

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035181.D
 Acq On : 19 Apr 2023 19:43
 Operator : JC/MD
 Sample : 02378-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ7

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: VX035181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	26	33	42	rBV	34131	111541	7.83%	1.016%
2	1.368	43	46	63	rVB	168300	196731	13.81%	1.792%
3	1.673	92	96	105	rBV	118764	155501	10.91%	1.416%
4	2.307	194	200	213	rBV	317372	496625	34.86%	4.523%
5	2.788	275	279	284	rBV4	1297	1599	0.11%	0.015%
6	2.941	295	304	314	rBV	27817	64535	4.53%	0.588%
7	3.038	319	320	324	rVV	211	179	0.01%	0.002%
8	3.123	332	334	335	rBV	224	179	0.01%	0.002%
9	3.288	360	361	365	rBV	245	276	0.02%	0.003%
10	3.349	369	371	372	rBV	310	185	0.01%	0.002%
11	3.386	375	377	382	rBV2	201	311	0.02%	0.003%
12	3.508	396	397	400	rVB2	324	246	0.02%	0.002%
13	3.715	430	431	434	rVB2	240	236	0.02%	0.002%
14	3.770	438	440	443	rBV3	301	275	0.02%	0.003%
15	3.843	449	452	453	rBV2	259	228	0.02%	0.002%
16	3.867	453	456	457	rBV2	255	233	0.02%	0.002%
17	3.940	462	468	469	rBV	1431	2117	0.15%	0.019%
18	4.227	514	515	516	rBV	412	172	0.01%	0.002%
19	4.245	516	518	519	rVV	331	210	0.01%	0.002%
20	4.263	519	521	523	rVB	328	302	0.02%	0.003%
21	4.367	536	538	540	rBV2	215	206	0.01%	0.002%
22	4.465	545	554	566	rBV	77372	247979	17.41%	2.259%
23	4.910	625	627	630	rVB3	301	228	0.02%	0.002%
24	5.056	639	651	666	rBV2	173982	540551	37.94%	4.923%
25	5.343	696	698	700	rVB2	273	215	0.02%	0.002%
26	5.391	700	706	715	rBV3	1612	4241	0.30%	0.039%
27	5.556	725	733	741	rBV4	3200	8653	0.61%	0.079%
28	5.660	748	750	752	rBV	154	171	0.01%	0.002%
29	5.727	760	761	765	rVB2	257	261	0.02%	0.002%
30	5.782	765	770	773	rBV2	191	299	0.02%	0.003%
31	5.971	789	801	819	rBV2	476516	1424742	100.00%	12.976%
32	6.220	840	842	844	rBV2	270	264	0.02%	0.002%
33	6.239	844	845	848	rVB2	359	184	0.01%	0.002%
34	6.306	854	856	858	rBV	389	306	0.02%	0.003%
35	6.330	858	860	862	rBV2	177	169	0.01%	0.002%
36	6.470	882	883	886	rVB2	318	173	0.01%	0.002%

