

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042570.D
 Acq On : 25 Jul 2024 16:35
 Operator : JC/MD
 Sample : P3334-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20E3

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	17	rVB	2103	2857	0.52%	0.065%
2	1.239	21	25	36	rBV	47936	58269	10.65%	1.331%
3	1.367	43	46	57	rVB2	51318	68466	12.52%	1.564%
4	1.648	88	92	101	rVB	39468	50267	9.19%	1.148%
5	2.233	186	188	192	rBV2	229	317	0.06%	0.007%
6	2.294	192	198	210	rVV	105963	169573	31.00%	3.874%
7	2.392	210	214	221	rVB	1967	3171	0.58%	0.072%
8	2.568	238	243	249	rBV3	1267	2236	0.41%	0.051%
9	2.733	269	270	273	rBV	126	140	0.03%	0.003%
10	2.788	274	279	285	rVB	1278	2371	0.43%	0.054%
11	2.946	298	305	311	rBV2	4536	9841	1.80%	0.225%
12	3.081	325	327	328	rBV2	155	118	0.02%	0.003%
13	3.129	333	335	337	rBV	194	178	0.03%	0.004%
14	3.306	362	364	366	rVB	107	73	0.01%	0.002%
15	3.343	366	370	373	rBV2	154	243	0.04%	0.006%
16	3.373	373	375	377	rBV	123	128	0.02%	0.003%
17	3.416	381	382	384	rBV	160	139	0.03%	0.003%
18	3.489	392	394	397	rVB	137	143	0.03%	0.003%
19	3.526	397	400	402	rBV	116	116	0.02%	0.003%
20	3.605	412	413	417	rVB2	127	164	0.03%	0.004%
21	3.660	417	422	424	rVB	126	172	0.03%	0.004%
22	3.721	428	432	433	rBV	150	149	0.03%	0.003%
23	3.739	433	435	437	rVB	106	84	0.02%	0.002%
24	3.794	442	444	448	rBV2	129	108	0.02%	0.002%
25	3.971	468	473	474	rBV2	147	270	0.05%	0.006%
26	4.251	515	519	520	rBV2	156	196	0.04%	0.004%
27	4.367	537	538	541	rBV2	137	148	0.03%	0.003%
28	4.471	546	555	573	rBV	42098	127793	23.36%	2.920%
29	4.867	618	620	621	rBV	145	130	0.02%	0.003%
30	5.062	640	652	669	rBV	72131	218130	39.88%	4.983%
31	5.208	674	676	680	rVB2	299	288	0.05%	0.007%
32	5.391	704	706	707	rBV	213	104	0.02%	0.002%
33	5.489	720	722	723	rVB	195	114	0.02%	0.003%
34	5.556	728	733	738	rBV3	290	747	0.14%	0.017%
35	5.781	767	770	772	rBV2	141	179	0.03%	0.004%
36	5.970	790	801	824	rBV2	185165	546998	100.00%	12.497%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

