

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
 Data File : VX025953.D
 Acq On : 21 Dec 2021 13:49
 Operator : JC/MD
 Sample : M5150-14DL 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBX2DL

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: VX025953.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	36	rBV	22954	29777	4.76%	0.515%
2	1.368	43	46	55	rVB	74475	76320	12.21%	1.319%
3	1.666	91	95	106	rVB	66982	86527	13.85%	1.496%
4	2.306	194	200	209	rBV	112915	190957	30.56%	3.301%
5	2.800	276	281	288	rVB4	1668	3285	0.53%	0.057%
6	2.953	300	306	312	rVB2	1650	3711	0.59%	0.064%
7	3.038	317	320	323	rVB3	226	331	0.05%	0.006%
8	3.544	401	403	408	rBV2	186	213	0.03%	0.004%
9	3.635	417	418	420	rVV	252	191	0.03%	0.003%
10	3.776	439	441	443	rVV	177	162	0.03%	0.003%
11	3.928	464	466	469	rBV2	183	180	0.03%	0.003%
12	4.026	480	482	485	rVB	288	196	0.03%	0.003%
13	4.068	485	489	491	rVB2	173	218	0.03%	0.004%
14	4.202	508	511	512	rBV	174	188	0.03%	0.003%
15	4.337	531	533	536	rVB2	248	253	0.04%	0.004%
16	4.373	538	539	542	rBV	168	170	0.03%	0.003%
17	4.458	544	553	566	rBV	48673	137626	22.02%	2.379%
18	4.647	582	584	585	rBV2	301	231	0.04%	0.004%
19	4.715	594	595	597	rVB	267	173	0.03%	0.003%
20	4.891	622	624	627	rVB	256	210	0.03%	0.004%
21	5.056	638	651	669	rBV	83134	252322	40.37%	4.362%
