

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035132.D
 Acq On : 18 Apr 2023 18:47
 Operator : JC/MD
 Sample : 02378-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMK1

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: VX035132.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	42	rBV	364302	587089	39.66%	4.670%
2	1.368	43	46	57	rVV	171214	196757	13.29%	1.565%
3	1.453	57	60	68	rVB	15464	21963	1.48%	0.175%
4	1.666	92	95	108	rVB	122360	165608	11.19%	1.317%
5	2.307	194	200	208	rBV	328784	499648	33.75%	3.975%
6	2.459	223	225	228	rVB2	476	239	0.02%	0.002%
7	2.508	228	233	238	rBV2	1029	1934	0.13%	0.015%
8	2.800	275	281	285	rVB6	1204	2497	0.17%	0.020%
9	2.934	297	303	304	rBV3	1790	2510	0.17%	0.020%
10	3.014	315	316	321	rBV2	245	363	0.02%	0.003%
11	3.111	326	332	333	rBV3	1111	1812	0.12%	0.014%
12	3.380	373	376	378	rBV	335	316	0.02%	0.003%
13	3.441	383	386	388	rBV3	361	477	0.03%	0.004%
14	3.508	395	397	400	rVB	385	330	0.02%	0.003%
15	3.642	416	419	422	rBV2	277	387	0.03%	0.003%
16	3.703	427	429	432	rVB2	284	243	0.02%	0.002%
17	3.934	465	467	469	rBV	365	254	0.02%	0.002%
18	3.995	474	477	479	rVB2	192	255	0.02%	0.002%
19	4.032	481	483	486	rVB	338	298	0.02%	0.002%
20	4.062	486	488	490	rBV	180	208	0.01%	0.002%
21	4.227	512	515	517	rBV	282	317	0.02%	0.003%
22	4.373	535	539	541	rBV2	280	410	0.03%	0.003%
23	4.459	544	553	572	rBV	90804	270068	18.24%	2.148%
24	4.861	617	619	623	rVB2	292	272	0.02%	0.002%
25	4.898	623	625	628	rVB2	280	351	0.02%	0.003%
26	4.946	631	633	637	rBB2	260	211	0.01%	0.002%
27	5.056	639	651	666	rBV	179149	547506	36.98%	4.355%
28	5.263	683	685	688	rVB3	378	386	0.03%	0.003%
29	5.306	688	692	694	rBV3	314	411	0.03%	0.003%
30	5.385	698	705	706	rBV3	822	1498	0.10%	0.012%
31	5.495	718	723	725	rBV2	382	585	0.04%	0.005%
32	5.556	725	733	739	rVV6	2196	5875	0.40%	0.047%
33	5.641	745	747	749	rVB	302	242	0.02%	0.002%
34	5.666	749	751	755	rBV3	288	453	0.03%	0.004%
35	5.751	760	765	766	rBV	125	199	0.01%	0.002%
36	5.794	770	772	774	rBV2	221	241	0.02%	0.002%

