

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035131.D
 Acq On : 18 Apr 2023 18:24
 Operator : JC/MD
 Sample : 02378-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMK0

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: VX035131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	24	30	37	rBV	39108	108568	7.59%	0.904%
2	1.368	43	46	56	rVB	173136	191059	13.36%	1.591%
3	1.666	92	95	107	rVB	115153	159398	11.15%	1.327%
4	2.307	194	200	209	rBV	318485	498674	34.87%	4.153%
5	2.514	230	234	240	rVB	4237	6673	0.47%	0.056%
6	2.599	247	248	250	rBV2	549	423	0.03%	0.004%
7	2.782	275	278	279	rBV3	936	1008	0.07%	0.008%
8	2.941	296	304	317	rVB	19668	45251	3.16%	0.377%
9	3.032	317	319	321	rBV	358	245	0.02%	0.002%
10	3.093	327	329	333	rBV2	379	328	0.02%	0.003%
11	3.142	336	337	338	rBV	475	243	0.02%	0.002%
12	3.325	363	367	370	rBV4	1263	2036	0.14%	0.017%
13	3.544	399	403	406	rBV2	145	226	0.02%	0.002%
14	3.587	406	410	413	rVB3	330	405	0.03%	0.003%
15	3.745	433	436	437	rBV2	254	196	0.01%	0.002%
16	3.764	437	439	442	rVB3	420	261	0.02%	0.002%
17	3.977	470	474	477	rBV2	224	401	0.03%	0.003%
18	4.105	494	495	498	rVB2	217	185	0.01%	0.002%
19	4.172	504	506	507	rBV	232	184	0.01%	0.002%
20	4.300	526	527	530	rVV2	315	276	0.02%	0.002%
