

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035153.D
 Acq On : 19 Apr 2023 03:15
 Operator : JC/MD
 Sample : 02397-17
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM9

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035153.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	42	rBV	102783	264032	1.09%	0.500%
2	1.367	43	46	58	rVB	235769	267653	1.10%	0.507%
3	1.672	92	96	108	rVB	183832	230227	0.95%	0.436%
4	2.306	194	200	211	rBV	443331	691739	2.85%	1.310%
5	2.501	230	232	233	rBV	651	523	0.00%	0.001%
6	2.788	277	279	286	rVB4	923	1229	0.01%	0.002%
7	2.940	302	304	307	rBV2	382	379	0.00%	0.001%
8	3.020	313	317	320	rBV2	322	503	0.00%	0.001%
9	3.050	320	322	324	rBV2	461	353	0.00%	0.001%
10	3.215	347	349	351	rVB2	225	180	0.00%	0.000%
11	3.446	385	387	388	rBV2	207	98	0.00%	0.000%
12	3.465	388	390	393	rBV2	300	319	0.00%	0.001%
13	3.574	406	408	409	rBV	87	43	0.00%	0.000%
14	3.593	409	411	413	rBV2	188	161	0.00%	0.000%
15	3.611	413	414	415	rVB	247	95	0.00%	0.000%
16	3.763	438	439	441	rVB	243	94	0.00%	0.000%
17	3.794	441	444	446	rBV3	163	205	0.00%	0.000%
18	3.824	448	449	450	rVB	163	63	0.00%	0.000%
19	3.885	458	459	462	rVB2	225	172	0.00%	0.000%
20	3.922	462	465	466	rBV2	211	259	0.00%	0.000%
