

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081122\
 Data File : VX030577.D
 Acq On : 11 Aug 2022 16:40
 Operator : JC/MD
 Sample : N4144-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EY162

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: VX030577.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	41	rBV	47880	109371	12.34%	1.414%
2	1.367	42	46	53	rVB	81300	83652	9.44%	1.081%
3	1.672	91	96	107	rVB	71426	93755	10.58%	1.212%
4	2.306	194	200	210	rVB	149228	228463	25.78%	2.953%
5	2.404	211	216	225	rVB4	3218	5872	0.66%	0.076%
6	2.581	243	245	246	rBV2	1072	807	0.09%	0.010%
7	2.788	275	279	280	rBV3	1572	1173	0.13%	0.015%
8	2.837	285	287	289	rBV2	418	406	0.05%	0.005%
9	2.940	301	304	305	rBV3	1038	1055	0.12%	0.014%
10	3.007	313	315	316	rBV	550	402	0.05%	0.005%
11	3.032	316	319	321	rVV4	492	555	0.06%	0.007%
12	3.074	321	326	327	rVB2	443	603	0.07%	0.008%
13	3.166	339	341	344	rBV2	336	469	0.05%	0.006%
14	3.507	394	397	399	rBV3	654	731	0.08%	0.009%
15	3.568	405	407	410	rBV	474	519	0.06%	0.007%
16	3.666	421	423	425	rBV2	577	484	0.05%	0.006%
17	3.952	467	470	472	rBV2	408	484	0.05%	0.006%
18	4.038	482	484	486	rBV2	570	407	0.05%	0.005%
19	4.336	530	533	534	rBV3	536	541	0.06%	0.007%
20	4.477	547	556	570	rBV	104979	312747	35.30%	4.042%
21	5.074	641	654	670	rVV2	122345	389110	43.91%	5.029%
22	5.202	673	675	679	rVB3	597	644	0.07%	0.008%
23	5.239	679	681	684	rBV2	620	533	0.06%	0.007%
24	5.403	702	708	711	rBV5	1122	1852	0.21%	0.024%
25	5.489	721	722	726	rBV3	654	814	0.09%	0.011%
26	5.544	728	731	732	rBV2	1353	1375	0.16%	0.018%
27	5.684	752	754	756	rVV2	522	410	0.05%	0.005%
28	5.726	758	761	763	rBV3	455	505	0.06%	0.007%
29	5.976	790	802	818	rBV2	305427	886056	100.00%	11.452%
30	6.610	904	906	908	rBV3	419	435	0.05%	0.006%
31	6.769	923	932	945	rBV	268696	642889	72.56%	8.309%
32	7.129	980	991	1004	rBV2	56538	134932	15.23%	1.744%
33	7.318	1013	1022	1032	rVV	192293	428736	48.39%	5.541%
34	7.476	1046	1048	1050	rBV2	765	567	0.06%	0.007%
35	7.598	1065	1068	1069	rBV	524	464	0.05%	0.006%
36	7.903	1115	1118	1119	rBV3	549	531	0.06%	0.007%

