

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081022\
 Data File : VX030543.D
 Acq On : 10 Aug 2022 11:28
 Operator : JC/MD
 Sample : N4114-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D75

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: VX030543.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	23	26	41	rBV	143718	261189	19.59%	2.494%
2	1.368	42	46	56	rVB2	279601	313551	23.52%	2.994%
3	1.666	92	95	105	rVB	133602	165565	12.42%	1.581%
4	2.307	194	200	212	rVB	268678	408936	30.67%	3.904%
5	2.788	277	279	281	rBV3	989	702	0.05%	0.007%
6	3.014	311	316	319	rVB5	708	1354	0.10%	0.013%
7	3.093	323	329	340	rVB3	22419	46456	3.48%	0.444%
8	3.276	356	359	360	rBV2	420	421	0.03%	0.004%
9	3.483	391	393	395	rBV3	439	393	0.03%	0.004%
10	3.587	408	410	413	rBV2	368	517	0.04%	0.005%
11	3.636	416	418	421	rVV2	442	457	0.03%	0.004%
12	3.843	447	452	453	rBV3	484	716	0.05%	0.007%
13	3.910	459	463	465	rVV2	494	674	0.05%	0.006%
14	4.166	503	505	507	rBV3	412	445	0.03%	0.004%
15	4.483	545	557	576	rBV2	173176	586310	43.98%	5.598%
16	4.696	590	592	594	rVB2	668	452	0.03%	0.004%
17	4.837	613	615	619	rBV2	552	846	0.06%	0.008%
18	5.062	641	652	668	rBV	177854	536377	40.23%	5.121%
19	5.196	672	674	676	rBV3	643	489	0.04%	0.005%
20	5.312	690	693	696	rVB3	489	672	0.05%	0.006%
21	5.385	703	705	707	rBV2	1206	1251	0.09%	0.012%
22	5.769	766	768	771	rVB	708	395	0.03%	0.004%
23	5.800	771	773	776	rVB2	455	399	0.03%	0.004%
24	5.977	788	802	828	rBV2	465103	1333127	100.00%	12.728%
25	6.385	868	869	874	rVB4	678	530	0.04%	0.005%
26	6.550	894	896	898	rBV2	510	359	0.03%	0.003%
27	6.763	922	931	944	rBV	284886	676887	50.77%	6.462%
28	7.117	981	989	999	rBV7	5769	14663	1.10%	0.140%
29	7.312	1012	1021	1038	rBV	267581	603366	45.26%	5.761%
30	7.635	1072	1074	1076	rVB2	491	485	0.04%	0.005%
31	7.738	1089	1091	1093	rVB2	516	385	0.03%	0.004%
32	7.763	1093	1095	1098	rBV2	630	592	0.04%	0.006%
33	7.915	1117	1120	1122	rBV2	493	452	0.03%	0.004%
34	7.940	1122	1124	1128	rVB4	509	663	0.05%	0.006%
35	8.330	1181	1188	1200	rBV	198073	314594	23.60%	3.004%
36	8.574	1226	1228	1230	rVV3	428	383	0.03%	0.004%