21	4.349	533	535	538	rVB	309	221	0.02%	0.002%
22	4.459	544	553	566	rBV	88835	266335	18.62%	2.218%
23	4.916	627	628	631	rVB2	340	265	0.02%	0.002%
24	4.940	631	632	633	rBV	342	190	0.01%	0.002%
25	5.056	638	651	672	rBV	176107	543583	38.01%	4.527%
26	5.288	687	689	691	rBV	286	275	0.02%	0.002%
27	5.312	691	693	694	rVV	298	225	0.02%	0.002%
28	5.361	698	701	702	rBV2	329	293	0.02%	0.002%
29	5.440	713	714	717	rBV	250	184	0.01%	0.002%
30	5.483	719	721	725	rBV4	316	425	0.03%	0.004%
31	5.550	729	732	742	rVB4	1475	3884	0.27%	0.032%
32	5.617	742	743	745	rBV	325	195	0.01%	0.002%
33	5.666	749	751	753	rVB	406	266	0.02%	0.002%
34	5.696	755	756	760	rVB2	287	251	0.02%	0.002%
35	5.733	760	762	765	rBV2	216	221	0.02%	0.002%
36	5.836	776	779	781	rBV2	213	219	0.02%	0.002%

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

37	5.971	787	801	816	rBV2	477269	1430019	100.00%	11.908%
38	6.214	839	841	842	rBV	455	252	0.02%	0.002%
39	6.355	861	864	867	rBV3	448	611	0.04%	0.005%
40	6.458	878	881	882	rBV2	298	327	0.02%	0.003%
41	6.605	903	905	906	rVB	374	185	0.01%	0.002%
42	6.629	906	909	911	rBV	335	282	0.02%	0.002%
43	6.653	911	913	916	rVV2	192	181	0.01%	0.002%
44	6.763	921	931	944	rBV	477227	1147819	80.27%	9.558%
45	7.117	984	989	995	rVB6	1345	2905	0.20%	0.024%
