

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
 Data File : VX025952.D
 Acq On : 21 Dec 2021 13:26
 Operator : JC/MD
 Sample : M5150-19DL 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBX7DL

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: VX025952.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	22	27	33	rBV	22174	29844	4.60%	0.539%
2	1.368	43	46	55	rVB	81657	86350	13.31%	1.560%
3	1.666	91	95	105	rVB	67676	89733	13.84%	1.621%
4	2.307	194	200	208	rBV	121734	199827	30.81%	3.610%
5	2.380	209	212	218	rVB2	3827	6007	0.93%	0.109%
6	2.489	228	230	232	rBV2	310	278	0.04%	0.005%
7	2.514	232	234	235	rVB2	504	347	0.05%	0.006%
8	2.788	276	279	285	rVB2	1542	2587	0.40%	0.047%
9	2.947	301	305	312	rVB2	934	1478	0.23%	0.027%
10	3.136	334	336	337	rVB	248	135	0.02%	0.002%
11	3.154	337	339	344	rBV2	175	221	0.03%	0.004%
12	3.227	349	351	354	rVV	247	277	0.04%	0.005%
13	3.276	357	359	360	rBV2	194	142	0.02%	0.003%
14	3.361	372	373	374	rBV	333	209	0.03%	0.004%
15	3.489	393	394	397	rVB2	274	203	0.03%	0.004%
16	3.526	397	400	403	rBV2	261	279	0.04%	0.005%
17	3.660	420	422	425	rVB	201	170	0.03%	0.003%
18	3.758	435	438	439	rBV2	166	227	0.04%	0.004%
19	3.806	444	446	448	rBV	166	140	0.02%	0.003%
20	4.014	478	480	484	rBV2	170	249	0.04%	0.004%
21	4.142	499	501	503	rBV2	181	158	0.02%	0.003%
22	4.459	543	553	569	rBV	51395	169229	26.09%	3.057%
23	4.715	593	595	597	rBB2	243	154	0.02%	0.003%
24	4.733	597	598	601	rBV	223	207	0.03%	0.004%
25	4.837	612	615	618	rVB2	170	214	0.03%	0.004%
26	5.062	639	652	668	rBV	87012	267748	41.28%	4.837%
27	5.324	693	695	697	rBV2	158	146	0.02%	0.003%
28	5.513	724	726	731	rBV2	151	221	0.03%	0.004%
29	5.971	789	801	815	rBV2	217059	648542	100.00%	11.715%
30	6.440	876	878	882	rBV	302	281	0.04%	0.005%
31	6.598	903	904	908	rBV	206	186	0.03%	0.003%
32	6.678	915	917	920	rVB	200	163	0.03%	0.003%
33	6.763	920	931	947	rBV	132818	319391	49.25%	5.769%
34	7.031	971	975	977	rBV2	187	238	0.04%	0.004%
35	7.129	982	991	1006	rBV	177113	384921	59.35%	6.953%
36	7.312	1012	1021	1037	rBV	135673	298816	46.08%	5.398%