21	3.940	466	468	471	rVB2	284	333	0.00%	0.001%
22	4.019	479	481	483	rVB3	195	103	0.00%	0.000%
23	4.099	492	494	498	rVB3	350	451	0.00%	0.001%
24	4.147	498	502	504	rBV3	403	491	0.00%	0.001%
25	4.300	525	527	530	rBV2	436	459	0.00%	0.001%
26	4.458	542	553	578	rBV	117203	363030	1.49%	0.688%
27	4.867	618	620	622	rBV2	266	203	0.00%	0.000%
28	4.964	634	636	637	rBV	239	234	0.00%	0.000%
29	5.056	639	651	668	rVV	254976	754275	3.11%	1.429%
30	5.294	688	690	691	rBV	209	135	0.00%	0.000%
31	5.367	700	702	703	rBV2	313	226	0.00%	0.000%
32	5.562	730	734	744	rVB5	1273	3242	0.01%	0.006%
33	5.641	744	747	750	rBV2	180	278	0.00%	0.001%
34	5.690	754	755	756	rBV	191	94	0.00%	0.000%
35	5.836	776	779	780	rBV2	202	254	0.00%	0.000%
36	5.879	785	786	788	rBV	259	107	0.00%	0.000%

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37	5.970	788	801	821	rBV2	661600	1995109	8.21%	3.779%
38	6.202	838	839	841	rBV	517	388	0.00%	0.001%
39	6.306	852	856	858	rVB3	250	299	0.00%	0.001%
40	6.446	875	879	881	rBV2	311	334	0.00%	0.001%
41	6.482	881	885	888	rVB3	442	646	0.00%	0.001%
42	6.513	888	890	891	rBV	241	146	0.00%	0.000%
43	6.531	891	893	895	rBV2	239	190	0.00%	0.000%
44	6.598	903	904	905	rBV	210	102	0.00%	0.000%
45	6.641	909	911	912	rVB	291	208	0.00%	0.000%