46	7.208	1001	1004	1007	rVB2	361	498	0.03%	0.004%
47	7.306	1011	1020	1039	rBV	287833	645595	45.15%	5.376%
48	7.574	1061	1064	1065	rBV	273	233	0.02%	0.002%
49	7.604	1067	1069	1075	rVB3	629	1180	0.08%	0.010%
50	7.891	1114	1116	1118	rBV	296	183	0.01%	0.002%
51	7.946	1123	1125	1132	rVB4	574	1098	0.08%	0.009%
52	8.110	1151	1152	1155	rBV2	246	302	0.02%	0.003%
53	8.153	1157	1159	1160	rBV2	359	283	0.02%	0.002%
54	8.324	1181	1187	1200	rBV	160116	269799	18.87%	2.247%
55	8.476	1211	1212	1214	rBV	575	433	0.03%	0.004%
56	8.647	1233	1240	1250	rBV	742142	1163290	81.35%	9.687%
57	8.952	1284	1290	1306	rBV	107326	168001	11.75%	1.399%
58	9.177	1325	1327	1330	rVB2	249	302	0.02%	0.003%
59	9.208	1330	1332	1336	rBV3	327	467	0.03%	0.004%
60	9.281	1340	1344	1350	rVB4	1139	1843	0.13%	0.015%
61	9.330	1350	1352	1353	rVB2	322	203	0.01%	0.002%
62	9.385	1355	1361	1379	rBV	407511	595153	41.62%	4.956%
63	9.525	1380	1384	1394	rVB2	8345	15242	1.07%	0.127%
64	9.811	1429	1431	1433	rVB2	340	298	0.02%	0.002%
65	9.842	1433	1436	1437	rBV	366	365	0.03%	0.003%
66	9.903	1444	1446	1450	rVV3	266	319	0.02%	0.003%
67	10.055	1465	1471	1472	rBV	1007110	1259369	88.07%	10.487%
68	10.287	1507	1509	1510	rBV	396	208	0.01%	0.002%
69	10.415	1526	1530	1532	rVV2	424	478	0.03%	0.004%
