

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030664.D
 Acq On : 17 Aug 2022 16:48
 Operator : JC/MD
 Sample : N4221-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN8

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: VX030664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	42	rBV3	17602	48304	1.10%	0.326%
2	1.368	42	46	55	rVB	189413	194131	4.42%	1.311%
3	1.666	91	95	103	rVB	134780	160180	3.65%	1.082%
4	2.307	193	200	211	rBV2	344984	610518	13.91%	4.123%
5	2.422	218	219	223	rBV2	985	1132	0.03%	0.008%
6	2.794	276	280	283	rVV3	987	1537	0.04%	0.010%
7	2.934	300	303	304	rBV2	673	736	0.02%	0.005%
8	3.093	323	329	335	rVV4	2355	5407	0.12%	0.037%
9	3.178	339	343	346	rBV	451	649	0.01%	0.004%
10	3.349	367	371	374	rBV2	486	638	0.01%	0.004%
11	3.556	403	405	407	rVV2	449	576	0.01%	0.004%
12	3.617	408	415	423	rVV3	8562	19615	0.45%	0.132%
13	3.715	429	431	435	rVV2	368	403	0.01%	0.003%
14	3.758	437	438	441	rVB2	349	344	0.01%	0.002%
15	3.800	441	445	446	rBV	445	507	0.01%	0.003%
16	3.812	446	447	450	rVB	477	423	0.01%	0.003%
17	3.953	469	470	472	rBV	464	346	0.01%	0.002%
18	3.977	472	474	477	rVV2	449	531	0.01%	0.004%
19	4.190	506	509	511	rBV2	411	583	0.01%	0.004%
20	4.264	520	521	525	rBV2	363	484	0.01%	0.003%