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

37	7.550	1059	1060	1065	rVB2	193	237	0.04%	0.004%
38	7.958	1125	1127	1129	rBV	244	176	0.03%	0.003%
39	8.092	1146	1149	1151	rBV2	182	210	0.03%	0.004%
40	8.147	1156	1158	1160	rBV	197	173	0.03%	0.003%
41	8.324	1181	1187	1195	rBV	99329	165856	25.57%	2.996%
42	8.409	1199	1201	1205	rVB2	555	503	0.08%	0.009%
43	8.562	1223	1226	1227	rBV2	371	355	0.05%	0.006%
44	8.580	1227	1229	1234	rBV2	182	134	0.02%	0.002%
45	8.653	1234	1241	1249	rBV	402798	642600	99.08%	11.608%
46	8.909	1281	1283	1284	rBV2	286	224	0.03%	0.004%
47	8.952	1284	1290	1301	rVV	80260	108416	16.72%	1.958%
48	9.165	1323	1325	1327	rBV2	281	208	0.03%	0.004%
49	9.275	1341	1343	1347	rBV4	681	806	0.12%	0.015%
50	9.342	1352	1354	1356	rBV2	233	250	0.04%	0.005%
51	9.385	1356	1361	1377	rBV	298302	429964	66.30%	7.767%
52	9.708	1412	1414	1416	rBV	233	187	0.03%	0.003%
53	9.793	1426	1428	1430	rBV	260	242	0.04%	0.004%
54	9.964	1454	1456	1460	rBV	201	246	0.04%	0.004%
55	10.055	1465	1471	1486	rVV	360113	489944	75.55%	8.850%
56	10.305	1508	1512	1517	rBV3	702	1167	0.18%	0.021%
57	10.451	1535	1536	1538	rBV	314	214	0.03%	0.004%
58	10.756	1583	1586	1589	rBV2	386	376	0.06%	0.007%
59	11.122	1643	1646	1652	rVB2	1837	2015	0.31%	0.036%
60	11.195	1652	1658	1665	rBV	290464	393059	60.61%	7.100%
61	11.390	1689	1690	1692	rVB2	320	214	0.03%	0.004%
62	11.482	1701	1705	1709	rVB5	671	1016	0.16%	0.018%
63	11.750	1745	1749	1755	rBV6	1274	1847	0.28%	0.033%
64	11.793	1755	1756	1759	rBV2	176	135	0.02%	0.002%
65	11.841	1762	1764	1765	rVV2	322	197	0.03%	0.004%
66	11.933	1776	1779	1783	rVB3	640	859	0.13%	0.016%
67	12.024	1788	1794	1804	rVB	284551	354906	54.72%	6.411%
68	12.122	1808	1810	1813	rBV3	515	775	0.12%	0.014%
69	12.201	1821	1823	1825	rBV	242	166	0.03%	0.003%
70	12.323	1836	1843	1853	rBV	325111	421876	65.05%	7.621%
71	12.421	1857	1859	1862	rBV3	213	206	0.03%	0.004%
72	12.567	1881	1883	1886	rVB2	237	234	0.04%	0.004%
73	12.616	1889	1891	1893	rBV	247	188	0.03%	0.003%
74	12.994	1951	1953	1955	rVB2	178	159	0.02%	0.003%
75	13.091	1967	1969	1971	rBV	201	188	0.03%	0.003%
76	13.164	1980	1981	1986	rVB	267	261	0.04%	0.005%

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

77	13.231	1990	1992	1993	rVB	274	144	0.02%	0.003%
78	13.335	2007	2009	2010	rVB	237	152	0.02%	0.003%
79	13.433	2023	2025	2028	rVB2	181	194	0.03%	0.004%
80	13.463	2028	2030	2031	rBV	161	137	0.02%	0.002%
81	13.628	2055	2057	2060	rBV	248	330	0.05%	0.006%
82	13.695	2065	2068	2069	rVB2	233	198	0.03%	0.004%
83	13.707	2069	2070	2073	rBV2	208	214	0.03%	0.004%
84	13.737	2073	2075	2079	rBV	166	255	0.04%	0.005%
85	13.872	2095	2097	2099	rBV2	271	230	0.04%	0.004%
86	13.896	2099	2101	2104	rBV	195	225	0.03%	0.004%
87	14.048	2124	2126	2128	rVV	188	156	0.02%	0.003%
88	14.256	2158	2160	2161	rVV	263	135	0.02%	0.002%
89	14.408	2181	2185	2188	rVB2	330	368	0.06%	0.007%
90	14.567	2209	2211	2212	rVB2	263	143	0.02%	0.003%
91	14.597	2215	2216	2217	rBV	267	142	0.02%	0.003%
92	14.749	2240	2241	2244	rVB2	192	164	0.03%	0.003%
93	14.932	2268	2271	2273	rBV2	221	240	0.04%	0.004%
94	15.487	2361	2362	2367	rVB	376	338	0.05%	0.006%
95	15.536	2367	2370	2372	rBV	379	380	0.06%	0.007%
96	15.798	2411	2413	2416	rBV2	256	281	0.04%	0.005%
97	16.322	2496	2499	2501	rBV2	274	365	0.06%	0.007%
98	16.469	2519	2523	2525	rBV3	339	420	0.06%	0.008%
99	16.633	2548	2550	2554	rBV3	302	345	0.05%	0.006%
100	16.780	2572	2574	2575	rVB	284	201	0.03%	0.004%