22	5.312	689	693	695	rVV2	246	271	0.04%	0.005%
23	5.330	695	696	699	rVB2	178	154	0.02%	0.003%
24	5.385	700	705	708	rBV2	237	289	0.05%	0.005%
25	5.440	712	714	715	rBV	253	209	0.03%	0.004%
26	5.531	727	729	731	rBV	254	200	0.03%	0.003%
27	5.629	742	745	746	rBV2	255	254	0.04%	0.004%
28	5.684	753	754	756	rBV	225	160	0.03%	0.003%
29	5.757	764	766	770	rVB	195	192	0.03%	0.003%
30	5.794	770	772	773	rBV2	194	182	0.03%	0.003%
31	5.891	785	788	789	rBV	155	153	0.02%	0.003%
32	5.970	789	801	818	rVV3	201067	606418	97.03%	10.484%
33	6.233	842	844	846	rBV2	180	162	0.03%	0.003%
34	6.647	910	912	914	rVB	328	221	0.04%	0.004%
35	6.684	914	918	919	rBV2	253	244	0.04%	0.004%
36	6.763	922	931	948	rBV	132165	316850	50.70%	5.478%

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

37	6.940	958	960	961	rBV	225	207	0.03%	0.004%
38	6.995	967	969	973	rVB2	205	219	0.04%	0.004%
39	7.129	981	991	1005	rBV	280932	619702	99.16%	10.714%
40	7.312	1013	1021	1032	rBV	149551	323687	51.79%	5.596%
41	7.458	1043	1045	1046	rBV2	289	207	0.03%	0.004%
42	7.702	1083	1085	1087	rBV2	291	248	0.04%	0.004%
43	7.812	1101	1103	1106	rVB2	346	247	0.04%	0.004%
44	8.001	1132	1134	1136	rVB	301	270	0.04%	0.005%
45	8.025	1136	1138	1139	rBV2	327	247	0.04%	0.004%
46	8.080	1145	1147	1149	rBV	326	327	0.05%	0.006%
47	8.324	1181	1187	1198	rBV	106527	165022	26.41%	2.853%