37	6.239	843	845	848	rVB2	157	113	0.02%	0.003%
38	6.263	848	849	852	rBV	104	101	0.02%	0.002%
39	6.330	858	860	862	rBV2	142	123	0.02%	0.003%
40	6.367	864	866	868	rBV2	183	139	0.03%	0.003%
41	6.452	879	880	883	rBV	173	180	0.03%	0.004%
42	6.495	885	887	890	rVB2	173	175	0.03%	0.004%
43	6.525	890	892	894	rBV	144	153	0.03%	0.003%
44	6.549	894	896	897	rBV2	107	99	0.02%	0.002%
45	6.653	912	913	915	rBV	130	83	0.02%	0.002%
46	6.763	922	931	952	rBV	167982	405715	74.17%	9.269%
47	7.135	985	992	1002	rVB5	4340	10527	1.92%	0.240%
48	7.220	1002	1006	1009	rBV3	330	637	0.12%	0.015%
49	7.312	1012	1021	1043	rVV	110165	246413	45.05%	5.630%
50	7.604	1067	1069	1071	rBV2	80	89	0.02%	0.002%
51	7.665	1078	1079	1082	rVB	120	91	0.02%	0.002%
52	7.702	1082	1085	1088	rBV2	132	227	0.04%	0.005%
53	7.805	1099	1102	1103	rVB2	96	94	0.02%	0.002%
54	8.086	1146	1148	1150	rVB	124	92	0.02%	0.002%
55	8.116	1150	1153	1156	rBV2	125	188	0.03%	0.004%
56	8.324	1181	1187	1199	rBV	67813	112560	20.58%	2.572%
57	8.543	1221	1223	1226	rBV	233	178	0.03%	0.004%
58	8.647	1234	1240	1250	rBV	278046	436349	79.77%	9.969%
59	8.878	1277	1278	1282	rBV2	208	195	0.04%	0.004%
60	8.951	1285	1290	1304	rBV	48231	72897	13.33%	1.665%
61	9.275	1339	1343	1347	rBV2	1043	1537	0.28%	0.035%
62	9.384	1356	1361	1381	rBV	172159	265893	48.61%	6.075%
63	9.750	1418	1421	1422	rBV	171	110	0.02%	0.003%
64	9.878	1439	1442	1444	rBV2	131	137	0.03%	0.003%
65	10.055	1465	1471	1488	rBV	341163	464923	85.00%	10.622%
66	10.244	1498	1502	1504	rBV2	243	342	0.06%	0.008%
67	10.311	1510	1513	1518	rVB	614	808	0.15%	0.018%
68	10.402	1527	1528	1531	rBV2	87	86	0.02%	0.002%
69	10.439	1532	1534	1537	rVB	91	82	0.01%	0.002%
70	10.652	1565	1569	1573	rVB3	297	381	0.07%	0.009%
71	10.762	1586	1587	1589	rBV	129	129	0.02%	0.003%
72	10.945	1615	1617	1618	rVB	216	133	0.02%	0.003%
73	10.963	1618	1620	1625	rBV2	253	480	0.09%	0.011%
74	11.189	1652	1657	1674	rBV	215975	285973	52.28%	6.533%
75	11.311	1674	1677	1681	rVB2	294	345	0.06%	0.008%
76	11.457	1699	1701	1703	rBV	244	152	0.03%	0.003%

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77	11.500	1706	1708	1709	rBV	101	77	0.01%	0.002%
78	11.756	1748	1750	1754	rBV2	266	342	0.06%	0.008%
79	11.902	1773	1774	1777	rBV	108	80	0.01%	0.002%
80	11.975	1784	1786	1788	rVB3	222	167	0.03%	0.004%
81	12.018	1788	1793	1806	rBV	315281	413427	75.58%	9.445%
82	12.219	1823	1826	1835	rVB2	2642	3468	0.63%	0.079%
83	12.317	1837	1842	1854	rVV	297720	383398	70.09%	8.759%
84	12.500	1870	1872	1873	rBV	126	92	0.02%	0.002%
85	12.579	1883	1885	1888	rVB2	125	76	0.01%	0.002%
86	13.036	1958	1960	1962	rBV	155	83	0.02%	0.002%
87	13.073	1965	1966	1967	rBV	140	74	0.01%	0.002%
88	13.152	1977	1979	1981	rVB2	137	99	0.02%	0.002%
89	13.378	2015	2016	2018	rBV2	109	92	0.02%	0.002%
90	13.597	2049	2052	2055	rVB3	297	308	0.06%	0.007%
91	13.786	2079	2083	2084	rBV2	313	341	0.06%	0.008%
92	13.884	2095	2099	2102	rBV3	174	368	0.07%	0.008%
93	13.963	2111	2112	2116	rBV3	206	182	0.03%	0.004%
94	14.005	2117	2119	2121	rVB	197	155	0.03%	0.004%
95	14.030	2121	2123	2124	rBV	132	90	0.02%	0.002%
96	14.127	2137	2139	2140	rVB	194	103	0.02%	0.002%
97	14.213	2152	2153	2155	rBV2	168	125	0.02%	0.003%
98	14.414	2184	2186	2188	rBV2	211	196	0.04%	0.004%
99	14.609	2217	2218	2220	rVB2	215	123	0.02%	0.003%
100	14.646	2222	2224	2229	rVB4	299	353	0.06%	0.008%

