

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042568.D
 Acq On : 25 Jul 2024 15:48
 Operator : JC/MD
 Sample : P3334-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20E1

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: VX042568.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	19	rVB2	5511	6970	1.29%	0.176%
2	1.240	22	25	39	rBV	49779	64037	11.90%	1.614%
3	1.374	43	47	57	rVV2	71723	96537	17.93%	2.433%
4	1.648	88	92	101	rVB	35476	48436	9.00%	1.221%
5	2.300	192	199	210	rBV	99542	162179	30.13%	4.087%
6	2.502	229	232	238	rBV	628	931	0.17%	0.023%
7	2.544	238	239	240	rBV	170	114	0.02%	0.003%
8	2.654	254	257	258	rBV2	196	179	0.03%	0.005%
9	2.721	264	268	271	rBV3	136	179	0.03%	0.005%
10	2.788	274	279	281	rBV2	1475	2327	0.43%	0.059%
11	2.947	298	305	313	rBV2	2076	4703	0.87%	0.119%
12	3.032	316	319	320	rBV	127	107	0.02%	0.003%
13	3.081	325	327	328	rBV	297	295	0.05%	0.007%
14	3.233	350	352	357	rBV	186	229	0.04%	0.006%
15	3.270	357	358	361	rBV	179	137	0.03%	0.003%
16	3.300	361	363	366	rBV2	90	95	0.02%	0.002%
17	3.355	370	372	374	rBV2	141	105	0.02%	0.003%
18	3.428	382	384	385	rBV	439	374	0.07%	0.009%
19	3.550	403	404	405	rBV	182	102	0.02%	0.003%
20	3.593	409	411	413	rVB	131	104	0.02%	0.003%
21	3.721	430	432	435	rVB	96	115	0.02%	0.003%
22	3.745	435	436	440	rBV2	144	189	0.04%	0.005%
23	3.867	454	456	458	rBV	114	117	0.02%	0.003%
24	4.233	515	516	519	rBV	153	165	0.03%	0.004%
25	4.288	524	525	532	rVB4	239	490	0.09%	0.012%
26	4.385	539	541	543	rBV	144	157	0.03%	0.004%
27	4.465	546	554	569	rBV	39497	118672	22.05%	2.990%
28	4.757	600	602	603	rBV	157	97	0.02%	0.002%
29	5.056	640	651	673	rBV	69830	217278	40.36%	5.475%
30	5.342	696	698	701	rBV2	77	85	0.02%	0.002%
31	5.391	702	706	709	rBV3	223	432	0.08%	0.011%
32	5.464	714	718	722	rBV3	469	1059	0.20%	0.027%
33	5.550	728	732	733	rBV2	304	352	0.07%	0.009%
34	5.629	742	745	746	rBV	179	183	0.03%	0.005%
35	5.727	757	761	763	rBV	130	220	0.04%	0.006%
36	5.879	784	786	788	rBV	179	168	0.03%	0.004%