48	8.653	1234	1241	1248	rBV	433840	624957	100.00%	10.805%
49	8.824	1268	1269	1271	rVB	437	189	0.03%	0.003%
50	8.952	1284	1290	1298	rBV	65509	93881	15.02%	1.623%
51	9.092	1311	1313	1314	rBV	397	229	0.04%	0.004%
52	9.110	1314	1316	1319	rVV2	174	158	0.03%	0.003%
53	9.275	1340	1343	1347	rVB3	2075	2703	0.43%	0.047%
54	9.384	1356	1361	1384	rBV	224366	344601	55.14%	5.958%
55	9.714	1414	1415	1418	rVB2	280	215	0.03%	0.004%
56	9.939	1451	1452	1454	rBV2	244	178	0.03%	0.003%
57	9.964	1454	1456	1458	rVV2	247	191	0.03%	0.003%
58	10.055	1465	1471	1487	rBV	387716	527044	84.33%	9.112%
59	10.305	1508	1512	1516	rVB3	803	1155	0.18%	0.020%
60	10.354	1516	1520	1523	rBV2	229	425	0.07%	0.007%
61	10.537	1548	1550	1551	rBV	268	193	0.03%	0.003%
62	11.122	1642	1646	1649	rVB2	1935	2314	0.37%	0.040%
63	11.195	1652	1658	1667	rBV	306273	386475	61.84%	6.682%
64	11.384	1687	1689	1691	rVB	308	213	0.03%	0.004%
65	11.750	1745	1749	1754	rVB4	1684	2153	0.34%	0.037%
66	11.847	1762	1765	1768	rBV3	320	514	0.08%	0.009%
67	11.933	1774	1779	1782	rVB2	807	1142	0.18%	0.020%
68	12.024	1788	1794	1805	rBV	394002	469330	75.10%	8.114%
69	12.323	1837	1843	1852	rVB	407293	498171	79.71%	8.613%
70	12.475	1866	1868	1869	rBV	242	212	0.03%	0.004%
71	12.670	1898	1900	1902	rBV2	214	154	0.02%	0.003%