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

37	6.544	893	895	896	rBV	365	200	0.01%	0.002%
38	6.653	911	913	915	rBV2	179	238	0.02%	0.002%
39	6.690	917	919	920	rBV	305	167	0.01%	0.002%
40	6.763	920	931	945	rBV	455587	1096557	76.97%	9.987%
41	7.062	978	980	983	rVB3	252	252	0.02%	0.002%
42	7.123	983	990	1000	rBV5	2174	6164	0.43%	0.056%
43	7.214	1003	1005	1007	rBV2	203	174	0.01%	0.002%
44	7.306	1011	1020	1040	rBV	287222	634043	44.50%	5.775%
45	7.470	1045	1047	1048	rBV2	395	320	0.02%	0.003%
46	7.543	1058	1059	1062	rVB2	278	175	0.01%	0.002%
47	7.867	1110	1112	1115	rVB2	302	303	0.02%	0.003%
48	7.952	1124	1126	1130	rVV3	462	545	0.04%	0.005%
49	8.098	1148	1150	1152	rVB	317	232	0.02%	0.002%
50	8.208	1167	1168	1169	rBV	273	167	0.01%	0.002%
51	8.324	1181	1187	1199	rBV	143272	236215	16.58%	2.151%
52	8.537	1220	1222	1224	rVB2	406	247	0.02%	0.002%
53	8.568	1224	1227	1230	rBV2	282	379	0.03%	0.003%
54	8.647	1234	1240	1257	rBV	733939	1162989	81.63%	10.592%
55	8.952	1284	1290	1303	rBV	94584	146169	10.26%	1.331%
56	9.141	1319	1321	1323	rVB2	299	192	0.01%	0.002%
57	9.275	1341	1343	1348	rVB2	1403	1473	0.10%	0.013%
58	9.385	1356	1361	1378	rBV	381904	555765	39.01%	5.062%
59	9.683	1408	1410	1413	rBV3	375	481	0.03%	0.004%
60	10.055	1465	1471	1491	rBV	890255	1243503	87.28%	11.326%
61	10.238	1499	1501	1503	rVB	467	304	0.02%	0.003%
62	10.329	1514	1516	1517	rBV2	328	269	0.02%	0.002%
63	10.403	1527	1528	1530	rBV	281	190	0.01%	0.002%
64	10.476	1538	1540	1542	rVB2	354	259	0.02%	0.002%
65	10.610	1558	1562	1563	rBV	228	237	0.02%	0.002%
66	11.061	1634	1636	1639	rBV	226	198	0.01%	0.002%
67	11.189	1652	1657	1668	rBV	460940	594181	41.70%	5.412%
68	11.317	1674	1678	1680	rVB3	1006	1249	0.09%	0.011%
69	11.451	1699	1700	1704	rVB2	346	206	0.01%	0.002%
70	11.537	1712	1714	1715	rBV	268	172	0.01%	0.002%
71	11.604	1723	1725	1729	rVB2	265	345	0.02%	0.003%
72	11.640	1729	1731	1734	rBV	337	222	0.02%	0.002%
73	11.665	1734	1735	1739	rBV2	326	286	0.02%	0.003%
74	11.750	1745	1749	1750	rBV2	466	380	0.03%	0.003%
75	11.793	1755	1756	1759	rBV	340	279	0.02%	0.003%
76	11.854	1764	1766	1768	rBV	408	312	0.02%	0.003%

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 Title : VOC Analysis

77	11.933	1777	1779	1781	rBV2	414	375	0.03%	0.003%
78	11.976	1781	1786	1788	rBV3	1676	2213	0.16%	0.020%
79	12.024	1788	1794	1807	rVV	816776	1085909	76.22%	9.890%
80	12.219	1822	1826	1833	rBV3	5823	9440	0.66%	0.086%
81	12.317	1837	1842	1864	rVB	682208	921339	64.67%	8.391%
82	12.671	1898	1900	1902	rVB	371	169	0.01%	0.002%
83	12.725	1905	1909	1912	rBV2	260	410	0.03%	0.004%
84	12.768	1912	1916	1918	rVB2	439	614	0.04%	0.006%
85	12.860	1928	1931	1934	rVB2	1191	1164	0.08%	0.011%
86	13.012	1953	1956	1957	rVB2	260	191	0.01%	0.002%
87	13.116	1971	1973	1975	rVV2	268	256	0.02%	0.002%
88	13.213	1987	1989	1993	rVB2	304	293	0.02%	0.003%
89	13.414	2019	2022	2023	rBV2	254	223	0.02%	0.002%
90	13.475	2030	2032	2034	rBV2	379	372	0.03%	0.003%
91	13.591	2047	2051	2056	rBV3	4018	5626	0.39%	0.051%
92	13.823	2087	2089	2090	rBV	431	228	0.02%	0.002%
93	13.969	2109	2113	2115	rBV3	1327	1575	0.11%	0.014%
94	14.243	2156	2158	2160	rVB2	566	397	0.03%	0.004%
95	14.268	2160	2162	2166	rBV2	447	723	0.05%	0.007%
96	14.341	2172	2174	2176	rVB	329	277	0.02%	0.003%
97	14.634	2221	2222	2224	rVB2	362	185	0.01%	0.002%
98	14.914	2266	2268	2270	rBV3	499	382	0.03%	0.003%
99	15.536	2368	2370	2372	rBV2	511	411	0.03%	0.004%
100	16.280	2491	2492	2495	rBV2	633	487	0.03%	0.004%