46	6.659	912	914	915	rBV	316	258	0.00%	0.000%
47	6.763	921	931	946	rBV	462789	1130694	4.65%	2.142%
48	7.031	973	975	976	rBV	232	215	0.00%	0.000%
49	7.116	983	989	996	rBV4	2035	4183	0.02%	0.008%
50	7.184	998	1000	1001	rBV2	389	163	0.00%	0.000%
51	7.305	1012	1020	1039	rBV	411191	889998	3.66%	1.686%
52	7.647	1075	1076	1077	rBV	395	166	0.00%	0.000%
53	7.683	1080	1082	1084	rBV	93	94	0.00%	0.000%
54	7.763	1093	1095	1097	rBV2	269	191	0.00%	0.000%
55	7.891	1115	1116	1121	rBV	267	395	0.00%	0.001%
56	7.939	1121	1124	1127	rBV3	1225	1912	0.01%	0.004%
57	8.007	1134	1135	1137	rBV	326	246	0.00%	0.000%
58	8.220	1168	1170	1172	rBV2	296	318	0.00%	0.001%
59	8.281	1179	1180	1181	rBV	276	153	0.00%	0.000%
60	8.324	1181	1187	1206	rVV	248675	410165	1.69%	0.777%
61	8.647	1233	1240	1250	rBV	1059957	1637148	6.74%	3.101%
62	8.872	1273	1277	1279	rBV3	336	454	0.00%	0.001%
63	8.951	1284	1290	1303	rBV	170379	260038	1.07%	0.493%
64	9.165	1323	1325	1328	rBV	478	461	0.00%	0.001%
65	9.275	1340	1343	1346	rBV5	835	995	0.00%	0.002%
66	9.384	1355	1361	1376	rBV	575858	801331	3.30%	1.518%
67	9.903	1445	1446	1448	rBV	342	236	0.00%	0.000%
68	9.939	1448	1452	1456	rBV2	612	1043	0.00%	0.002%
69	10.079	1465	1475	1492	rBV2	5282081	8520380	35.08%	16.141%