Sum of corrected areas: 4377168

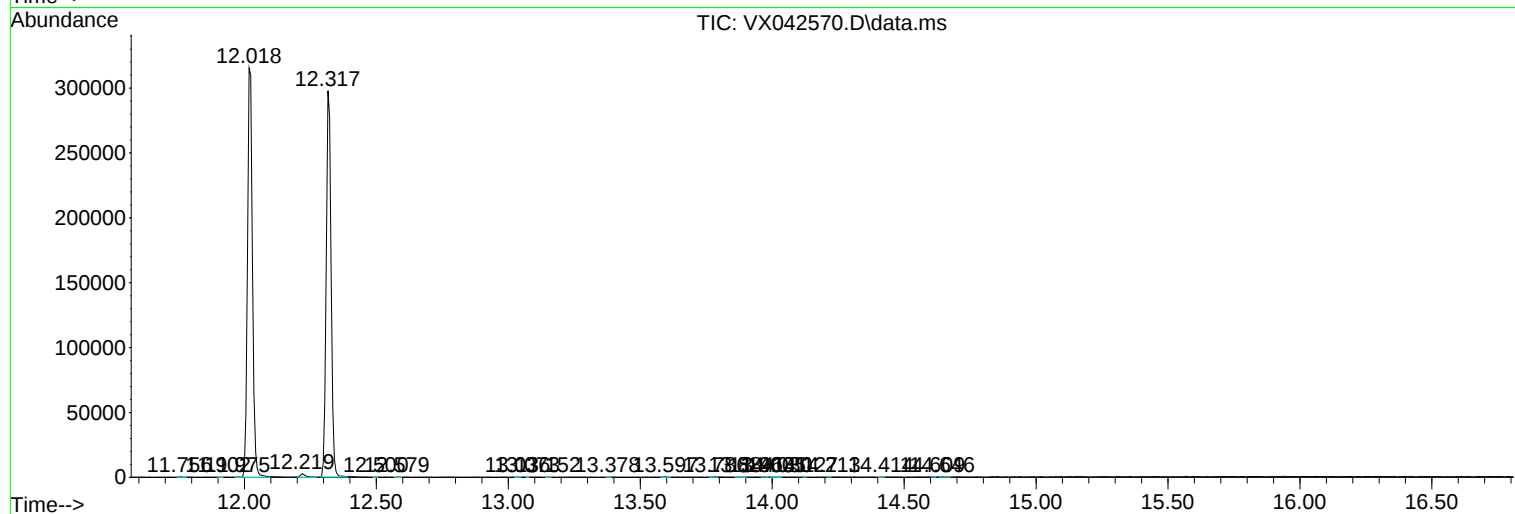
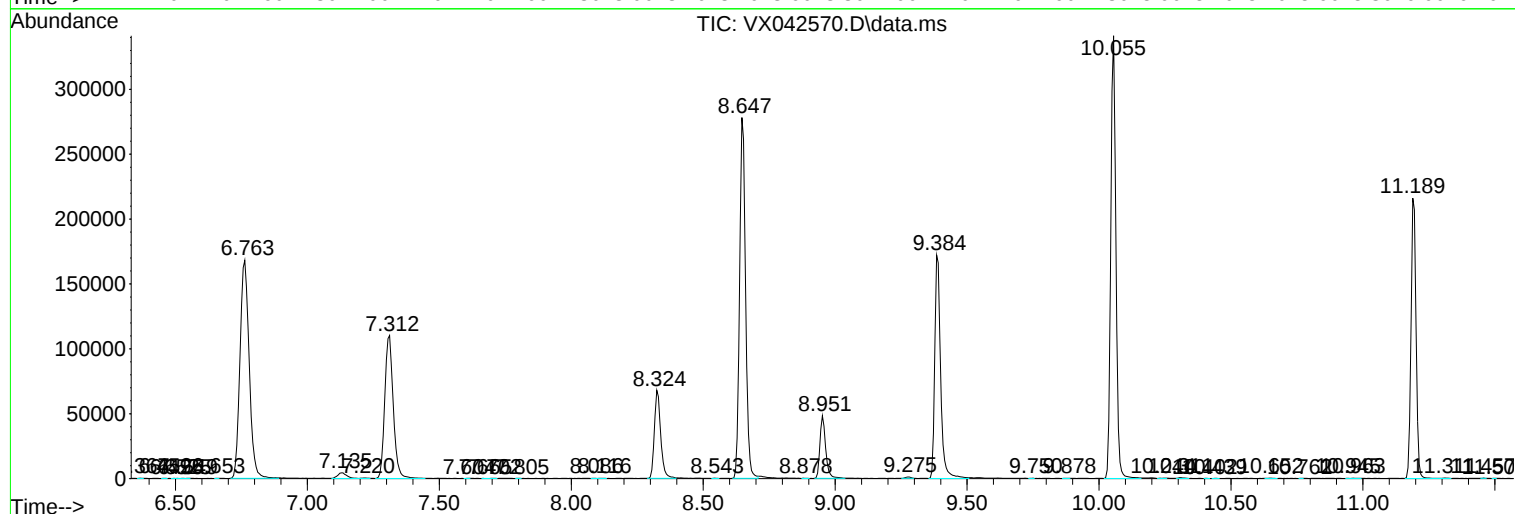
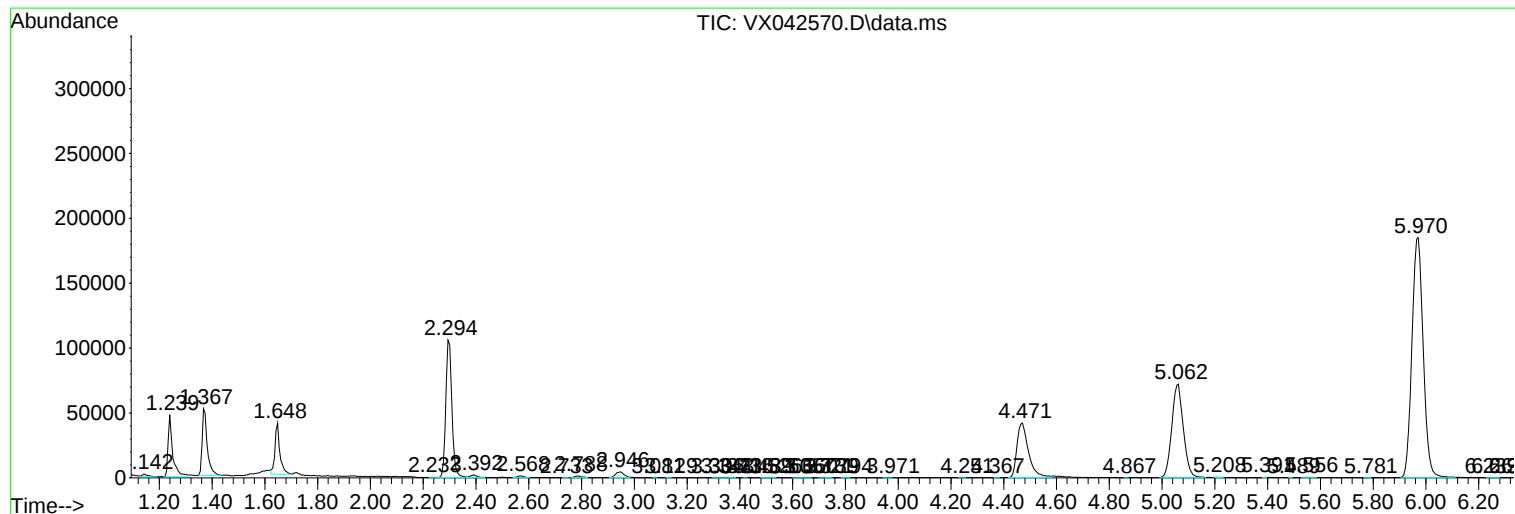
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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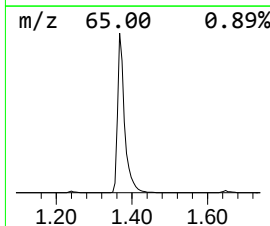
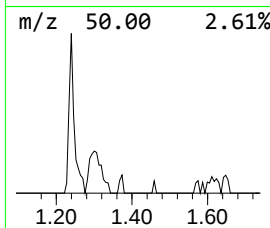
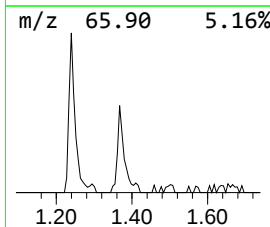
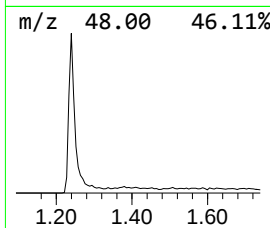
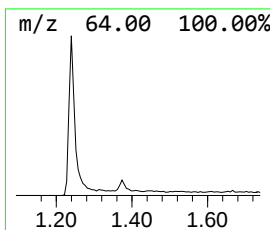
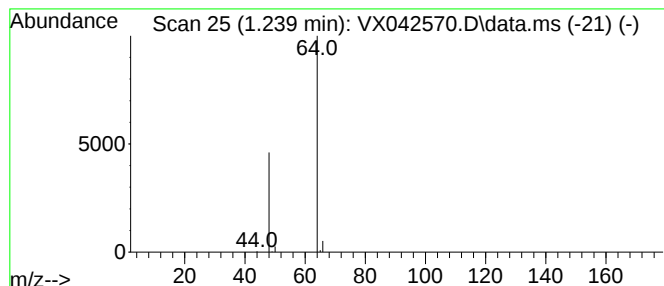
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.239	7.18 ug/L	58269	1,4-Difluorobenzene	6.763

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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	7.2	ug/L	58269	1	6.763	405715	50.0