

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
 Data File : VX025950.D
 Acq On : 21 Dec 2021 12:39
 Operator : JC/MD
 Sample : M5150-13DL 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBX1DL

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\SFAMXML122021WMA.M
 Title : VOC Analysis

Signal : TIC: VX025950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	34	rBV2	19530	32961	5.31%	0.595%
2	1.368	43	46	57	rVB	83584	82271	13.25%	1.484%
3	1.666	91	95	104	rBV	65276	87081	14.03%	1.571%
4	2.313	194	201	209	rBV	115523	192850	31.06%	3.479%
5	2.788	276	279	285	rVB2	1702	2604	0.42%	0.047%
6	3.032	316	319	320	rBV	166	151	0.02%	0.003%
7	3.081	323	327	329	rBV2	204	230	0.04%	0.004%
8	3.148	337	338	342	rBV	272	249	0.04%	0.004%
9	3.264	356	357	360	rVB	284	184	0.03%	0.003%
10	3.312	363	365	366	rVB2	151	74	0.01%	0.001%
11	3.550	403	404	407	rBV	211	170	0.03%	0.003%
12	3.757	436	438	440	rBV	267	246	0.04%	0.004%
13	3.818	447	448	452	rVB2	198	180	0.03%	0.003%
14	3.855	452	454	455	rBV	106	59	0.01%	0.001%
15	3.946	468	469	470	rBV	201	108	0.02%	0.002%
16	4.020	480	481	483	rBV	112	79	0.01%	0.001%
17	4.123	495	498	502	rVB2	238	336	0.05%	0.006%
18	4.160	502	504	505	rBV2	107	67	0.01%	0.001%
19	4.209	510	512	513	rBV	203	112	0.02%	0.002%
20	4.300	525	527	530	rBV2	139	109	0.02%	0.002%
21	4.349	534	535	537	rBV2	132	112	0.02%	0.002%
22	4.373	537	539	541	rVB	240	121	0.02%	0.002%
23	4.398	541	543	544	rBV2	158	147	0.02%	0.003%
24	4.459	545	553	567	rBV	47372	131348	21.16%	2.369%
25	4.849	615	617	618	rVB	233	111	0.02%	0.002%
26	4.940	629	632	633	rBV	244	149	0.02%	0.003%
27	5.062	639	652	669	rBV2	89121	256382	41.29%	4.625%
28	5.391	704	706	711	rVB2	269	390	0.06%	0.007%
29	5.477	715	720	725	rVV3	616	1135	0.18%	0.020%
30	5.544	728	731	732	rBV	158	119	0.02%	0.002%
31	5.690	753	755	758	rBV2	111	123	0.02%	0.002%
32	5.977	790	802	820	rBV2	207226	620862	100.00%	11.200%
33	6.190	836	837	839	rBV	162	130	0.02%	0.002%
34	6.233	842	844	846	rVB2	174	92	0.01%	0.002%
35	6.251	846	847	848	rBV	159	94	0.02%	0.002%
36	6.300	854	855	856	rBV	194	86	0.01%	0.002%