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 Title : VOC Analysis

37	5.971	788	801	808	rBV2	481401	1456290	98.37%	11.584%
38	6.361	862	865	869	rBV2	179	257	0.02%	0.002%
39	6.483	883	885	888	rVB	303	307	0.02%	0.002%
40	6.519	888	891	893	rBV2	182	250	0.02%	0.002%
41	6.647	910	912	916	rVB2	278	301	0.02%	0.002%
42	6.763	921	931	948	rBV	491086	1190471	80.42%	9.470%
43	7.117	983	989	991	rBV5	1035	2044	0.14%	0.016%
44	7.165	995	997	999	rVB	344	243	0.02%	0.002%
45	7.306	1012	1020	1037	rBV	287635	644017	43.50%	5.123%
46	7.489	1045	1050	1056	rVV5	958	1841	0.12%	0.015%
47	7.763	1093	1095	1096	rVB	352	201	0.01%	0.002%
48	7.824	1103	1105	1107	rBV2	266	225	0.02%	0.002%
49	7.934	1121	1123	1124	rBV2	363	341	0.02%	0.003%
50	7.958	1124	1127	1128	rVV2	618	692	0.05%	0.006%
51	8.153	1158	1159	1163	rVB	359	323	0.02%	0.003%
52	8.190	1163	1165	1168	rBV2	258	264	0.02%	0.002%
53	8.324	1180	1187	1200	rBV	156903	266149	17.98%	2.117%
54	8.464	1208	1210	1213	rBV4	347	223	0.02%	0.002%
55	8.580	1227	1229	1231	rBV2	394	367	0.02%	0.003%
56	8.647	1234	1240	1251	rBV	755780	1167115	78.84%	9.284%
57	8.952	1284	1290	1300	rBV	109024	165108	11.15%	1.313%
58	9.098	1312	1314	1316	rVB	491	370	0.02%	0.003%
59	9.122	1316	1318	1320	rBV	304	281	0.02%	0.002%
60	9.275	1339	1343	1348	rVB4	2004	2822	0.19%	0.022%
61	9.385	1355	1361	1381	rBV	413817	596721	40.31%	4.747%
62	9.708	1413	1414	1416	rBV	322	203	0.01%	0.002%
63	9.781	1423	1426	1427	rVB2	306	247	0.02%	0.002%
64	9.805	1427	1430	1433	rVB3	376	490	0.03%	0.004%
65	9.830	1433	1434	1436	rBV2	309	261	0.02%	0.002%
66	9.884	1440	1443	1446	rBV2	353	615	0.04%	0.005%
67	9.915	1446	1448	1454	rVB3	311	233	0.02%	0.002%
68	10.055	1465	1471	1473	rBV	991912	1480373	100.00%	11.776%
69	10.299	1509	1511	1515	rVB2	387	538	0.04%	0.004%
70	10.397	1526	1527	1530	rBV2	285	281	0.02%	0.002%
71	10.573	1554	1556	1561	rBV2	191	294	0.02%	0.002%
72	10.866	1601	1604	1610	rVB4	762	1298	0.09%	0.010%
73	10.921	1610	1613	1615	rVB2	234	236	0.02%	0.002%
74	10.964	1618	1620	1622	rBB3	433	417	0.03%	0.003%
75	11.043	1631	1633	1636	rVB2	342	249	0.02%	0.002%
76	11.092	1638	1641	1645	rBV2	378	426	0.03%	0.003%

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 Title : VOC Analysis

77	11.189	1652	1657	1666	rBV	471740	619114	41.82%	4.925%
78	11.311	1674	1677	1681	rVB3	2006	2448	0.17%	0.019%
79	11.482	1703	1705	1708	rBV2	272	240	0.02%	0.002%
80	11.598	1722	1724	1726	rBV2	278	220	0.01%	0.002%
81	11.689	1737	1739	1740	rBV	287	206	0.01%	0.002%
82	11.707	1740	1742	1744	rVB	414	325	0.02%	0.003%
83	11.750	1747	1749	1750	rBV	569	338	0.02%	0.003%
84	11.933	1776	1779	1781	rVB3	1310	1379	0.09%	0.011%
85	11.969	1781	1785	1789	rVV3	16655	21014	1.42%	0.167%
86	12.024	1789	1794	1809	rVB2	920926	1433344	96.82%	11.402%
87	12.219	1822	1826	1834	rBV2	2638	5178	0.35%	0.041%
88	12.323	1837	1843	1854	rBV2	778169	1165562	78.73%	9.272%
89	12.677	1899	1901	1903	rBV2	248	247	0.02%	0.002%
90	12.756	1912	1914	1922	rVB2	621	983	0.07%	0.008%
91	12.860	1926	1931	1936	rBV2	4232	6313	0.43%	0.050%
92	13.109	1970	1972	1973	rBV2	530	408	0.03%	0.003%
93	13.152	1976	1979	1981	rBV2	274	273	0.02%	0.002%
94	13.329	2005	2008	2010	rVB2	249	217	0.01%	0.002%
95	13.591	2046	2051	2059	rVB	10088	12958	0.88%	0.103%
96	13.786	2079	2083	2090	rBV4	555	1192	0.08%	0.009%
97	13.853	2090	2094	2095	rVB2	448	373	0.03%	0.003%
98	13.969	2108	2113	2118	rVB4	1569	2282	0.15%	0.018%
99	14.506	2199	2201	2202	rBV	361	253	0.02%	0.002%
100	15.792	2410	2412	2415	rBV2	769	837	0.06%	0.007%