70	10.598	1558	1560	1561	rBV	412	246	0.00%	0.000%
71	10.793	1591	1592	1594	rBV2	521	409	0.00%	0.001%
72	10.847	1599	1601	1603	rVV2	234	197	0.00%	0.000%
73	11.018	1627	1629	1630	rBV2	298	209	0.00%	0.000%
74	11.079	1638	1639	1641	rVB	330	216	0.00%	0.000%
75	11.110	1641	1644	1645	rBV2	188	206	0.00%	0.000%
76	11.189	1652	1657	1672	rBV	645513	851153	3.50%	1.612%

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 Title : VOC Analysis

77	11.360	1684	1685	1689	rVB3	506	583	0.00%	0.001%
78	11.421	1692	1695	1697	rBV2	221	348	0.00%	0.001%
79	11.573	1719	1720	1722	rBV	237	137	0.00%	0.000%
80	11.603	1724	1725	1726	rBV	309	131	0.00%	0.000%
81	11.634	1726	1730	1731	rBV3	243	256	0.00%	0.000%
82	11.707	1740	1742	1745	rBV2	731	823	0.00%	0.002%
83	11.969	1780	1785	1789	rBV	549871	672161	2.77%	1.273%
84	12.042	1789	1797	1818	rVB2	2089912	3812754	15.70%	7.223%
85	12.219	1823	1826	1835	rBV2	5023	9552	0.04%	0.018%
86	12.335	1837	1845	1851	rBV	17813671	24291317	100.00%	46.016%
87	12.804	1920	1922	1925	rBV3	387	357	0.00%	0.001%
88	12.920	1936	1941	1949	rBV	25854	33953	0.14%	0.064%
89	13.061	1959	1964	1969	rVB3	3964	7609	0.03%	0.014%
90	13.115	1969	1973	1977	rVB3	3349	4383	0.02%	0.008%