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 Title : VOC Analysis

37	6.367	864	866	868	rBV	257	178	0.03%	0.003%
38	6.592	902	903	904	rBV	94	53	0.01%	0.001%
39	6.763	922	931	946	rBV	165028	398752	64.23%	7.193%
40	7.129	982	991	1001	rBV	280514	594390	95.74%	10.723%
41	7.312	1013	1021	1033	rBV	147875	331467	53.39%	5.980%
42	7.696	1083	1084	1085	rBV	171	107	0.02%	0.002%
43	8.177	1162	1163	1164	rBV	214	119	0.02%	0.002%
44	8.281	1179	1180	1181	rBV	230	159	0.03%	0.003%
45	8.324	1181	1187	1199	rVV	96747	153045	24.65%	2.761%
46	8.580	1226	1229	1233	rBV3	327	458	0.07%	0.008%
47	8.653	1233	1241	1249	rBV	363417	588376	94.77%	10.614%
48	8.952	1285	1290	1301	rBV	66152	90740	14.62%	1.637%
49	9.275	1339	1343	1348	rVB2	2620	3872	0.62%	0.070%
50	9.385	1356	1361	1377	rBV	233312	341786	55.05%	6.166%
51	9.994	1459	1461	1465	rBV	257	274	0.04%	0.005%
52	10.055	1465	1471	1489	rVB	354951	502739	80.97%	9.069%
53	10.299	1508	1511	1518	rBV3	809	1190	0.19%	0.021%
54	10.543	1549	1551	1552	rVB	263	109	0.02%	0.002%
55	11.122	1642	1646	1652	rVB3	1768	2460	0.40%	0.044%
56	11.195	1652	1658	1666	rBV	275090	361214	58.18%	6.516%
57	11.671	1735	1736	1737	rVB	238	87	0.01%	0.002%
58	11.689	1737	1739	1741	rBV	294	222	0.04%	0.004%
59	11.823	1760	1761	1762	rVB	139	51	0.01%	0.001%
60	11.841	1762	1764	1766	rVB	337	293	0.05%	0.005%
61	11.908	1773	1775	1776	rBV	166	127	0.02%	0.002%
62	11.927	1776	1778	1783	rVB2	607	775	0.12%	0.014%
63	12.024	1789	1794	1801	rBV	287535	357698	57.61%	6.453%
64	12.183	1819	1820	1823	rBV	193	196	0.03%	0.004%
65	12.225	1825	1827	1830	rBV2	245	313	0.05%	0.006%
66	12.323	1837	1843	1851	rVB	300762	394214	63.49%	7.112%
67	12.482	1866	1869	1873	rBV2	293	393	0.06%	0.007%
68	12.597	1887	1888	1891	rVB2	315	199	0.03%	0.004%
69	12.628	1891	1893	1896	rBV2	208	218	0.04%	0.004%
70	12.695	1902	1904	1906	rVB2	334	253	0.04%	0.005%
71	12.731	1908	1910	1911	rVB	146	62	0.01%	0.001%
72	12.774	1916	1917	1919	rVV	376	210	0.03%	0.004%
73	12.829	1923	1926	1927	rBV2	213	173	0.03%	0.003%
74	12.884	1934	1935	1937	rBV	183	120	0.02%	0.002%
75	13.049	1959	1962	1966	rBV2	333	492	0.08%	0.009%
76	13.116	1972	1973	1975	rVB2	144	70	0.01%	0.001%

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 Title : VOC Analysis

77	13.134	1975	1976	1977	rBV	158	100	0.02%	0.002%
78	13.420	2020	2023	2029	rBV2	294	530	0.09%	0.010%
79	13.463	2029	2030	2033	rBV2	255	224	0.04%	0.004%
80	13.555	2043	2045	2046	rBV	136	76	0.01%	0.001%
81	13.603	2051	2053	2054	rVB	194	78	0.01%	0.001%
82	13.652	2059	2061	2065	rVB2	200	230	0.04%	0.004%
83	13.713	2069	2071	2073	rBV	276	245	0.04%	0.004%
84	13.786	2080	2083	2085	rBV	255	230	0.04%	0.004%
85	13.847	2091	2093	2095	rBV	183	183	0.03%	0.003%
86	14.073	2128	2130	2132	rBV	115	85	0.01%	0.002%
87	14.121	2136	2138	2140	rVB2	271	149	0.02%	0.003%
88	14.359	2176	2177	2181	rBV2	147	149	0.02%	0.003%
89	14.402	2183	2184	2187	rVB	199	155	0.02%	0.003%
90	14.682	2228	2230	2232	rBV2	172	193	0.03%	0.003%
91	14.756	2241	2242	2243	rBV	289	143	0.02%	0.003%
92	14.847	2255	2257	2258	rVB	152	59	0.01%	0.001%
93	14.890	2263	2264	2265	rVB	247	90	0.01%	0.002%
94	14.938	2267	2272	2274	rBV3	315	422	0.07%	0.008%
95	15.780	2408	2410	2413	rBV3	397	450	0.07%	0.008%
96	15.963	2439	2440	2442	rBV	365	163	0.03%	0.003%
97	16.432	2515	2517	2518	rBV	206	184	0.03%	0.003%