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 Title : VOC Analysis

37	8.653	1234	1241	1260	rVB	670949	1044701	78.36%	9.974%
38	8.952	1285	1290	1300	rBV	140339	208997	15.68%	1.995%
39	9.202	1327	1331	1332	rBV3	667	756	0.06%	0.007%
40	9.281	1342	1344	1349	rVB4	1032	1174	0.09%	0.011%
41	9.391	1356	1362	1373	rBV	557958	807159	60.55%	7.706%
42	9.830	1430	1434	1435	rBV3	590	675	0.05%	0.006%
43	9.897	1442	1445	1447	rBV3	569	539	0.04%	0.005%
44	10.055	1465	1471	1481	rBV	590697	795710	59.69%	7.597%
45	10.232	1499	1500	1503	rVB3	824	525	0.04%	0.005%
46	10.476	1537	1540	1541	rBV3	331	411	0.03%	0.004%
47	10.500	1541	1544	1546	rVV3	406	399	0.03%	0.004%
48	10.939	1614	1616	1619	rBV3	405	484	0.04%	0.005%
49	11.061	1634	1636	1639	rVB3	484	530	0.04%	0.005%
50	11.092	1639	1641	1642	rBV2	774	496	0.04%	0.005%
51	11.195	1652	1658	1668	rBV	502032	641365	48.11%	6.123%
52	11.329	1678	1680	1682	rVB	557	392	0.03%	0.004%
53	11.524	1710	1712	1714	rBV2	342	358	0.03%	0.003%
54	11.628	1728	1729	1734	rVB3	567	517	0.04%	0.005%
55	11.665	1734	1735	1738	rBV3	746	615	0.05%	0.006%
56	11.756	1747	1750	1753	rBV4	675	893	0.07%	0.009%
57	11.811	1757	1759	1762	rVB2	507	471	0.04%	0.004%
58	11.847	1762	1765	1766	rBV	506	424	0.03%	0.004%
59	11.969	1783	1785	1788	rVB2	592	495	0.04%	0.005%
60	12.024	1788	1794	1802	rBV	595625	748691	56.16%	7.148%
61	12.219	1824	1826	1830	rVB3	1399	1363	0.10%	0.013%
62	12.323	1837	1843	1852	rBV	716142	918629	68.91%	8.770%
63	12.555	1877	1881	1883	rBV4	604	841	0.06%	0.008%
64	12.744	1910	1912	1914	rBV3	432	447	0.03%	0.004%
65	12.866	1930	1932	1933	rBV2	362	383	0.03%	0.004%
66	12.945	1943	1945	1950	rVB2	575	796	0.06%	0.008%
67	13.158	1978	1980	1982	rBV	531	373	0.03%	0.004%
68	13.311	2001	2005	2007	rBV3	981	1425	0.11%	0.014%
69	13.414	2019	2022	2023	rBV2	478	526	0.04%	0.005%
70	13.585	2049	2050	2055	rVB4	491	407	0.03%	0.004%
71	13.628	2055	2057	2060	rBV3	445	488	0.04%	0.005%
72	13.652	2060	2061	2064	rVB	773	535	0.04%	0.005%
73	13.676	2064	2065	2067	rBV	558	523	0.04%	0.005%
74	13.774	2079	2081	2082	rBV	656	471	0.04%	0.004%
75	13.939	2105	2108	2109	rBV3	442	530	0.04%	0.005%
76	13.969	2111	2113	2115	rVV2	673	495	0.04%	0.005%

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Peak Location: TOP

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 Title : VOC Analysis

77	14.018	2119	2121	2124	rVB2	747	612	0.05%	0.006%
78	14.060	2126	2128	2131	rVB3	391	405	0.03%	0.004%
79	14.097	2131	2134	2135	rBV3	407	483	0.04%	0.005%
80	14.378	2179	2180	2182	rBV2	677	629	0.05%	0.006%
81	14.512	2200	2202	2204	rBV2	796	567	0.04%	0.005%
82	14.536	2204	2206	2207	rBV2	649	573	0.04%	0.005%
83	14.548	2207	2208	2209	rVV	1024	426	0.03%	0.004%
84	14.566	2209	2211	2213	rVB3	504	447	0.03%	0.004%
85	14.676	2227	2229	2231	rVV2	560	444	0.03%	0.004%
86	14.707	2232	2234	2236	rVB	651	510	0.04%	0.005%
87	14.731	2236	2238	2241	rBV3	449	585	0.04%	0.006%
88	14.987	2279	2280	2284	rBV3	672	702	0.05%	0.007%
89	15.036	2286	2288	2294	rVV3	616	828	0.06%	0.008%
90	15.085	2294	2296	2300	rBV3	579	789	0.06%	0.008%
91	15.310	2331	2333	2334	rVB	712	431	0.03%	0.004%
92	15.432	2350	2353	2358	rBV4	836	1224	0.09%	0.012%
93	15.481	2359	2361	2364	rVV4	666	638	0.05%	0.006%
94	15.542	2370	2371	2373	rVB2	754	371	0.03%	0.004%
95	15.658	2387	2390	2392	rBV2	792	838	0.06%	0.008%
96	16.219	2481	2482	2485	rBV2	529	593	0.04%	0.006%
97	16.432	2516	2517	2519	rBV	677	551	0.04%	0.005%
98	16.475	2522	2524	2525	rBV	620	464	0.03%	0.004%
99	16.530	2531	2533	2536	rBV2	384	432	0.03%	0.004%
100	16.749	2567	2569	2572	rBV3	521	514	0.04%	0.005%