70	10.451	1535	1536	1540	rVB2	531	566	0.04%	0.005%
71	10.781	1589	1590	1592	rBV	254	195	0.01%	0.002%
72	10.860	1598	1603	1608	rBV4	1350	2412	0.17%	0.020%
73	10.903	1608	1610	1611	rVV2	366	220	0.02%	0.002%
74	10.921	1611	1613	1615	rVV2	262	202	0.01%	0.002%
75	10.957	1617	1619	1622	rVV2	328	345	0.02%	0.003%
76	11.189	1652	1657	1670	rBV	463393	609449	42.62%	5.075%

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 Title : VOC Analysis

77	11.305	1674	1676	1682	rVB2	1010	1553	0.11%	0.013%
78	11.451	1696	1700	1703	rBV2	528	783	0.05%	0.007%
79	11.555	1715	1717	1718	rBV	351	226	0.02%	0.002%
80	11.750	1746	1749	1750	rBV2	567	570	0.04%	0.005%
81	11.927	1776	1778	1780	rBV2	457	468	0.03%	0.004%
82	11.969	1780	1785	1789	rBV	168830	216067	15.11%	1.799%
83	12.024	1789	1794	1795	rBV	1005787	1215177	84.98%	10.119%
84	12.219	1823	1826	1833	rVB5	1655	2964	0.21%	0.025%
85	12.323	1837	1843	1857	rVV2	803165	1402882	98.10%	11.682%
86	12.561	1881	1882	1884	rBV2	268	197	0.01%	0.002%
87	12.658	1897	1898	1900	rBV	248	231	0.02%	0.002%
88	12.762	1913	1915	1921	rVB3	887	1120	0.08%	0.009%
89	12.811	1921	1923	1925	rBV2	182	203	0.01%	0.002%
90	12.866	1928	1932	1934	rBV3	939	1151	0.08%	0.010%
91	12.945	1943	1945	1946	rBV	303	267	0.02%	0.002%