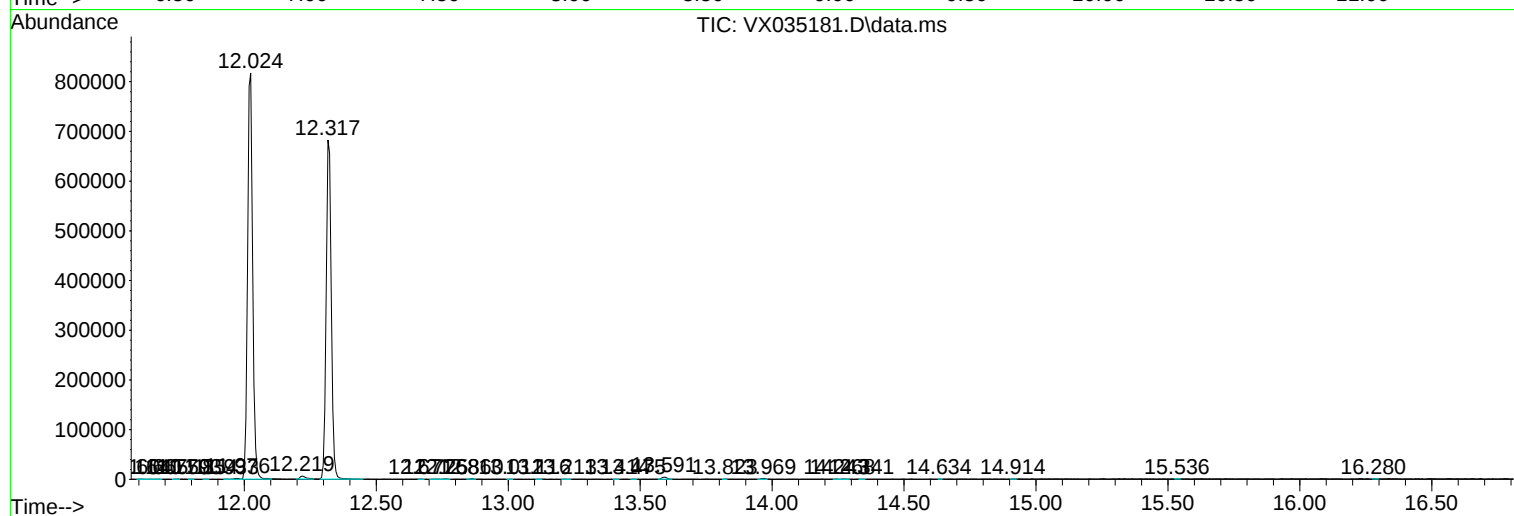
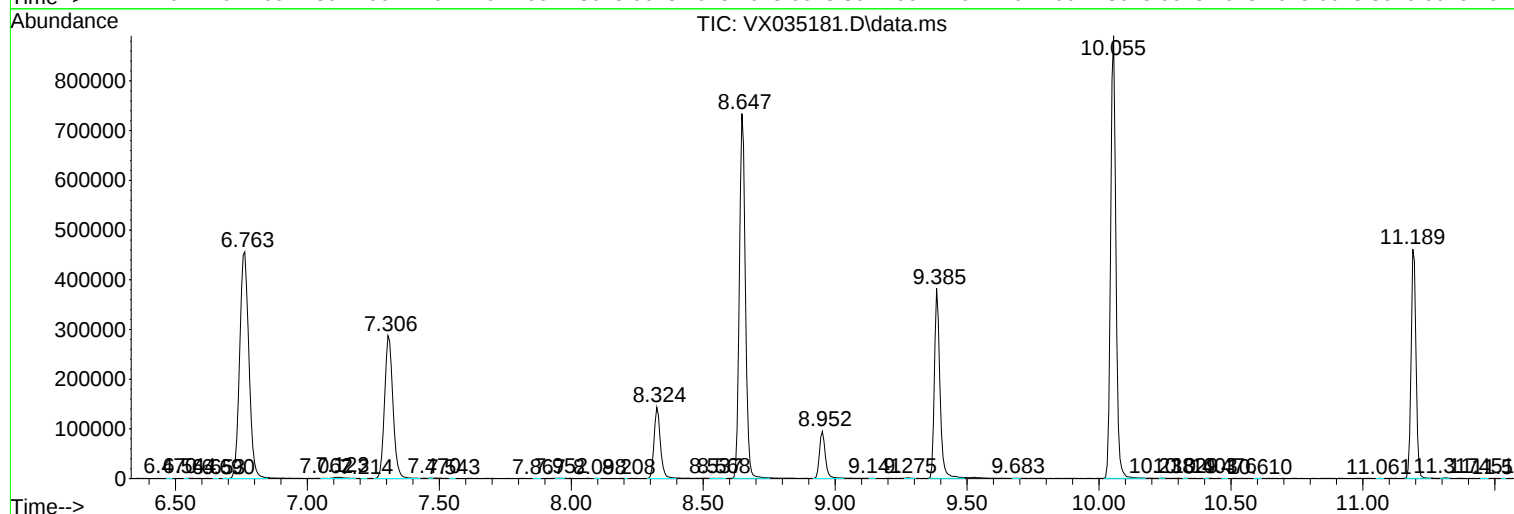
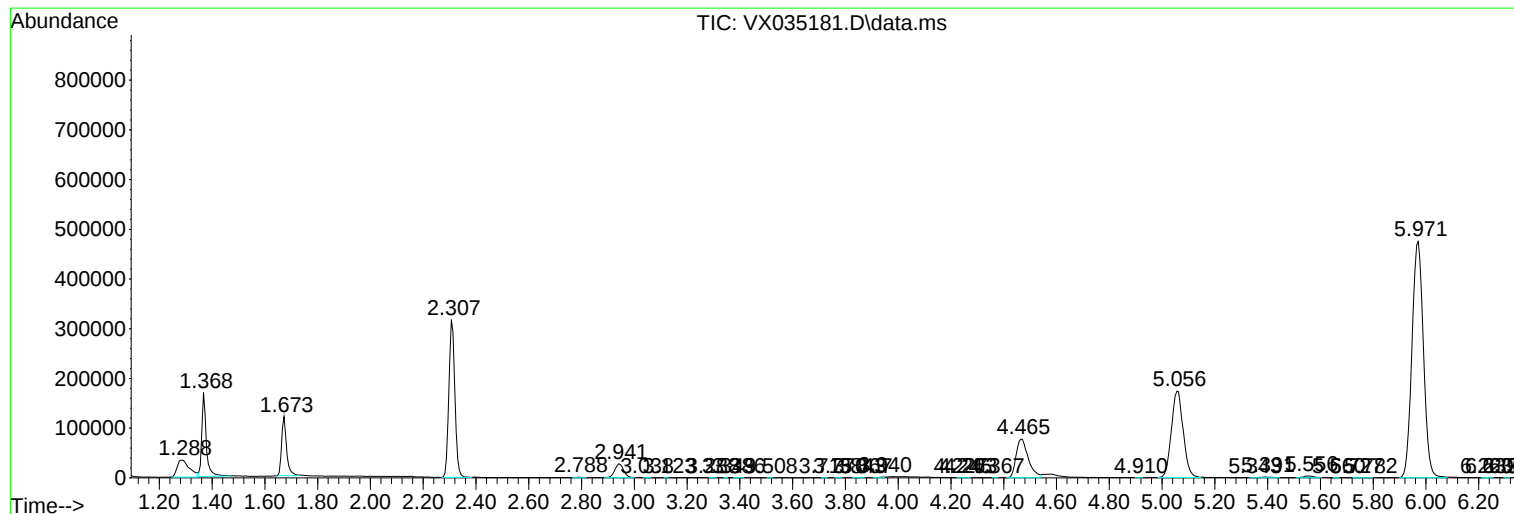
Sum of corrected areas: 10979621

