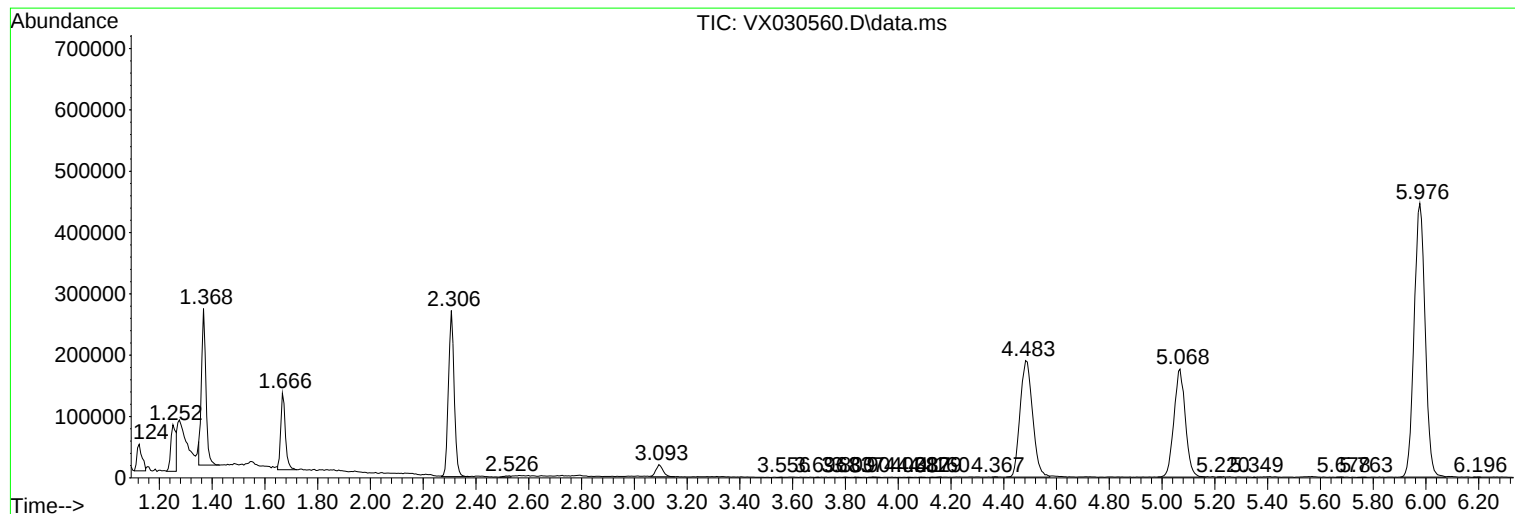
Sum of corrected areas: 9908765

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Instrument :
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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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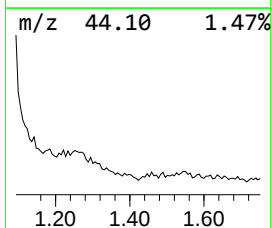
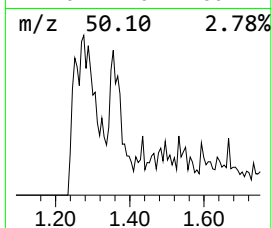
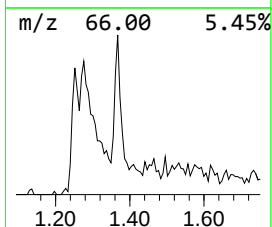
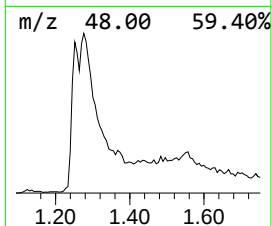
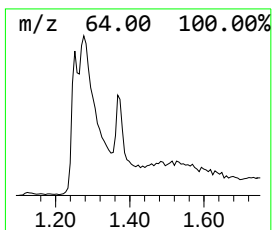
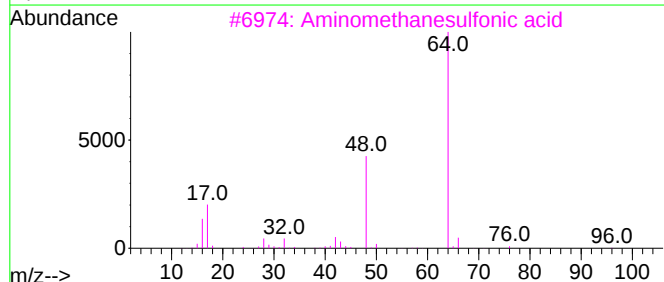
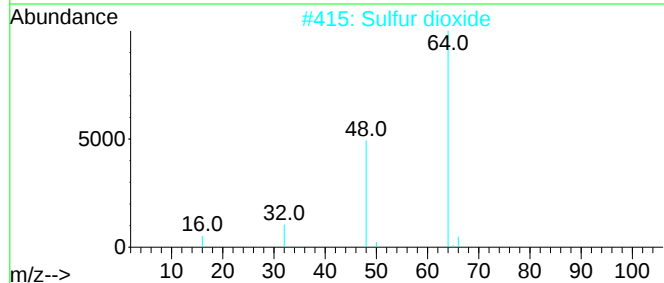
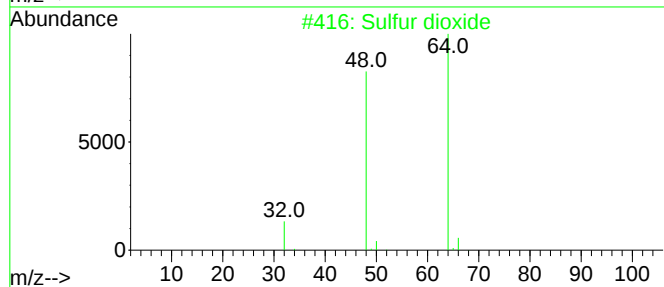
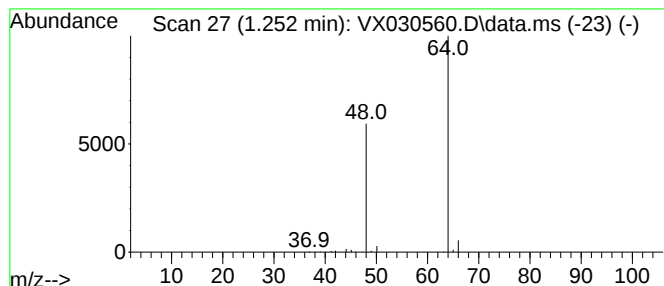
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	7.69 ug/L	105226	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
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	1.252	7.7	ug/L	105226	1	6.769	683900	50.0