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 Title : VOC Analysis

37	7.933	1122	1123	1124	rBV	709	399	0.05%	0.005%
38	8.037	1139	1140	1143	rVB2	666	454	0.05%	0.006%
39	8.232	1167	1172	1175	rBV2	475	736	0.08%	0.010%
40	8.330	1182	1188	1200	rVB	126976	209873	23.69%	2.712%
41	8.488	1210	1214	1220	rBV5	2093	4069	0.46%	0.053%
42	8.653	1234	1241	1250	rBV	392390	611521	69.02%	7.904%
43	8.958	1285	1291	1308	rBV	91566	142501	16.08%	1.842%
44	9.092	1311	1313	1316	rVV2	427	558	0.06%	0.007%
45	9.140	1319	1321	1324	rVB2	514	403	0.05%	0.005%
46	9.171	1324	1326	1329	rBV3	622	634	0.07%	0.008%
47	9.275	1339	1343	1348	rVB4	4158	6249	0.71%	0.081%
48	9.317	1348	1350	1351	rBV2	537	381	0.04%	0.005%
49	9.390	1356	1362	1375	rBV	473957	673686	76.03%	8.707%
50	9.683	1408	1410	1411	rVV	584	418	0.05%	0.005%
51	9.842	1435	1436	1439	rBV2	623	469	0.05%	0.006%
52	9.933	1448	1451	1452	rVB2	560	447	0.05%	0.006%
53	9.957	1452	1455	1456	rBV	328	366	0.04%	0.005%
54	9.970	1456	1457	1460	rVB2	519	394	0.04%	0.005%
55	10.000	1460	1462	1465	rBV2	341	376	0.04%	0.005%
56	10.055	1466	1471	1484	rVV	572538	760959	85.88%	9.835%
57	10.305	1509	1512	1514	rBV2	1215	1111	0.13%	0.014%
58	10.366	1520	1522	1525	rVB2	533	505	0.06%	0.007%
59	10.415	1525	1530	1533	rBV	583	909	0.10%	0.012%
60	10.518	1545	1547	1550	rVB2	518	487	0.05%	0.006%
61	10.549	1550	1552	1556	rBV	538	738	0.08%	0.010%
62	10.634	1564	1566	1567	rBV2	421	384	0.04%	0.005%
63	10.787	1590	1591	1593	rVB	792	417	0.05%	0.005%
64	10.854	1601	1602	1605	rBV	479	421	0.05%	0.005%
65	11.079	1636	1639	1642	rBV3	679	1023	0.12%	0.013%
66	11.128	1645	1647	1651	rBV3	474	380	0.04%	0.005%
67	11.195	1652	1658	1667	rBV	429497	543101	61.29%	7.019%
68	11.677	1735	1737	1740	rVB	680	569	0.06%	0.007%
69	11.701	1740	1741	1742	rBV	713	380	0.04%	0.005%
70	11.762	1750	1751	1755	rVB3	936	735	0.08%	0.009%
71	11.872	1765	1769	1776	rVB4	2546	4037	0.46%	0.052%
72	11.933	1777	1779	1780	rVB2	692	362	0.04%	0.005%
73	12.024	1789	1794	1802	rBV	607898	719251	81.17%	9.296%
74	12.225	1823	1827	1834	rVV3	6156	10515	1.19%	0.136%
75	12.323	1837	1843	1857	rBV	564901	690866	77.97%	8.929%
76	12.652	1895	1897	1898	rBV2	504	400	0.05%	0.005%

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 Title : VOC Analysis

77	12.719	1905	1908	1909	rBV2	402	362	0.04%	0.005%
78	12.835	1925	1927	1928	rBV	596	586	0.07%	0.008%
79	12.939	1943	1944	1947	rVB2	817	520	0.06%	0.007%
80	12.981	1949	1951	1953	rVV2	723	505	0.06%	0.007%
81	13.048	1957	1962	1963	rBV2	569	740	0.08%	0.010%
82	13.128	1972	1975	1977	rBV3	493	586	0.07%	0.008%
83	13.213	1986	1989	1991	rBV3	439	458	0.05%	0.006%
84	13.329	2005	2008	2010	rBV2	878	1048	0.12%	0.014%
85	13.469	2028	2031	2034	rVB3	411	433	0.05%	0.006%
86	13.512	2034	2038	2039	rBV3	475	671	0.08%	0.009%
87	13.560	2045	2046	2049	rBV2	537	366	0.04%	0.005%
88	13.627	2056	2057	2062	rVB3	662	723	0.08%	0.009%
89	13.695	2064	2068	2071	rBV2	691	649	0.07%	0.008%
90	14.140	2138	2141	2143	rBV3	632	698	0.08%	0.009%
91	14.274	2161	2163	2168	rVB3	497	488	0.06%	0.006%
92	14.530	2203	2205	2207	rBV	829	777	0.09%	0.010%
93	14.658	2224	2226	2228	rBV3	567	504	0.06%	0.007%
94	14.749	2238	2241	2242	rBV3	566	500	0.06%	0.006%
95	15.237	2319	2321	2325	rVB3	532	513	0.06%	0.007%
96	15.341	2336	2338	2340	rVB3	664	371	0.04%	0.005%
97	15.408	2348	2349	2350	rBV	713	362	0.04%	0.005%
98	15.725	2399	2401	2403	rBV2	890	604	0.07%	0.008%
99	16.505	2527	2529	2531	rVB3	594	374	0.04%	0.005%
100	16.590	2541	2543	2545	rVB2	960	614	0.07%	0.008%