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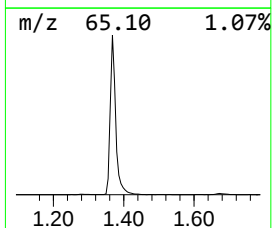
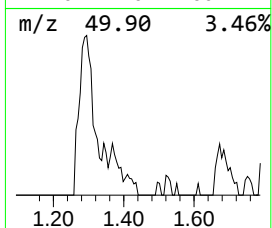
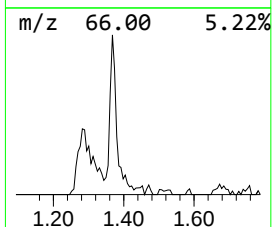
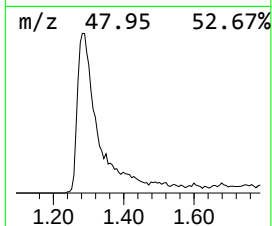
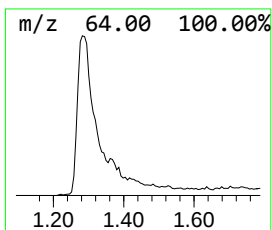
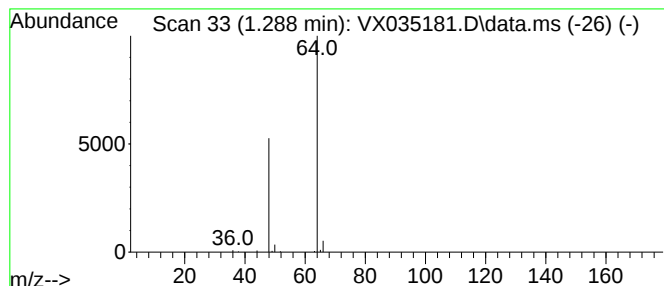
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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.
1.288	5.09 ug/L	111541	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 Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.288	5.1	ug/L	111541	1	6.763	1096560	50.0