92	13.109	1969	1972	1977	rVB3	1657	2316	0.16%	0.019%
93	13.238	1991	1993	1994	rVB2	373	272	0.02%	0.002%
94	13.268	1996	1998	2000	rVV	287	230	0.02%	0.002%
95	13.305	2002	2004	2005	rVB	421	192	0.01%	0.002%
96	13.591	2047	2051	2056	rBV3	4162	5251	0.37%	0.044%
97	13.695	2066	2068	2071	rBV2	230	320	0.02%	0.003%
98	13.780	2080	2082	2085	rVV2	695	704	0.05%	0.006%
99	13.963	2110	2112	2115	rVB2	958	970	0.07%	0.008%
100	14.164	2143	2145	2147	rVB2	422	306	0.02%	0.003%

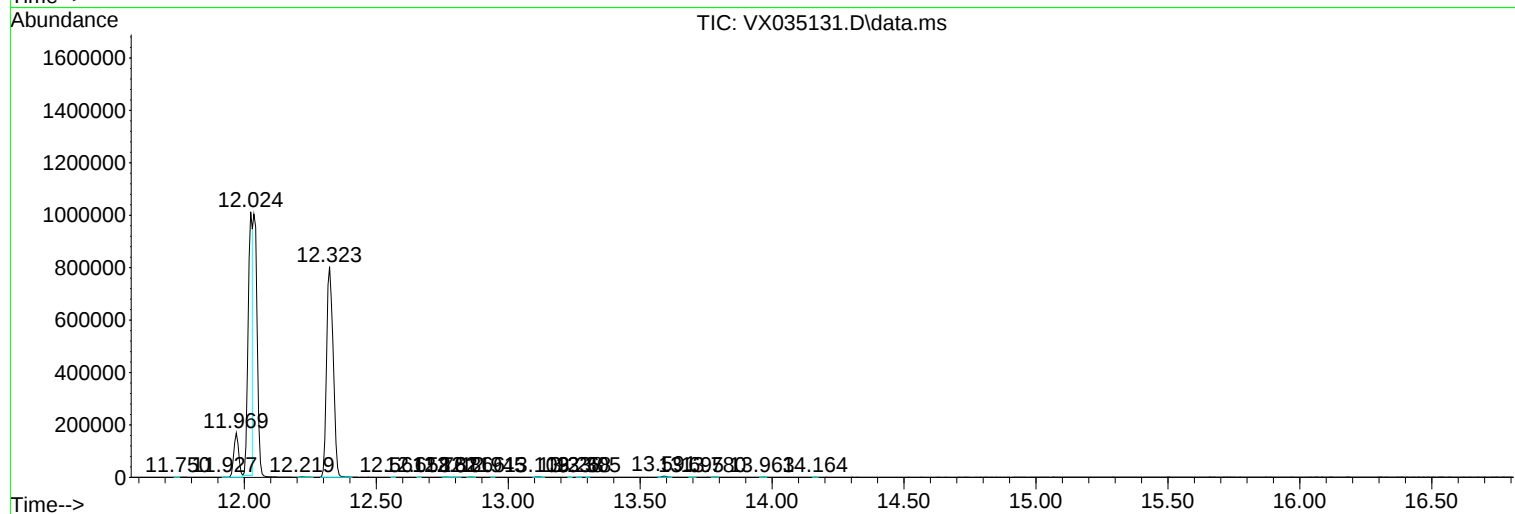
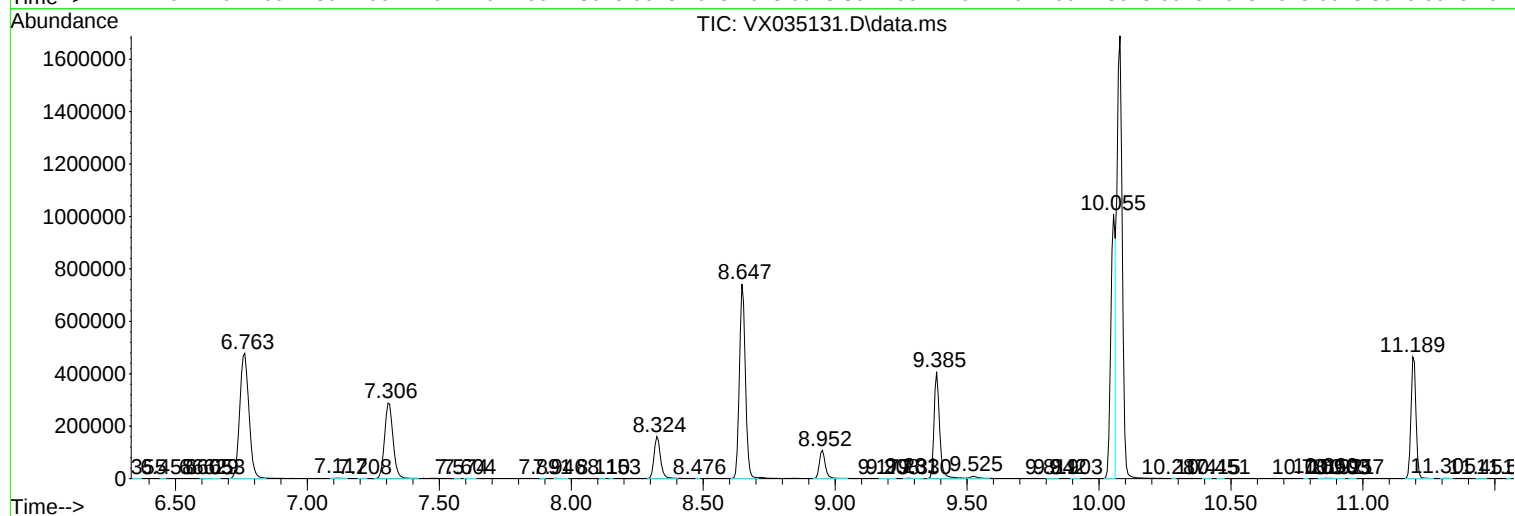
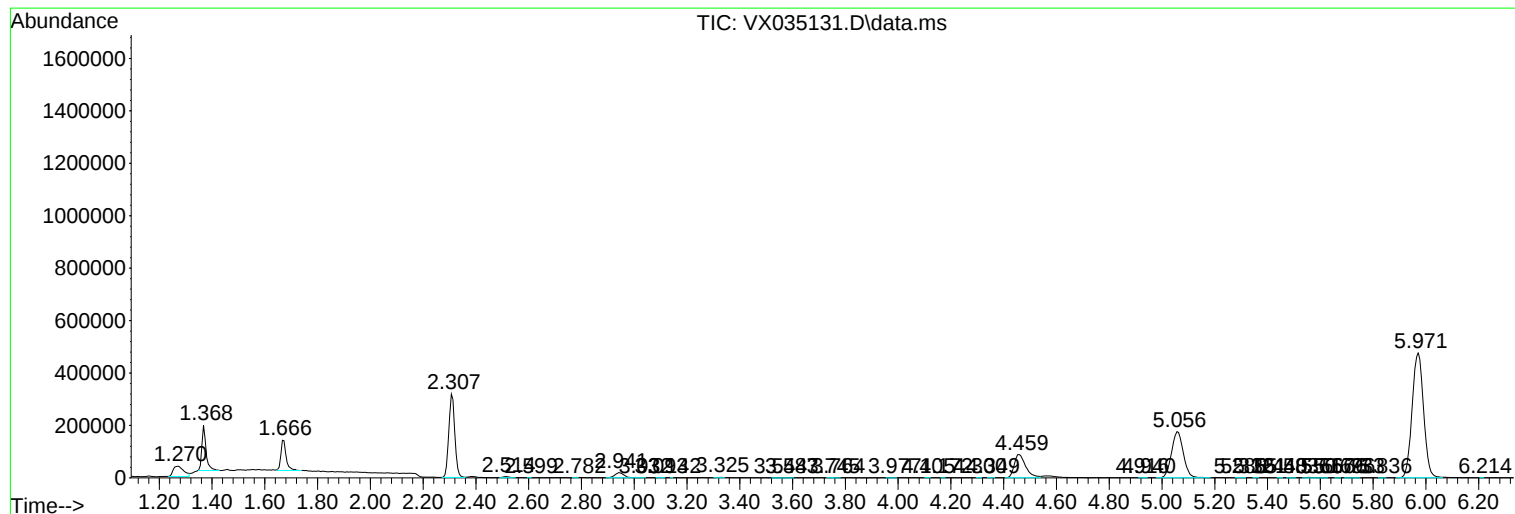
Sum of corrected areas: 12008604

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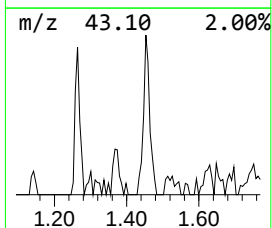
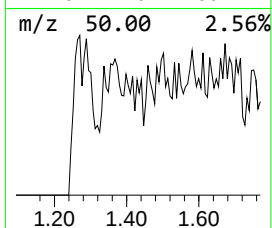
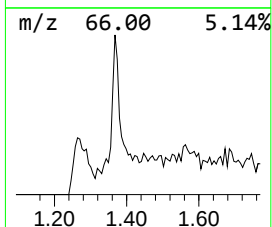
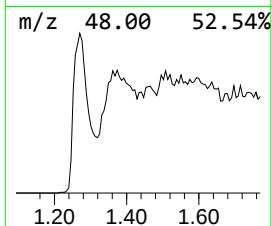
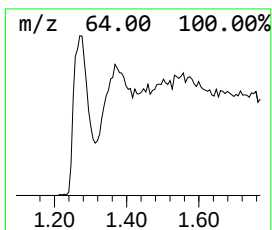
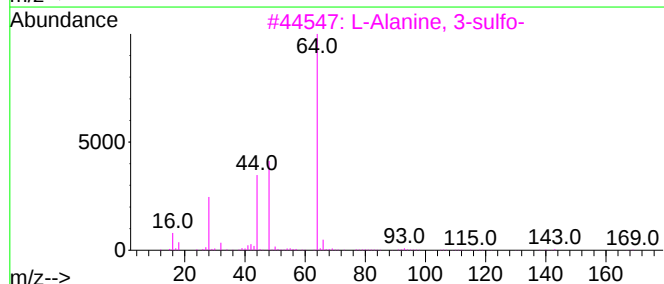
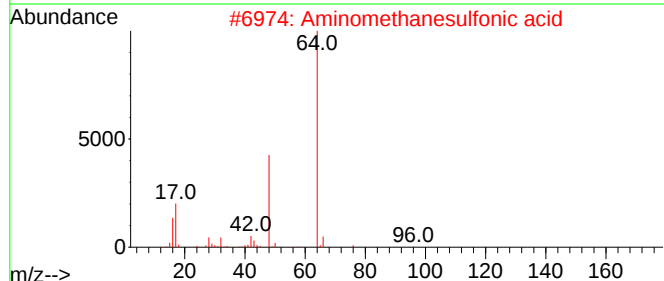
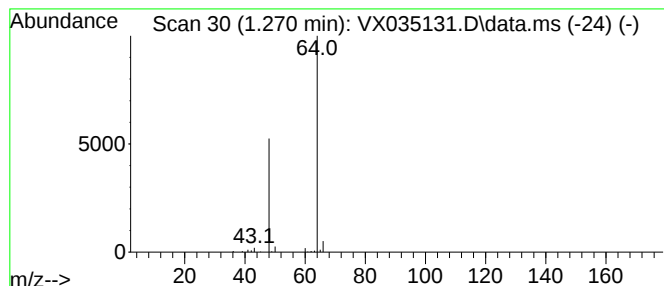
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	4.73 ug/L	108568	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			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	1.270	4.7	ug/L	108568	1	6.763	1147820	50.0