72	12.695	1902	1904	1909	rVB2	323	395	0.06%	0.007%
73	12.817	1920	1924	1927	rBV2	242	391	0.06%	0.007%
74	13.067	1963	1965	1966	rBV	240	227	0.04%	0.004%
75	13.128	1973	1975	1978	rVB2	220	278	0.04%	0.005%
76	13.152	1978	1979	1982	rBV	237	263	0.04%	0.005%

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77	13.420	2022	2023	2027	rBV2	231	262	0.04%	0.005%
78	13.689	2065	2067	2069	rVB2	207	185	0.03%	0.003%
79	13.853	2093	2094	2099	rVB	283	350	0.06%	0.006%
80	14.085	2129	2132	2133	rBV	181	189	0.03%	0.003%
81	14.213	2151	2153	2156	rVB	313	337	0.05%	0.006%
82	14.243	2156	2158	2162	rBV2	236	379	0.06%	0.007%
83	14.341	2172	2174	2175	rBV	218	189	0.03%	0.003%
84	14.408	2183	2185	2188	rBV2	305	334	0.05%	0.006%
85	14.475	2194	2196	2197	rBV	235	154	0.02%	0.003%
86	14.493	2197	2199	2204	rVB2	182	250	0.04%	0.004%
87	14.585	2211	2214	2216	rBV	193	219	0.04%	0.004%
88	14.713	2233	2235	2237	rBV	333	250	0.04%	0.004%
89	14.737	2237	2239	2241	rVV	275	267	0.04%	0.005%
90	14.981	2276	2279	2281	rBV2	275	327	0.05%	0.006%
91	15.121	2299	2302	2303	rVB	197	160	0.03%	0.003%
92	15.146	2305	2306	2310	rBV2	247	280	0.04%	0.005%
93	15.261	2324	2325	2328	rBV2	294	211	0.03%	0.004%
94	15.536	2368	2370	2371	rBV2	232	228	0.04%	0.004%
95	16.060	2454	2456	2459	rBV	245	214	0.03%	0.004%
96	16.097	2459	2462	2463	rBV	303	249	0.04%	0.004%