21	4.331	530	532	536	rVB2	464	548	0.01%	0.004%
22	4.489	545	558	578	rBV2	363211	1177121	26.83%	7.950%
23	4.898	623	625	627	rBV2	400	390	0.01%	0.003%
24	5.062	641	652	668	rVV	163423	513150	11.70%	3.465%
25	5.233	677	680	683	rBV2	463	628	0.01%	0.004%
26	5.397	696	707	720	rVB4	17025	54186	1.23%	0.366%
27	5.556	725	733	738	rBV3	1997	5169	0.12%	0.035%
28	5.647	746	748	751	rBV	443	391	0.01%	0.003%
29	5.812	773	775	778	rVB2	460	396	0.01%	0.003%
30	5.861	781	783	785	rBV3	302	375	0.01%	0.003%
31	5.977	790	802	822	rVV2	442990	1304630	29.73%	8.811%
32	6.233	843	844	847	rBV2	824	706	0.02%	0.005%
33	6.409	872	873	876	rBV2	474	452	0.01%	0.003%
34	6.464	881	882	887	rVB2	476	394	0.01%	0.003%
35	6.617	904	907	910	rBV2	364	401	0.01%	0.003%
36	6.763	923	931	947	rBV	136037	330769	7.54%	2.234%

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 Title : VOC Analysis

37	6.915	954	956	958	rBV3	461	406	0.01%	0.003%
38	6.958	961	963	964	rBV2	442	374	0.01%	0.003%
39	7.056	976	979	982	rBV2	307	500	0.01%	0.003%
40	7.129	982	991	1004	rBV	428892	952779	21.72%	6.434%
41	7.312	1013	1021	1033	rBV	262923	577047	13.15%	3.897%
42	7.464	1044	1046	1047	rBV	646	370	0.01%	0.002%
43	7.690	1079	1083	1086	rBV3	510	764	0.02%	0.005%
44	7.873	1108	1113	1114	rVB3	277	374	0.01%	0.003%