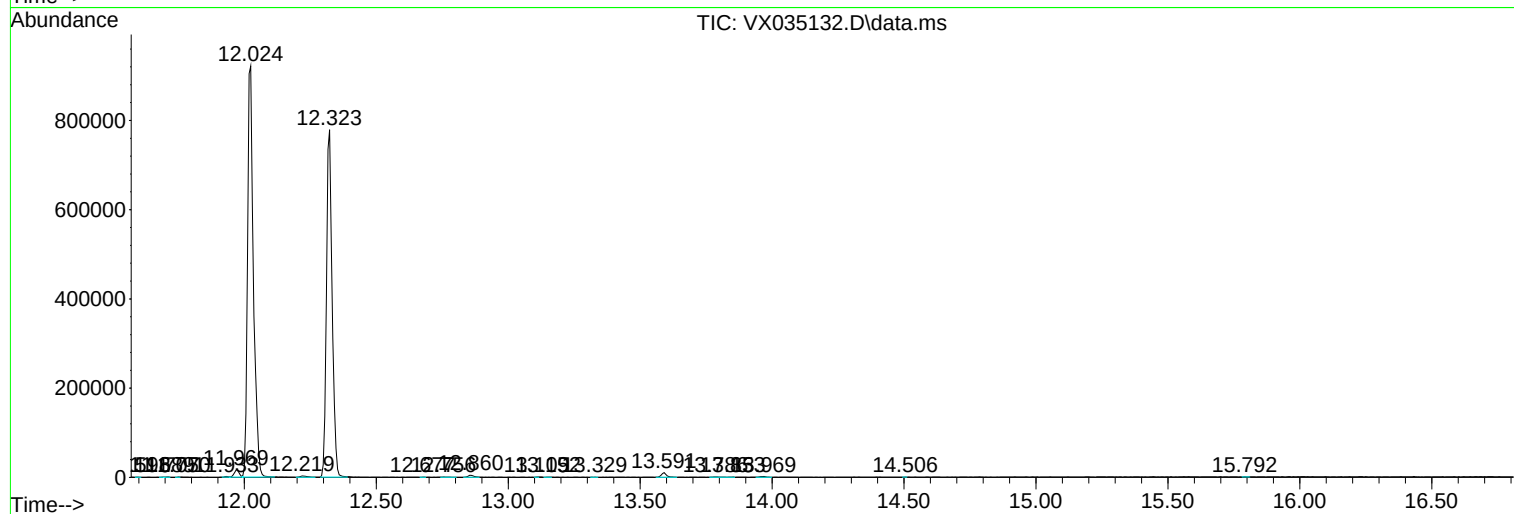
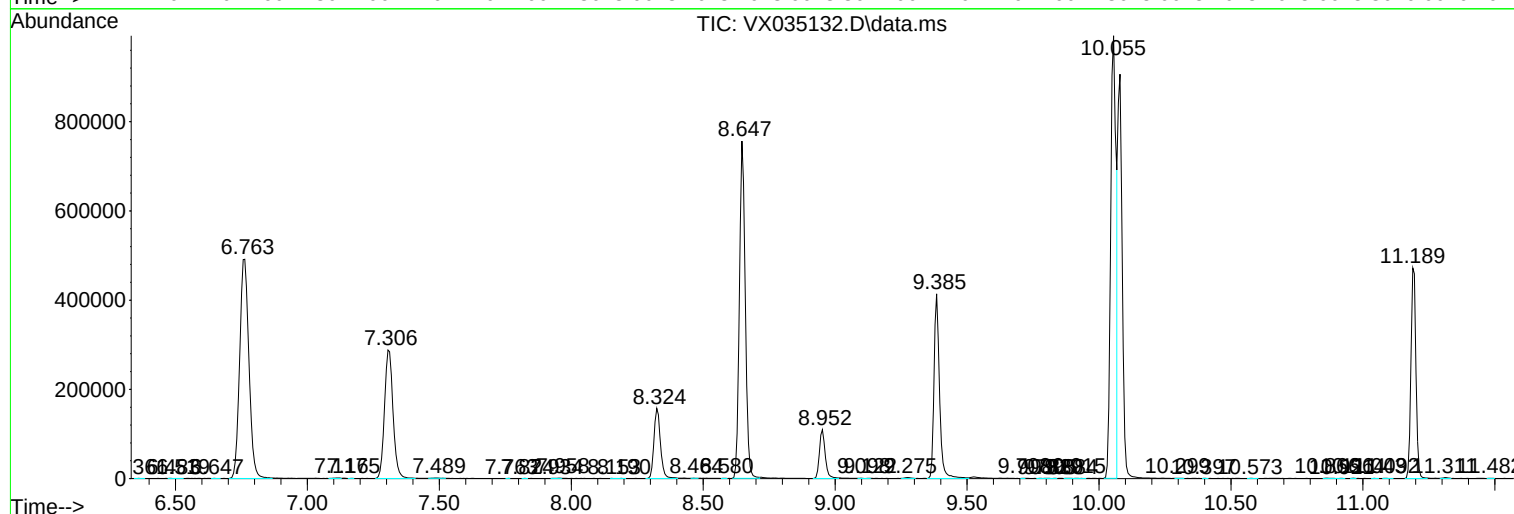