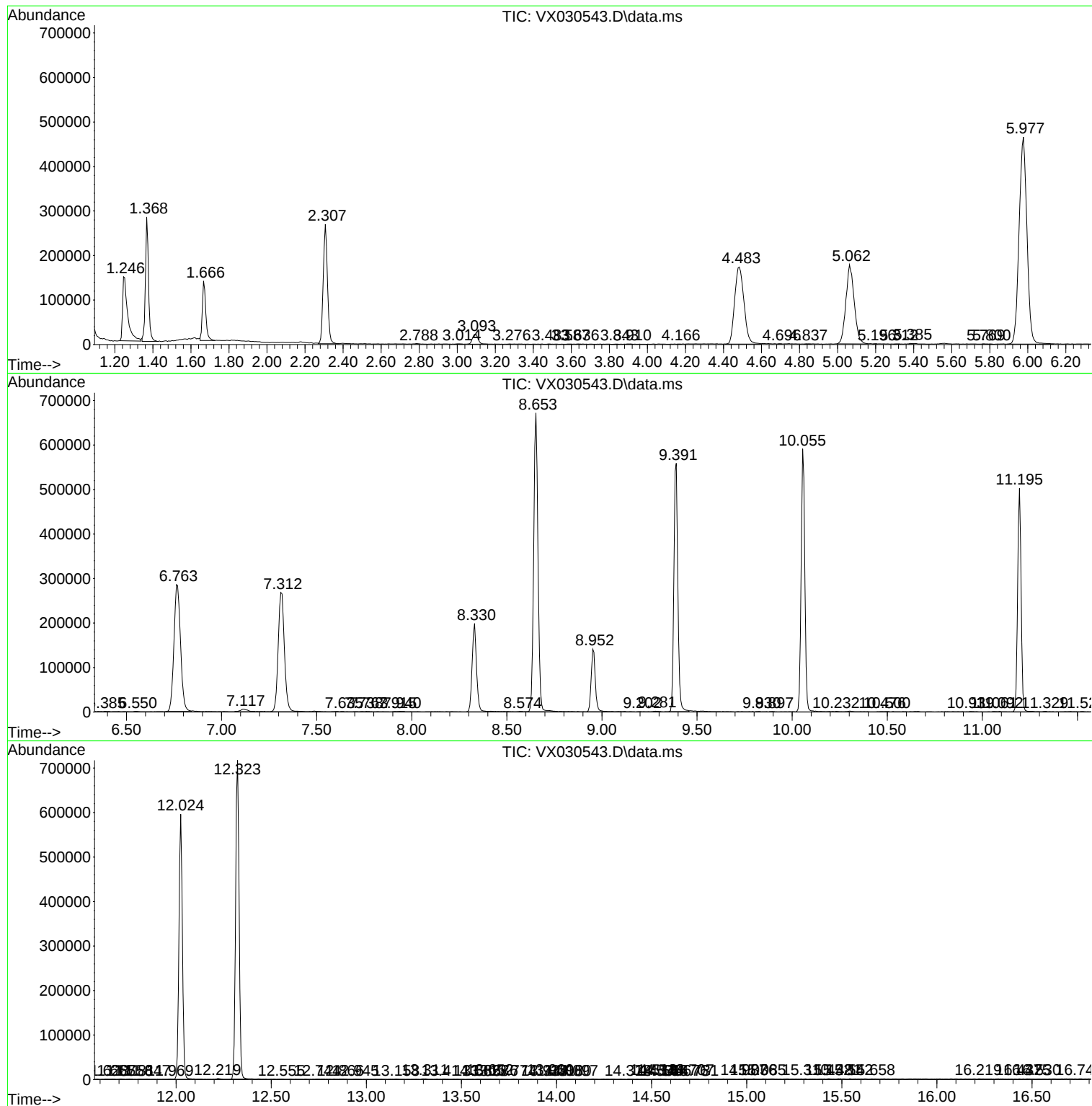
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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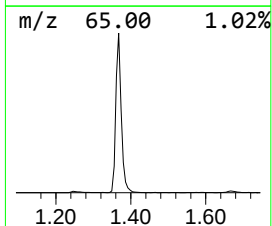
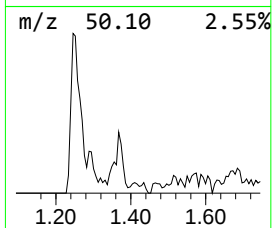
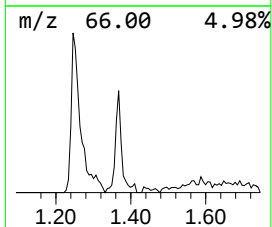
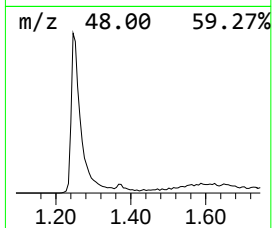
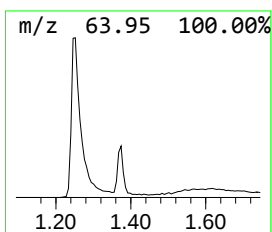