45	7.934	1119	1123	1128	rBV4	1162	2195	0.05%	0.015%
46	8.074	1144	1146	1151	rVB	473	454	0.01%	0.003%
47	8.129	1153	1155	1157	rBV	528	480	0.01%	0.003%
48	8.269	1177	1178	1181	rBV2	475	432	0.01%	0.003%
49	8.330	1181	1188	1198	rBV	178208	291485	6.64%	1.969%
50	8.482	1210	1213	1217	rVB2	799	1163	0.03%	0.008%
51	8.653	1234	1241	1254	rBV	677425	1048272	23.89%	7.079%
52	8.952	1285	1290	1300	rBV	127304	188727	4.30%	1.275%
53	9.153	1321	1323	1324	rBV	710	695	0.02%	0.005%
54	9.275	1336	1343	1356	rBV	3018225	4387652	100.00%	29.631%
55	9.391	1356	1362	1373	rVB	460140	665676	15.17%	4.496%
56	9.805	1426	1430	1432	rVB2	565	561	0.01%	0.004%
57	10.055	1466	1471	1488	rVB	280028	416487	9.49%	2.813%
58	10.366	1521	1522	1526	rVB2	448	403	0.01%	0.003%
59	10.525	1546	1548	1549	rBV2	426	413	0.01%	0.003%
60	10.555	1552	1553	1556	rVV2	466	378	0.01%	0.003%
61	10.616	1561	1563	1564	rVV2	548	350	0.01%	0.002%
62	10.695	1574	1576	1578	rVB	860	606	0.01%	0.004%
63	10.726	1578	1581	1582	rBV	439	409	0.01%	0.003%
64	10.811	1593	1595	1598	rBV3	332	432	0.01%	0.003%
65	10.964	1618	1620	1624	rVB3	560	749	0.02%	0.005%
66	11.146	1648	1650	1652	rBV	368	451	0.01%	0.003%
67	11.195	1652	1658	1667	rBV	476323	593648	13.53%	4.009%
68	11.311	1675	1677	1682	rVB3	1331	1923	0.04%	0.013%