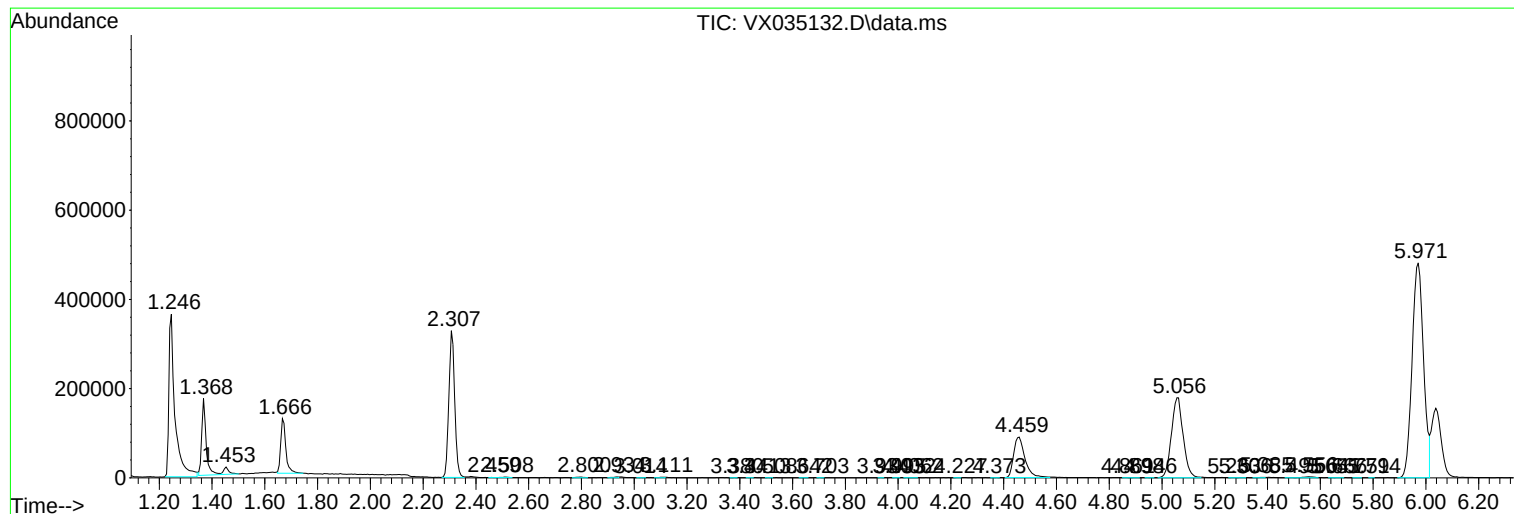
Sum of corrected areas: 12571301