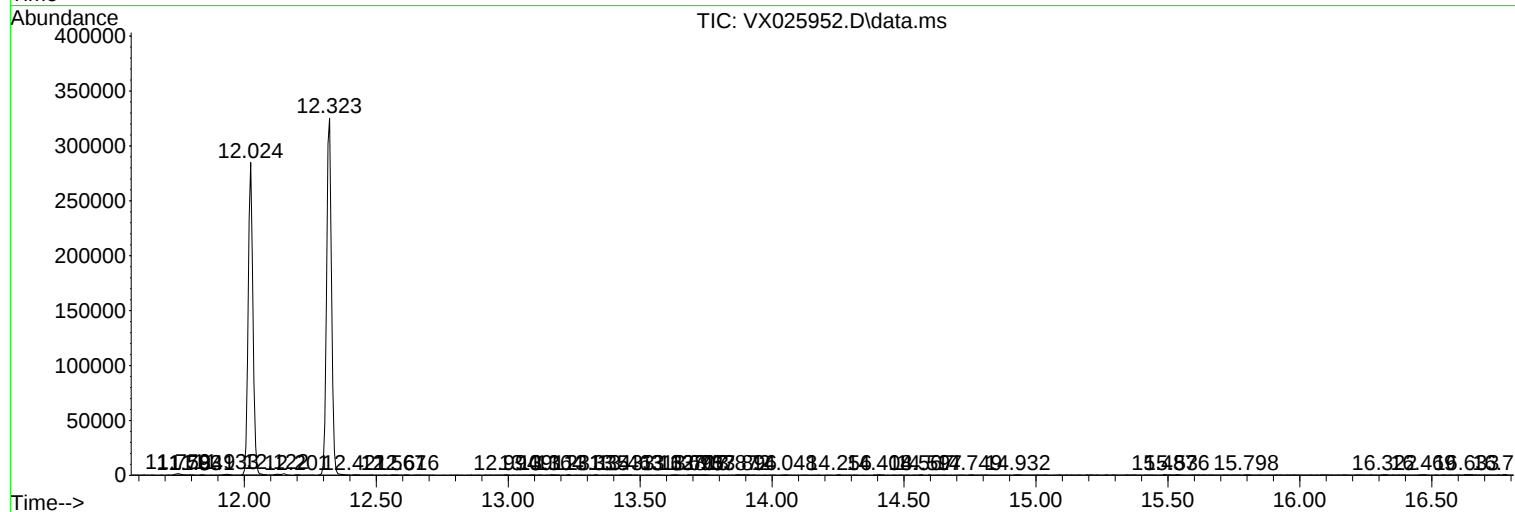
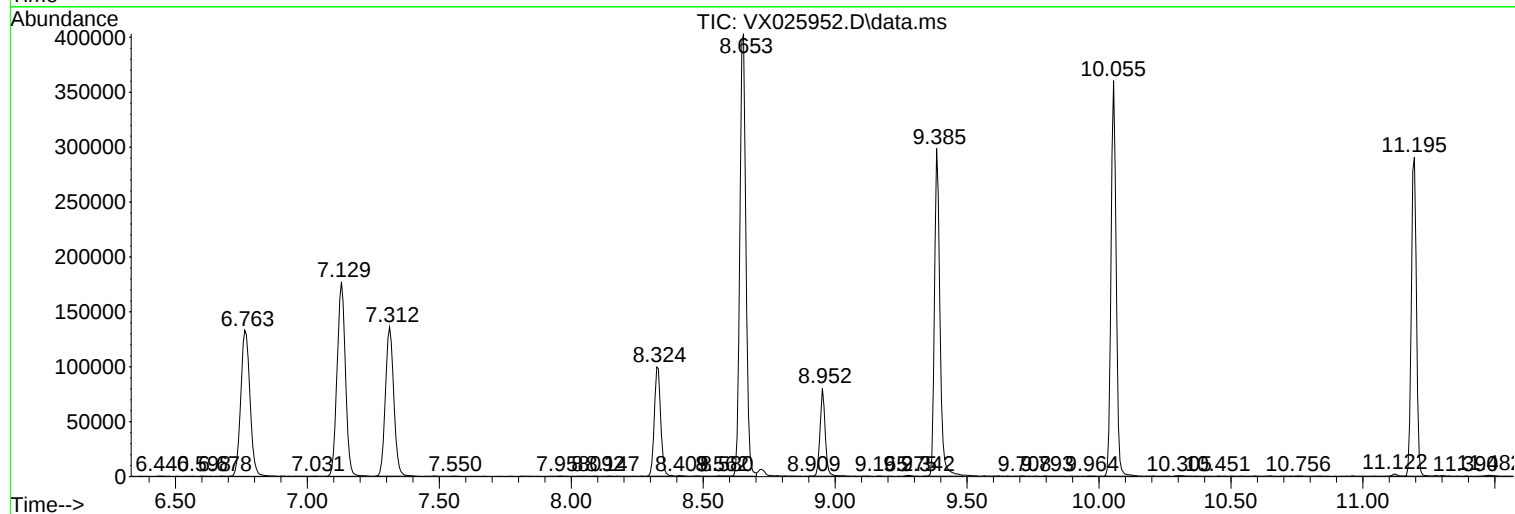