69	11.427	1694	1696	1699	rBV2	414	352	0.01%	0.002%
70	11.463	1699	1702	1703	rBV2	451	391	0.01%	0.003%
71	11.518	1710	1711	1715	rVB2	506	400	0.01%	0.003%
72	11.555	1715	1717	1721	rVB2	641	651	0.01%	0.004%
73	11.634	1728	1730	1732	rBV2	606	451	0.01%	0.003%
74	11.707	1741	1742	1745	rBV	668	568	0.01%	0.004%
75	11.799	1753	1757	1761	rVB2	2075	2580	0.06%	0.017%
76	11.878	1765	1770	1771	rBV2	668	896	0.02%	0.006%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : VOC Analysis

77	11.921	1775	1777	1779	rBV2	322	357	0.01%	0.002%
78	12.024	1788	1794	1801	rBV	280082	345739	7.88%	2.335%
79	12.104	1805	1807	1809	rBV2	624	519	0.01%	0.004%
80	12.323	1837	1843	1852	rBV	704061	870928	19.85%	5.882%
81	12.433	1860	1861	1864	rBV2	522	486	0.01%	0.003%
82	12.805	1919	1922	1925	rVB2	713	575	0.01%	0.004%
83	12.829	1925	1926	1928	rBV	506	410	0.01%	0.003%
84	12.896	1935	1937	1940	rVB	416	399	0.01%	0.003%
85	12.963	1946	1948	1949	rVV	484	389	0.01%	0.003%
86	13.006	1953	1955	1957	rBV2	507	398	0.01%	0.003%
87	13.073	1964	1966	1967	rBV	632	392	0.01%	0.003%
88	13.122	1973	1974	1976	rBV	628	373	0.01%	0.003%
89	13.207	1986	1988	1989	rBV	771	446	0.01%	0.003%
90	13.353	2010	2012	2016	rVB2	501	474	0.01%	0.003%
91	13.530	2040	2041	2044	rBV	523	473	0.01%	0.003%
92	13.762	2076	2079	2082	rBV2	587	818	0.02%	0.006%