91	13.201	1982	1987	1992	rVB	10293	13281	0.05%	0.025%
92	13.585	2045	2050	2070	rBV	3290534	4097827	16.87%	7.763%
93	13.957	2106	2111	2123	rBV	494237	662637	2.73%	1.255%
94	14.091	2131	2133	2134	rBV	435	270	0.00%	0.001%
95	14.786	2240	2247	2252	rVB2	30814	44177	0.18%	0.084%
96	15.249	2318	2323	2329	rBV	31378	42259	0.17%	0.080%
97	15.359	2339	2341	2342	rBV2	669	412	0.00%	0.001%

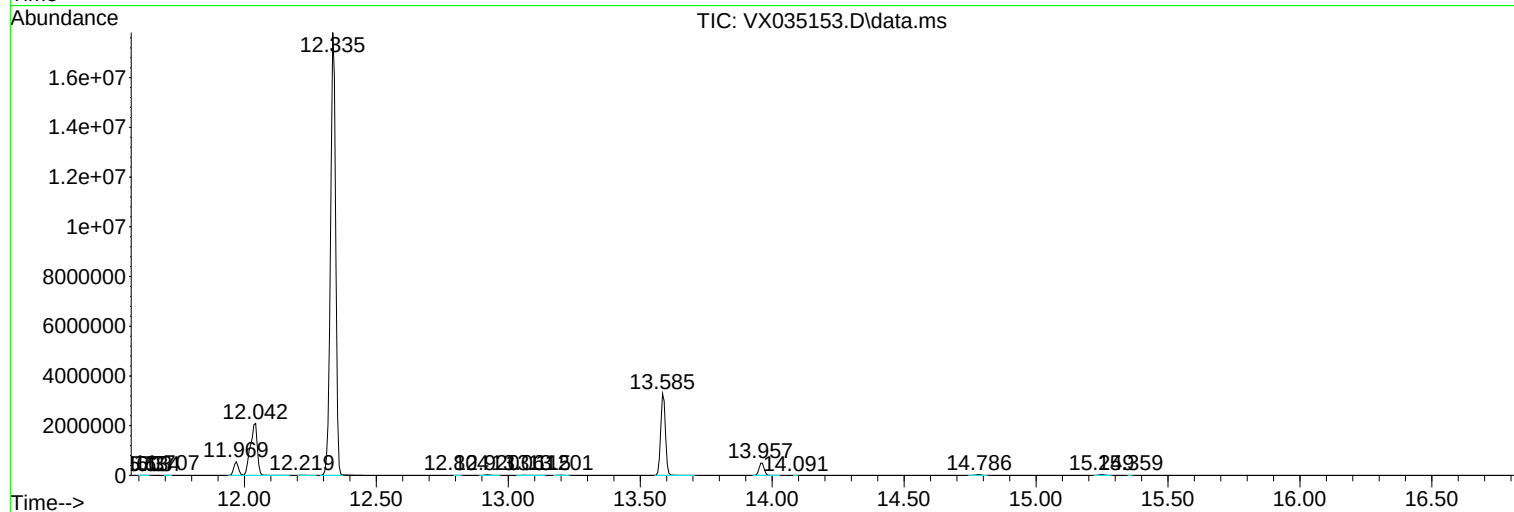
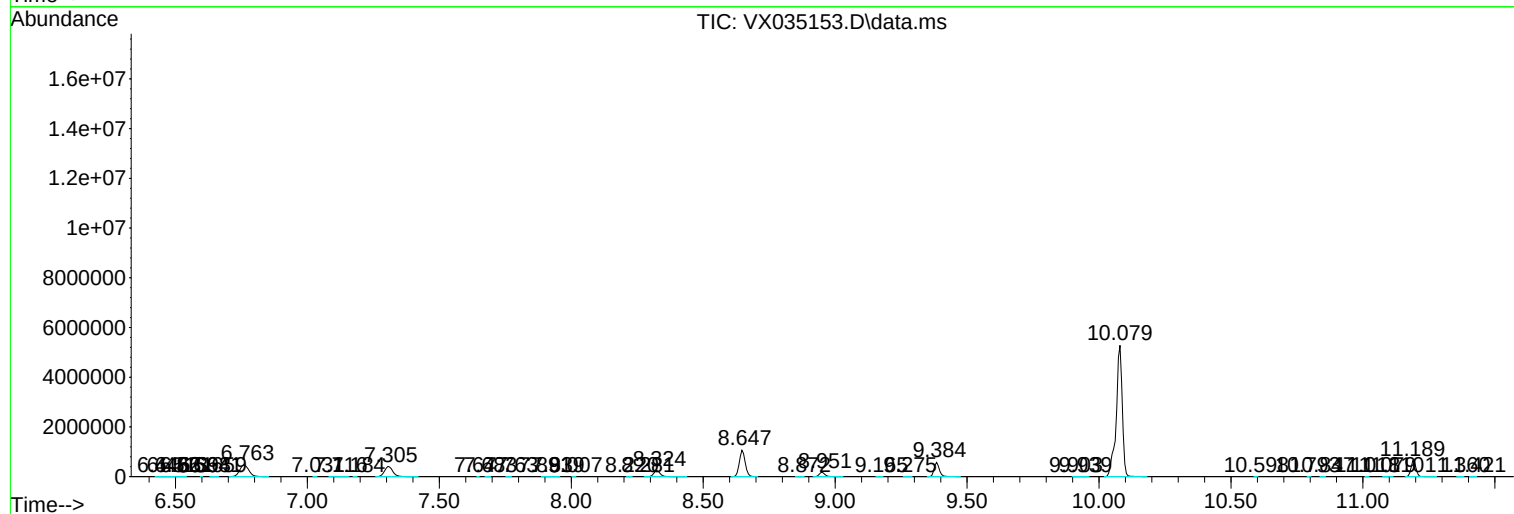
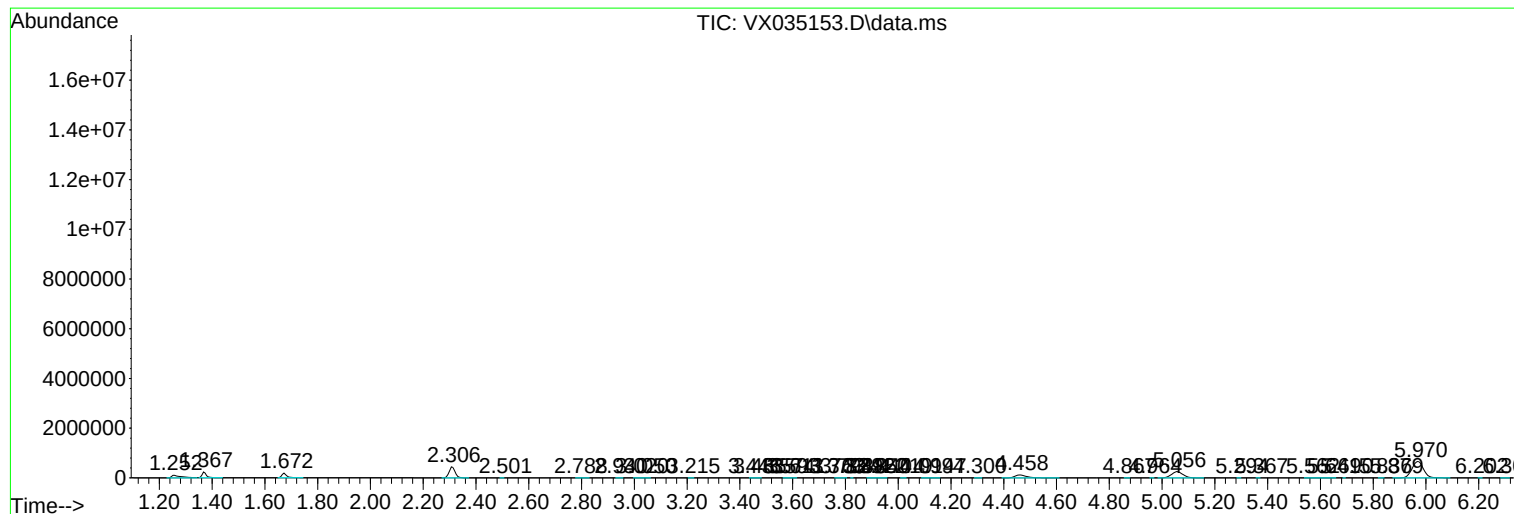
Sum of corrected areas: 52788764

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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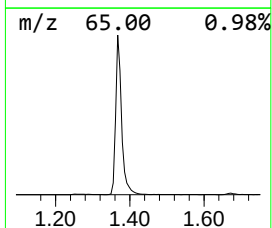
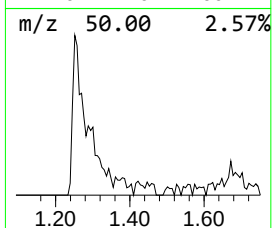
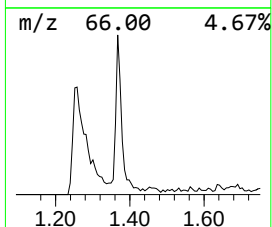
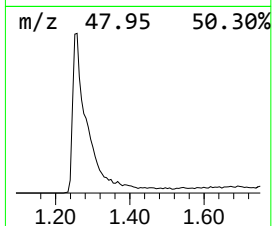
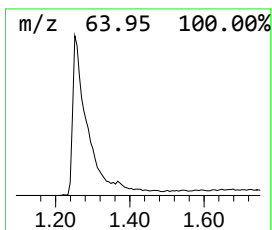
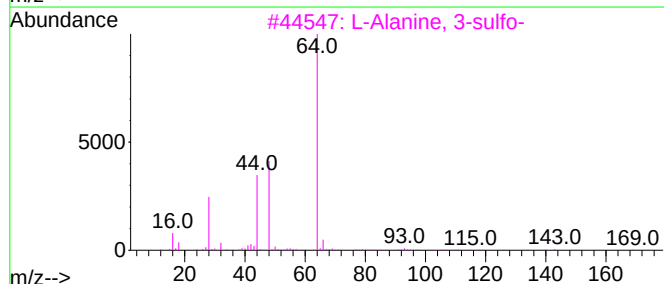
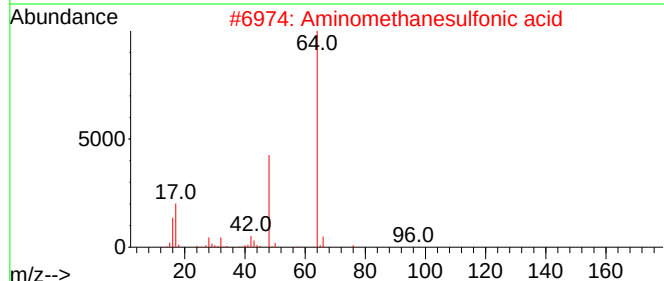
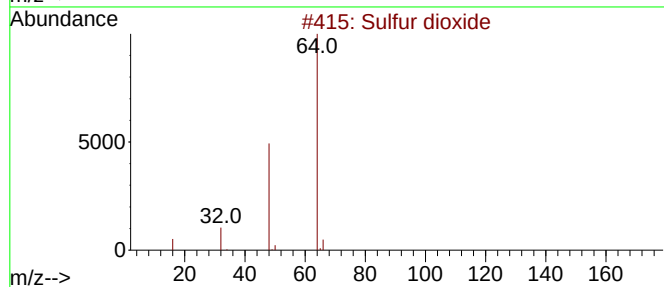
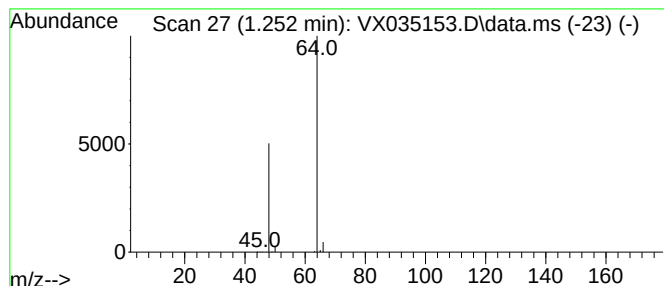
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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	11.68 ug/L	264032	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.252	11.7	ug/L	264032	1	6.763	1130690	50.0