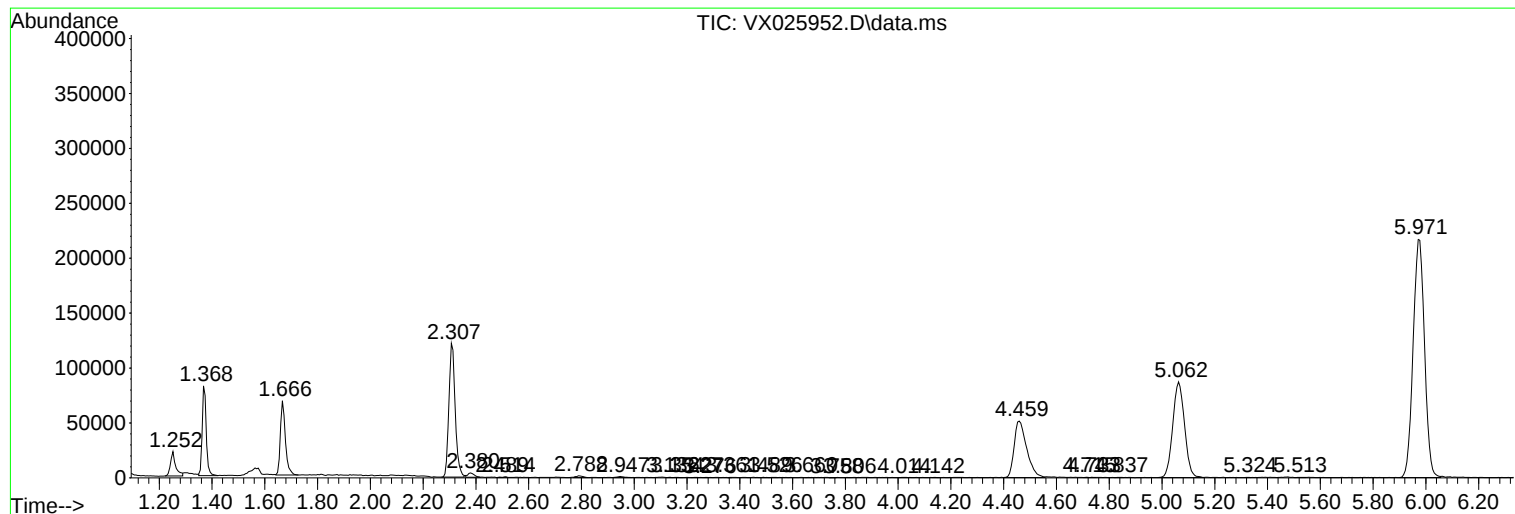
Sum of corrected areas: 5535864