93	13.847	2091	2093	2096	rVB3	718	471	0.01%	0.003%
94	14.170	2145	2146	2150	rBV	581	639	0.01%	0.004%
95	14.292	2163	2166	2171	rBV3	579	716	0.02%	0.005%
96	14.335	2171	2173	2175	rVB2	641	489	0.01%	0.003%
97	14.506	2198	2201	2202	rBV2	632	524	0.01%	0.004%
98	15.359	2340	2341	2344	rBV2	1044	800	0.02%	0.005%
99	15.457	2355	2357	2358	rBV	645	430	0.01%	0.003%
100	16.164	2471	2473	2474	rBV	887	509	0.01%	0.003%

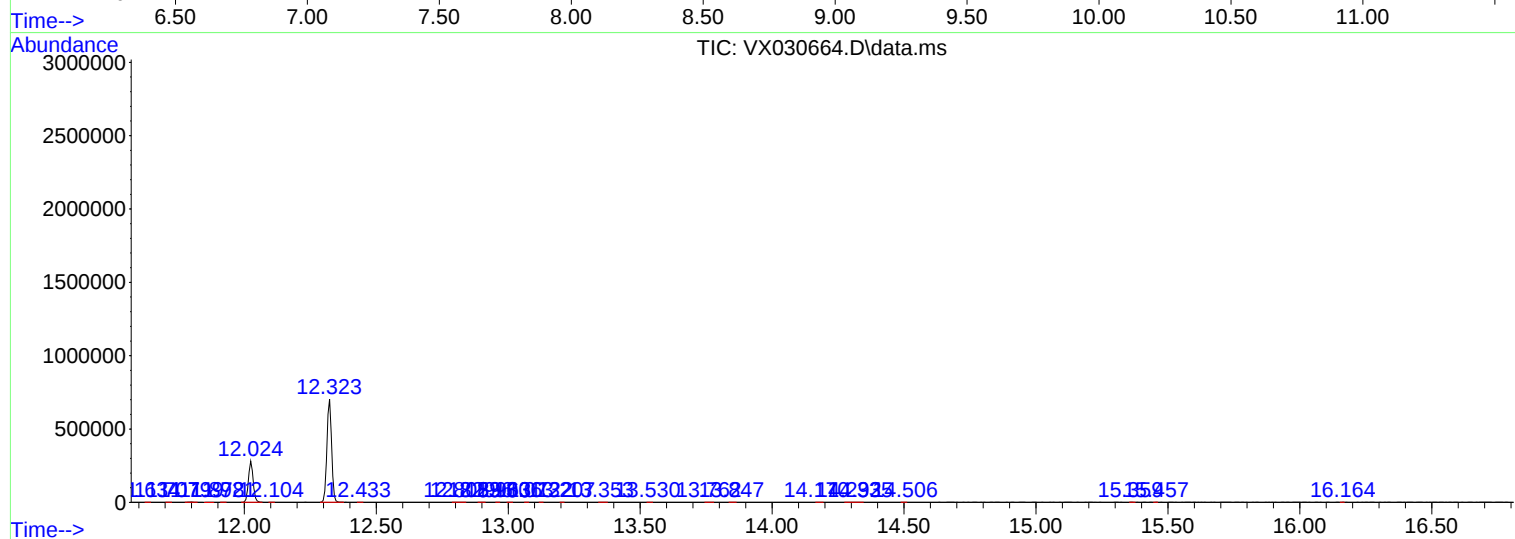
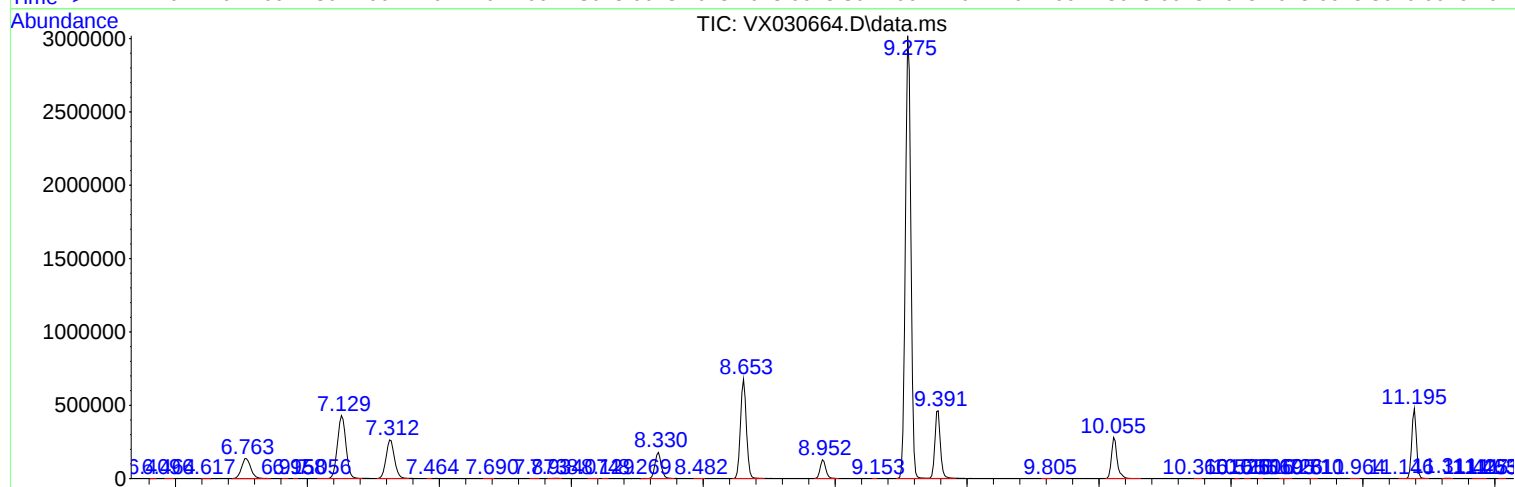
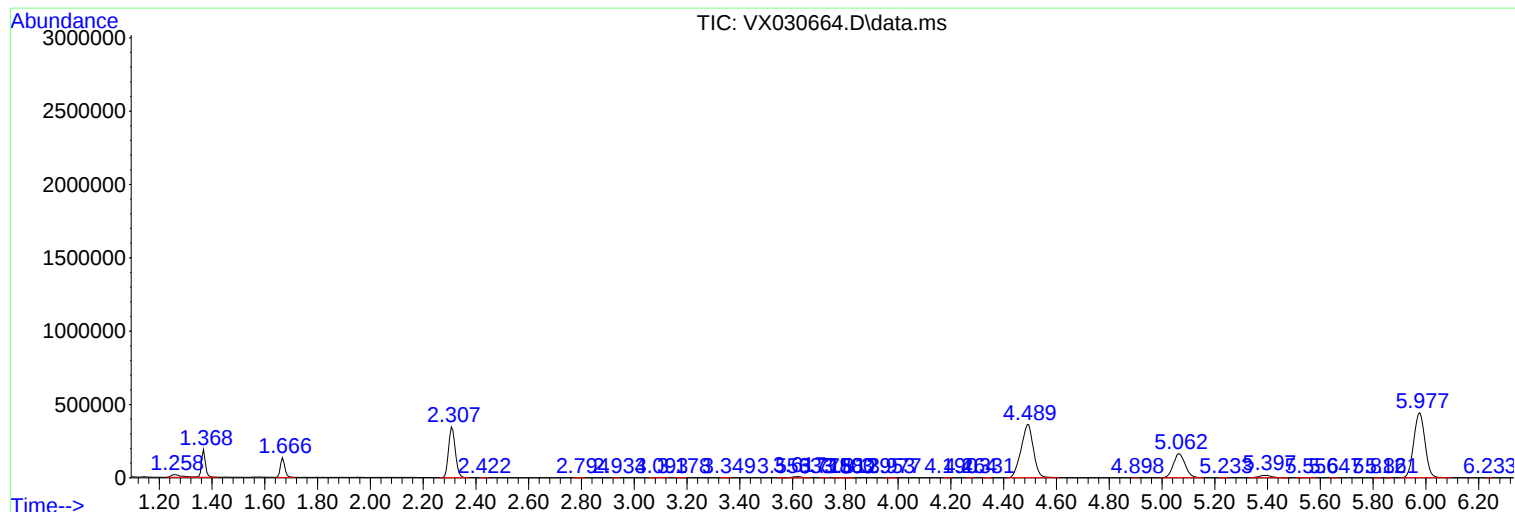
Sum of corrected areas: 14807448

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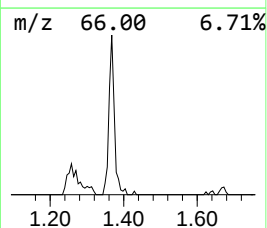
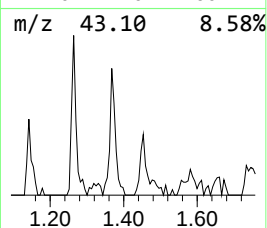
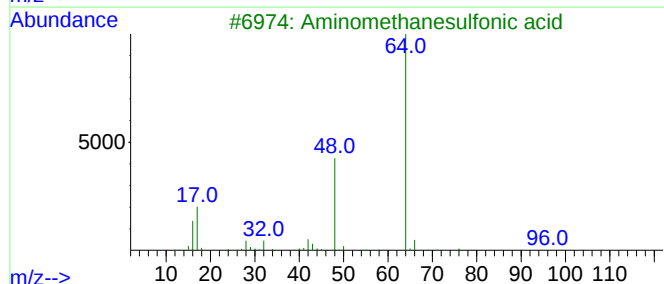
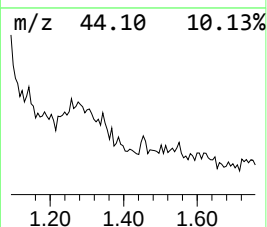
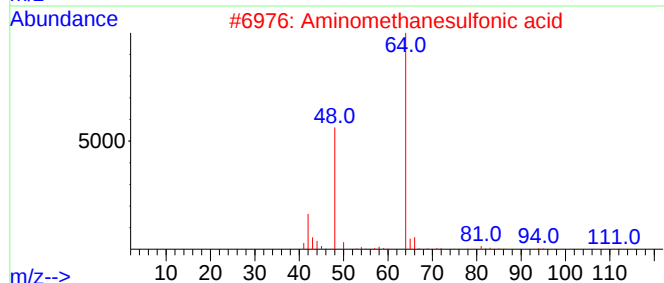
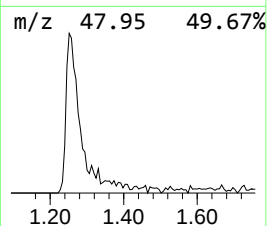
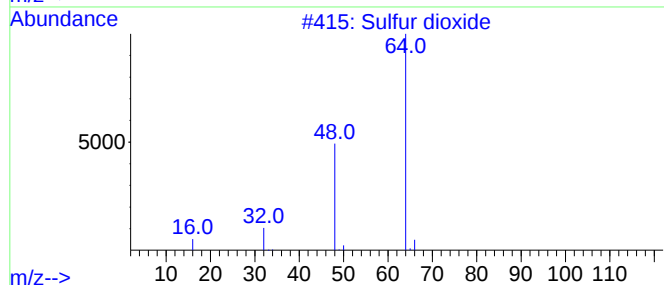
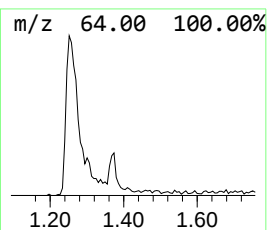
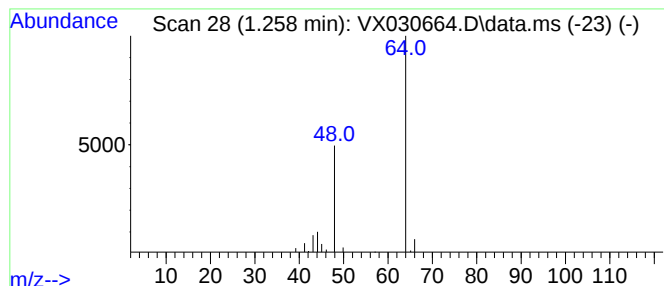
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
1.258	7.30 ug/L	48304	1,4-Difluorobenzene	6.769

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	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	7.3	ug/L	48304	1	6.769	330769	50.0