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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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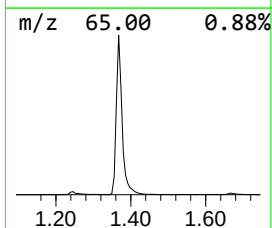
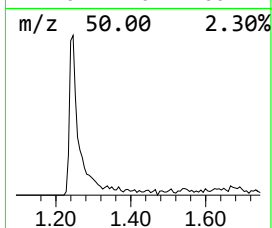
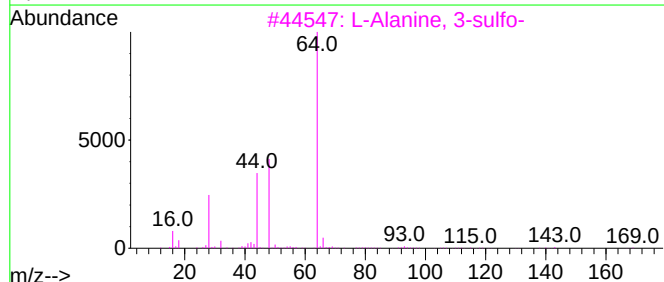
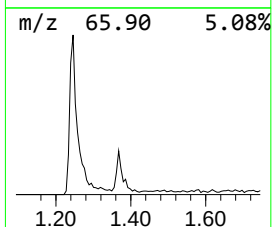
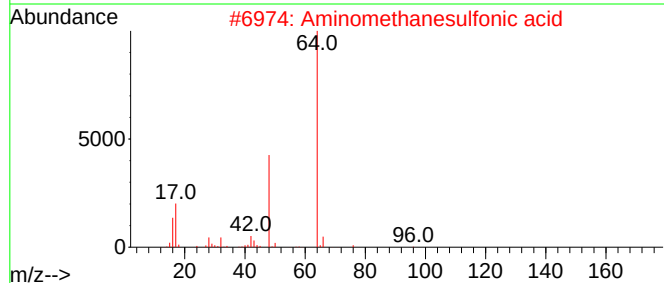
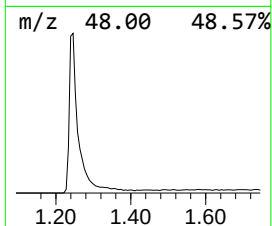
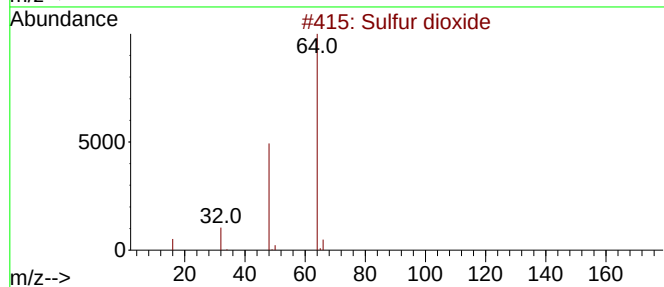
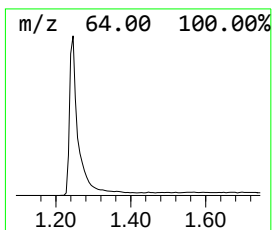
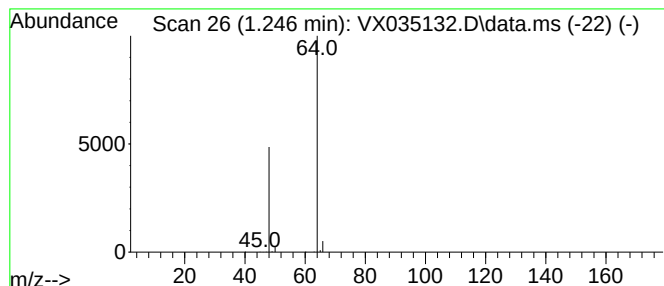
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	24.66 ug/L	587089	1,4-Difluorobenzene	6.763

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	24.7	ug/L	587089	1	6.763	1190470	50.0