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GBBX7DL

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



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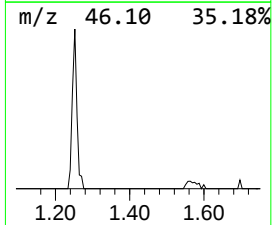
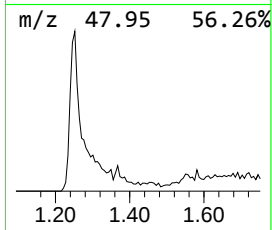
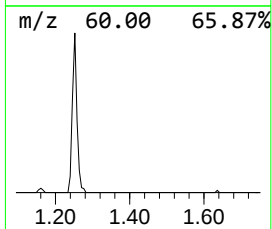
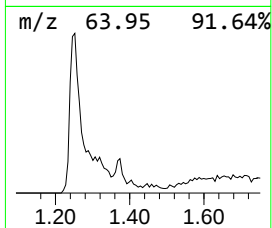
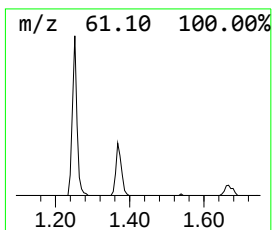
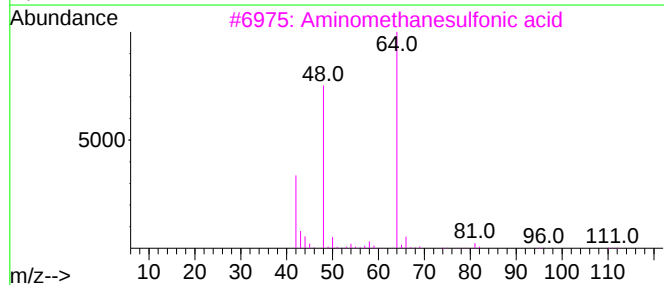
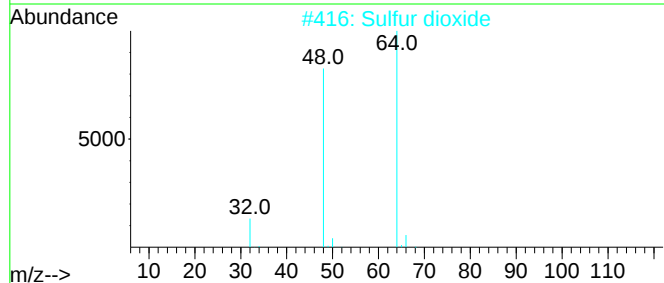
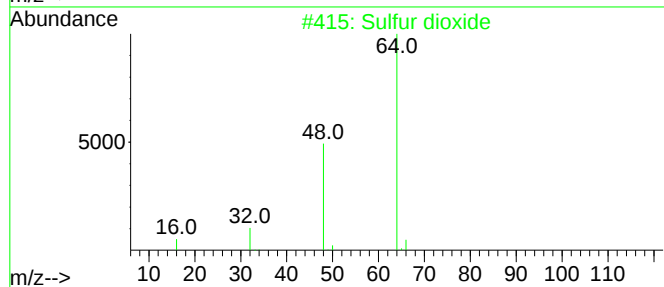
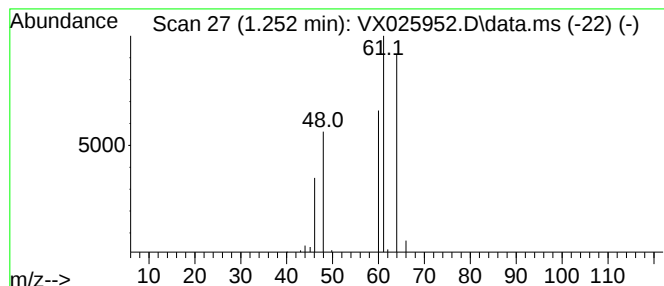
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	4.67 ug/L	29844	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	42
2			Sulfur dioxide	64	O2S	007446-09-5	42
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	36
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
unknown-01	1.252	4.7	ug/L	29844	1	6.763	319391	50.0