Sum of corrected areas: 5543314

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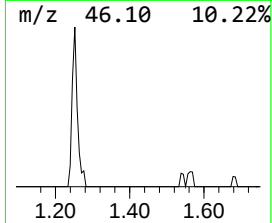
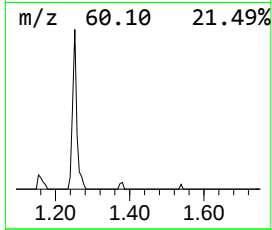
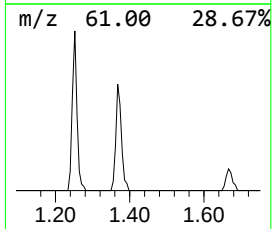
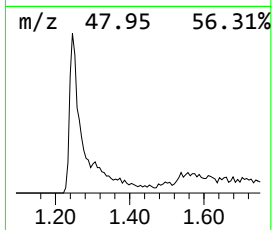
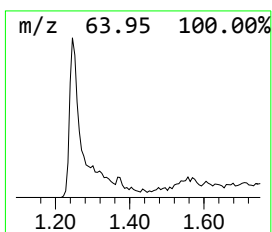
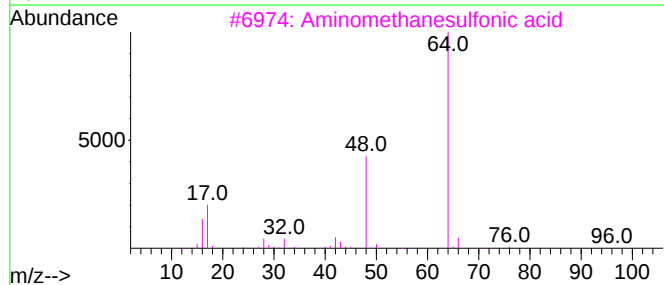
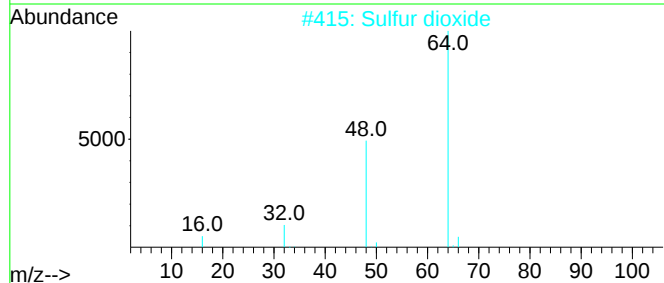
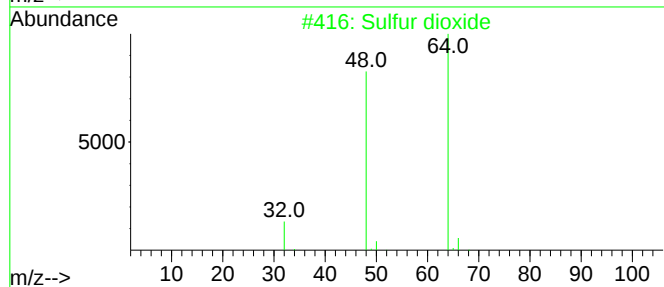
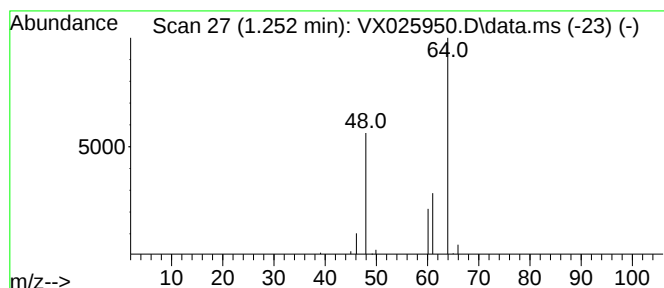
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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.
1.252	4.13 ug/L	32961	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	72
2			Sulfur dioxide	64	O2S	007446-09-5	72
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	56
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	4.1	ug/L	32961	1	6.769	398752	50.0