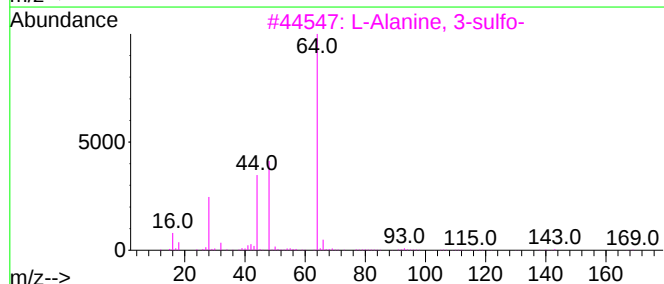
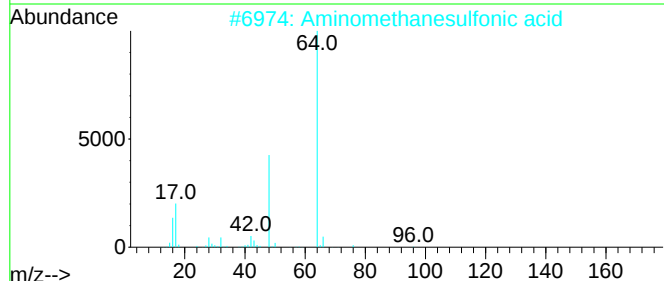
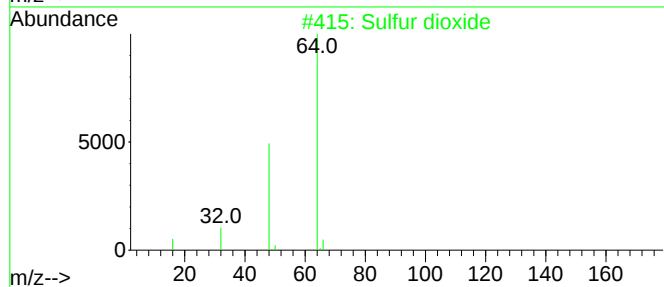
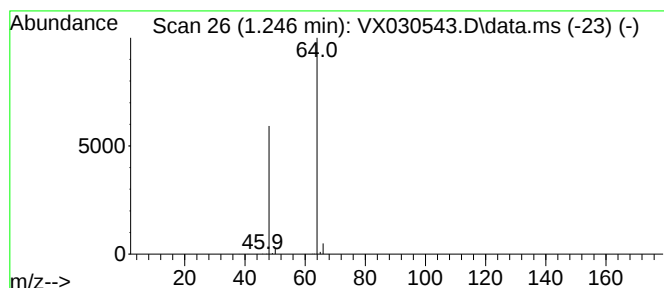
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
1.246	19.29 ug/L	261189	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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	19.3	ug/L	261189	1	6.763	676887	50.0