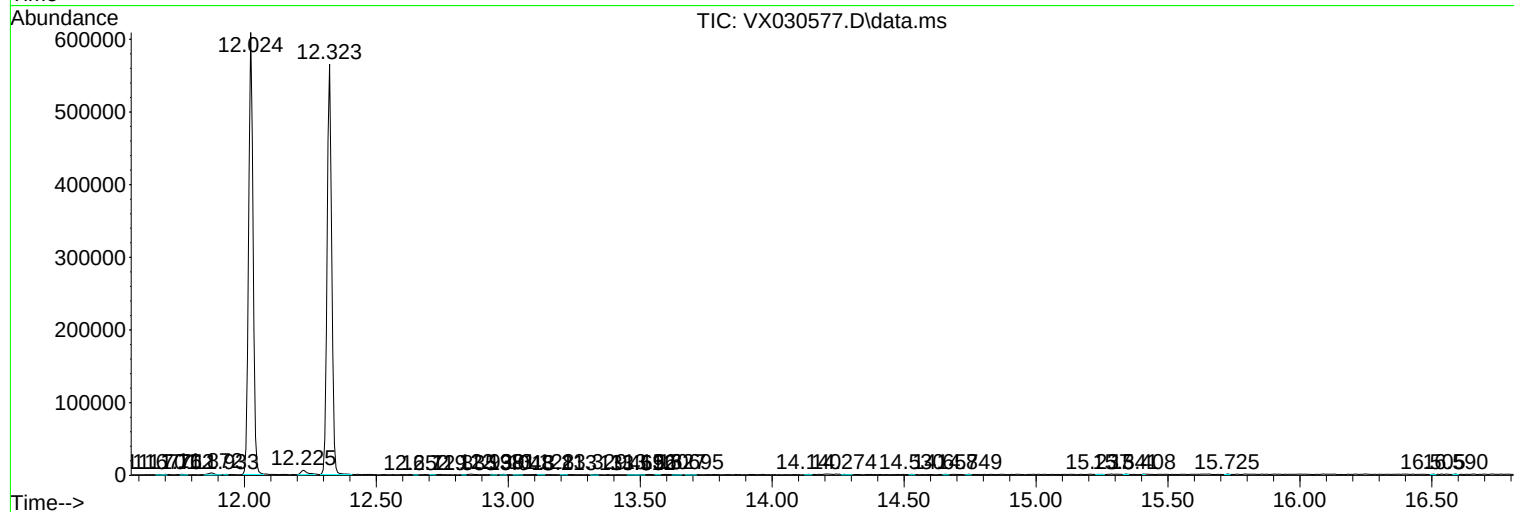
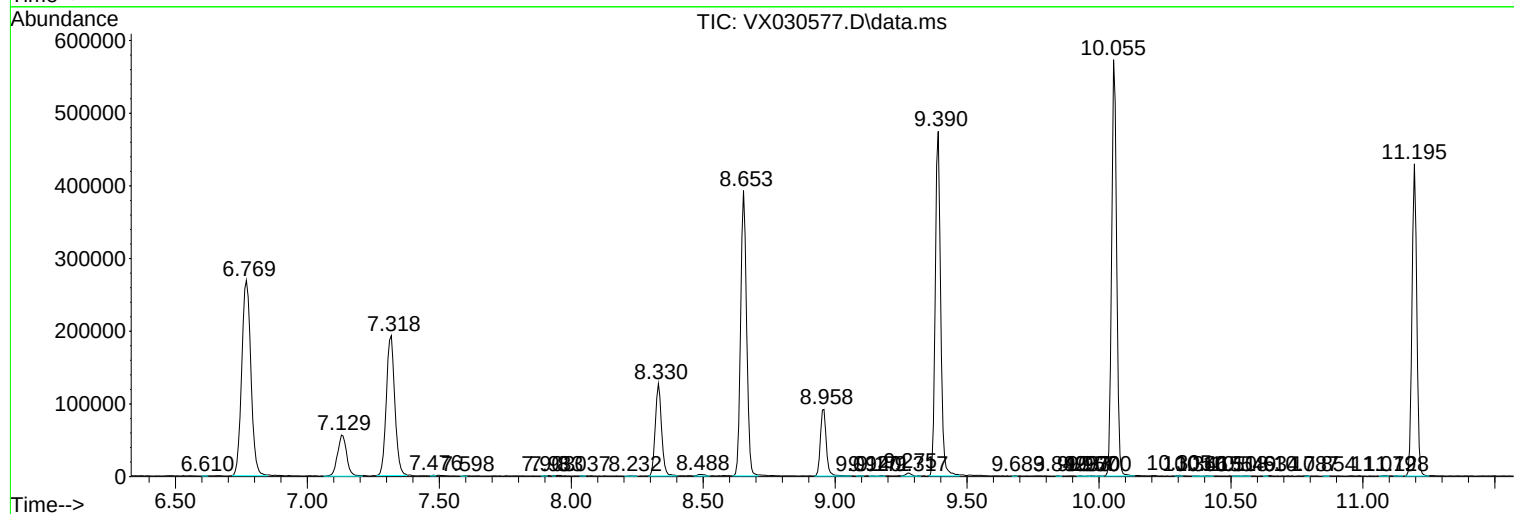