97	16.176	2474	2475	2478	rBV2	383	307	0.05%	0.005%
98	16.255	2486	2488	2489	rVB	294	155	0.02%	0.003%
99	16.444	2515	2519	2520	rBV3	337	337	0.05%	0.006%
100	16.578	2540	2541	2542	rBV	507	248	0.04%	0.004%

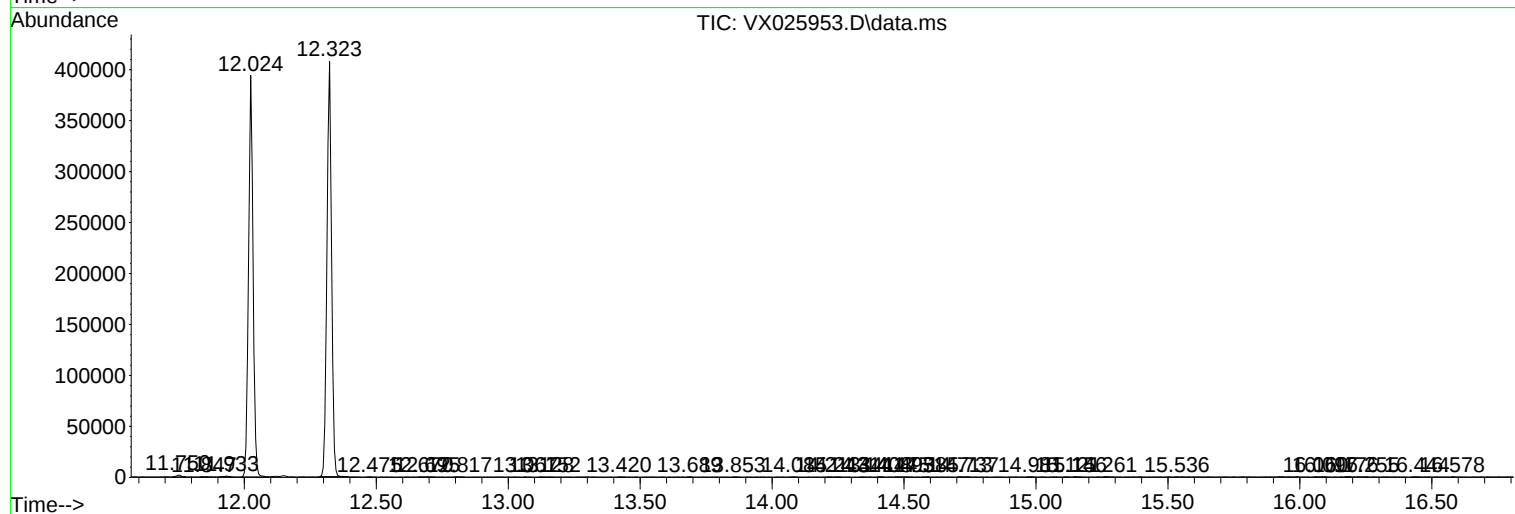
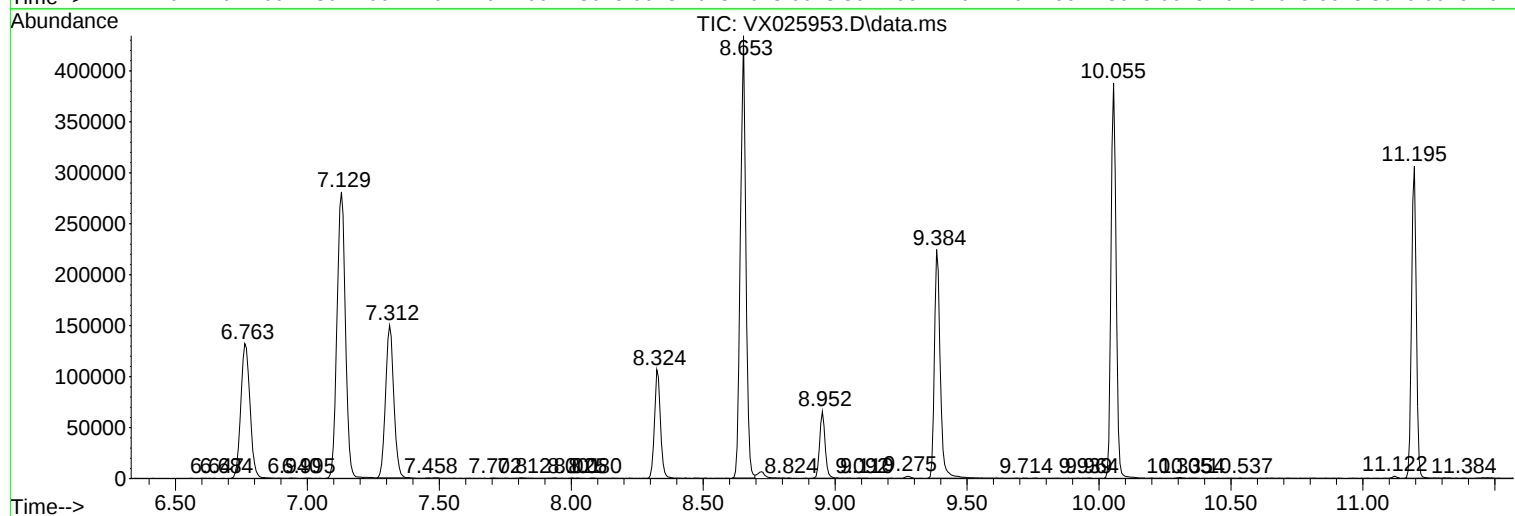
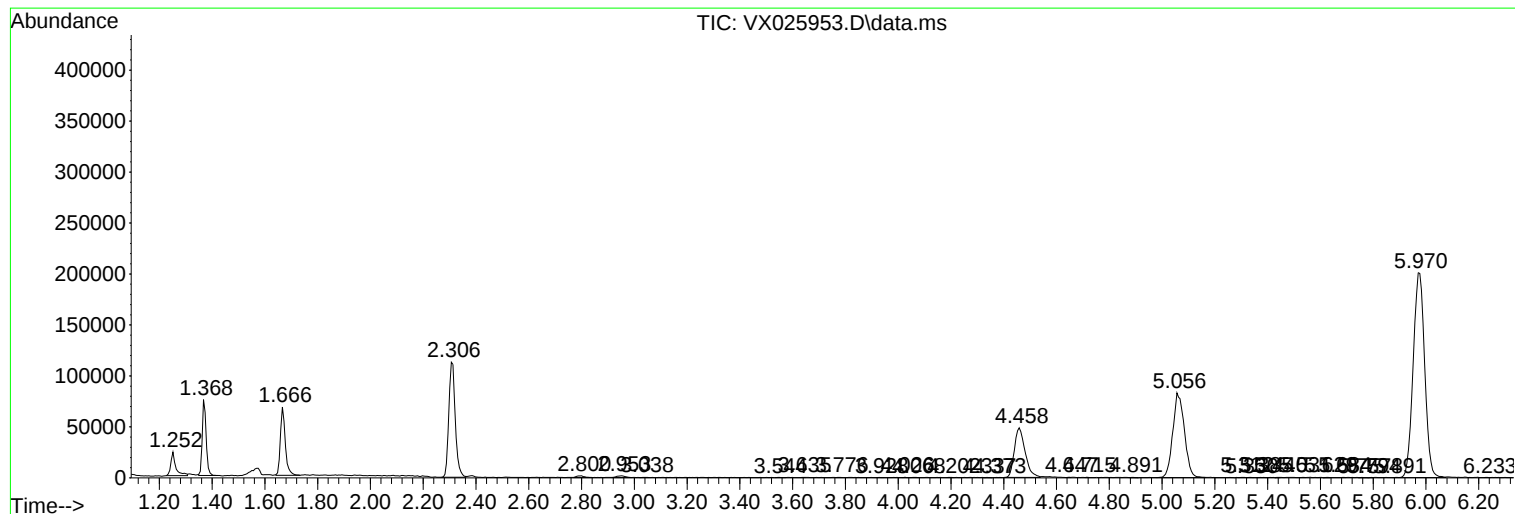
Sum of corrected areas: 5784015

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Instrument :
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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



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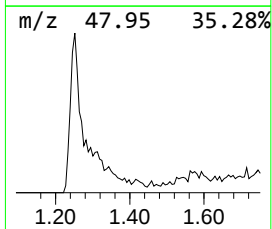
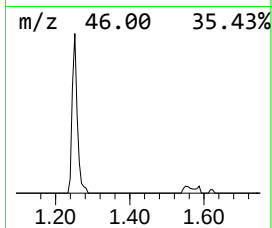
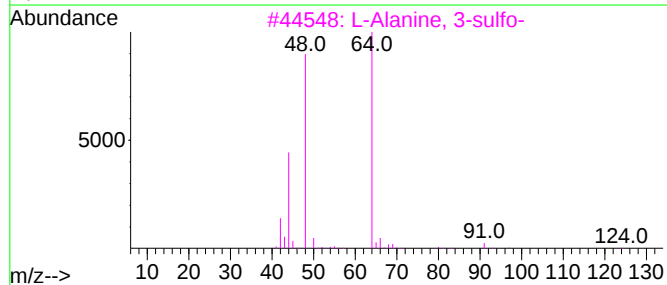
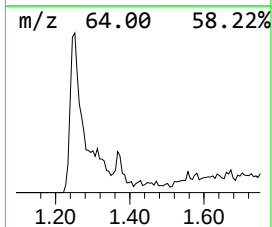
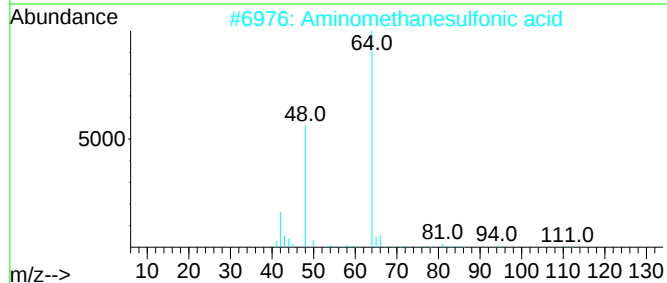
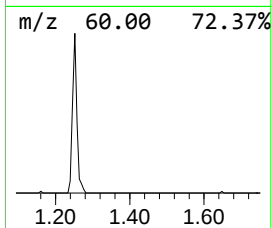
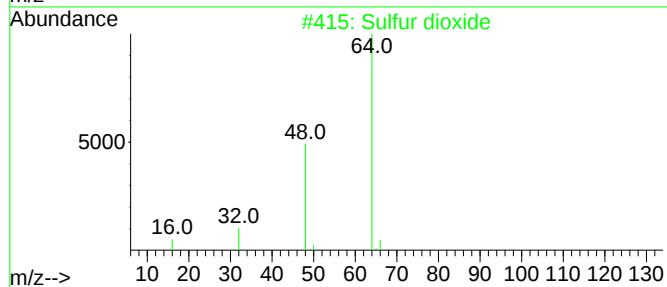
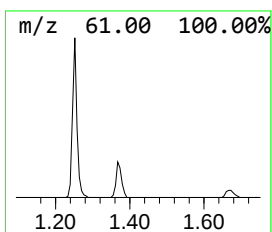
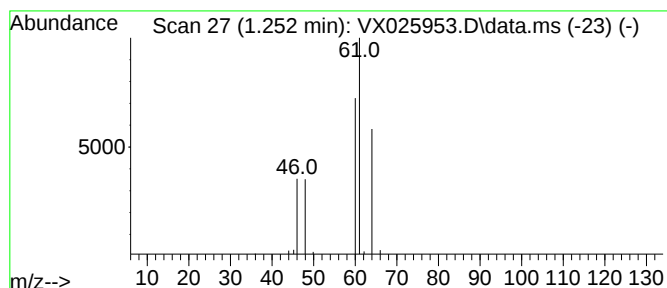
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	4.70 ug/L	29777	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	37
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	25
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			Pentaborane(11)	66	B5H11	018433-84-6	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	29777	1	6.763	316850	50.0