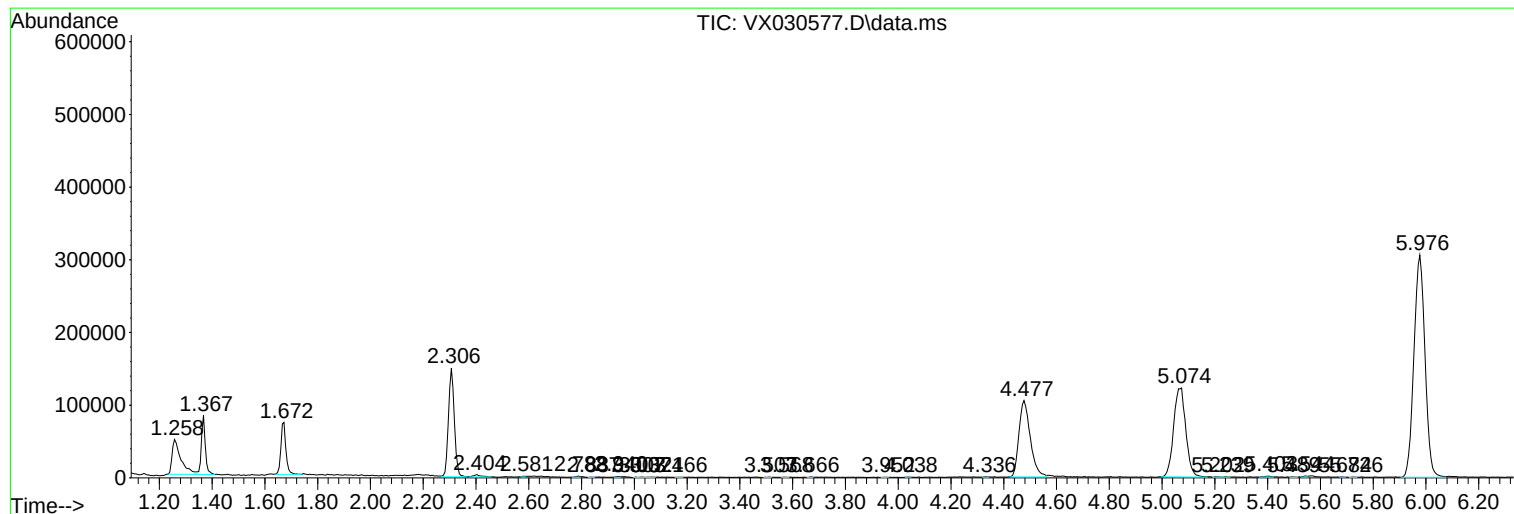
Sum of corrected areas: 7737285

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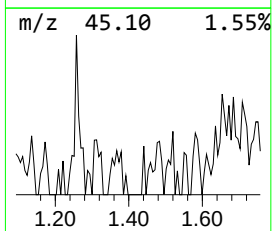
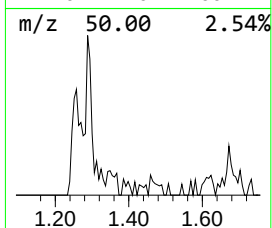
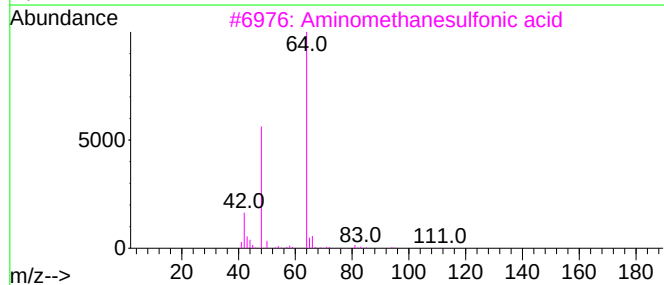
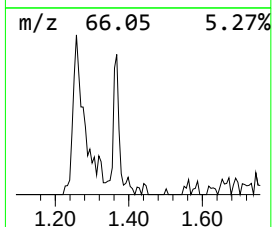
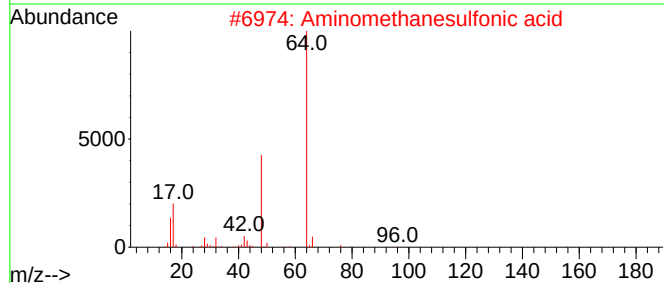
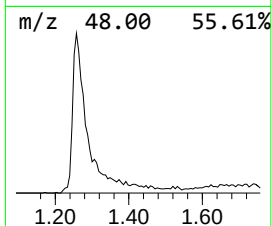
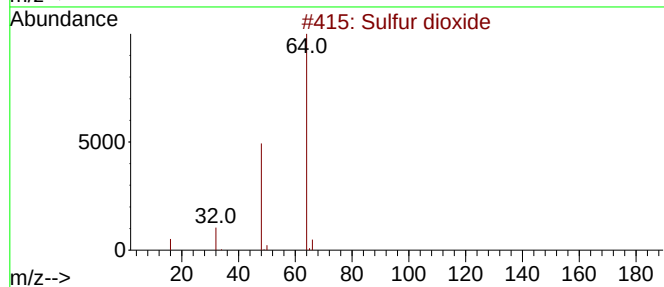
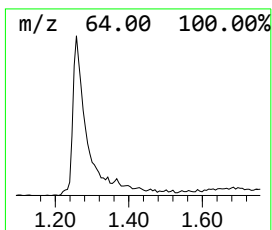
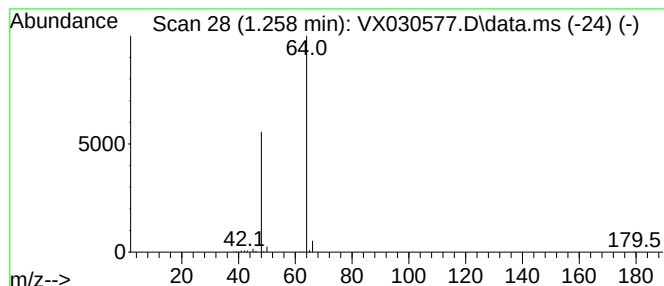
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
1.258	8.51 ug/L	109371	1,4-Difluorobenzene	6.769

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



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	8.5	ug/L	109371	1	6.769	642889	50.0