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 Title : VOC Analysis

37	5.970	789	801	819	rVV2	181048	538303	100.00%	13.564%
38	6.184	834	836	838	rBV	264	228	0.04%	0.006%
39	6.226	841	843	845	rBV2	134	97	0.02%	0.002%
40	6.312	855	857	859	rBV	132	121	0.02%	0.003%
41	6.354	863	864	865	rBV	157	94	0.02%	0.002%
42	6.385	867	869	871	rVB	200	154	0.03%	0.004%
43	6.537	892	894	895	rBV2	174	113	0.02%	0.003%
44	6.556	895	897	898	rVV2	176	108	0.02%	0.003%
45	6.629	907	909	910	rBV2	101	79	0.01%	0.002%
46	6.763	922	931	946	rBV	134490	321792	59.78%	8.109%
47	7.080	981	983	984	rBV	115	99	0.02%	0.002%
48	7.129	984	991	1003	rVV2	14357	32457	6.03%	0.818%
49	7.306	1012	1020	1037	rBV	106658	241665	44.89%	6.090%
50	7.799	1100	1101	1103	rVB2	188	118	0.02%	0.003%
51	7.824	1103	1105	1106	rBV	120	93	0.02%	0.002%
52	7.964	1124	1128	1130	rBV2	245	380	0.07%	0.010%
53	8.092	1146	1149	1150	rBV2	94	96	0.02%	0.002%
54	8.244	1172	1174	1176	rBV2	206	187	0.03%	0.005%
55	8.281	1178	1180	1181	rVV	135	71	0.01%	0.002%
56	8.324	1182	1187	1201	rVV	53823	93634	17.39%	2.359%
57	8.519	1215	1219	1221	rBV2	291	348	0.06%	0.009%
58	8.586	1229	1230	1234	rBV	204	163	0.03%	0.004%
59	8.647	1234	1240	1250	rBV	262915	414146	76.94%	10.436%
60	8.909	1281	1283	1285	rBV	135	110	0.02%	0.003%
61	8.952	1285	1290	1300	rVV	39989	59534	11.06%	1.500%
62	9.092	1311	1313	1316	rBV2	148	155	0.03%	0.004%
63	9.189	1327	1329	1330	rBV	105	90	0.02%	0.002%
64	9.275	1339	1343	1347	rBV3	1068	1323	0.25%	0.033%
65	9.384	1356	1361	1378	rBV	170184	263995	49.04%	6.652%
66	9.933	1449	1451	1452	rVB2	174	83	0.02%	0.002%
67	10.000	1460	1462	1465	rBV2	111	155	0.03%	0.004%
68	10.055	1465	1471	1487	rVV	259441	360170	66.91%	9.076%
69	10.201	1491	1495	1500	rVB	1111	1694	0.31%	0.043%
70	10.305	1509	1512	1517	rBV2	1489	2367	0.44%	0.060%
71	10.646	1564	1568	1571	rBV	891	1183	0.22%	0.030%
72	10.695	1574	1576	1578	rVV2	95	79	0.01%	0.002%
73	10.738	1582	1583	1586	rVB	104	68	0.01%	0.002%
74	10.890	1606	1608	1610	rBV	140	116	0.02%	0.003%
75	10.933	1613	1615	1616	rVV2	126	77	0.01%	0.002%
76	10.970	1618	1621	1625	rVB	364	343	0.06%	0.009%

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 Title : VOC Analysis

77	11.055	1633	1635	1637	rBV	123	77	0.01%	0.002%
78	11.195	1652	1658	1672	rBV	213207	288179	53.53%	7.262%
79	11.384	1687	1689	1693	rVB	345	359	0.07%	0.009%
80	11.463	1697	1702	1707	rVB3	333	545	0.10%	0.014%
81	11.549	1715	1716	1719	rBV2	94	106	0.02%	0.003%
82	11.756	1746	1750	1754	rBV	671	1056	0.20%	0.027%
83	11.957	1781	1783	1784	rBV	133	78	0.01%	0.002%
84	11.975	1784	1786	1789	rVV	393	457	0.08%	0.012%
85	12.024	1789	1794	1810	rVV	213186	277870	51.62%	7.002%
86	12.219	1823	1826	1837	rBV3	1849	3077	0.57%	0.078%
87	12.323	1837	1843	1851	rBV	244558	328215	60.97%	8.270%
88	13.122	1971	1974	1978	rVB2	482	402	0.07%	0.010%
89	13.189	1982	1985	1986	rBV	123	100	0.02%	0.003%
90	13.201	1986	1987	1989	rBV	125	107	0.02%	0.003%
91	13.292	1999	2002	2004	rBV2	216	218	0.04%	0.005%
92	13.597	2049	2052	2054	rVB2	381	367	0.07%	0.009%
93	13.786	2079	2083	2089	rVB3	647	1017	0.19%	0.026%
94	13.969	2110	2113	2119	rVB2	429	578	0.11%	0.015%
95	14.048	2123	2126	2128	rBV	337	318	0.06%	0.008%
96	14.127	2137	2139	2141	rBV2	226	166	0.03%	0.004%
97	14.329	2169	2172	2174	rBV2	222	322	0.06%	0.008%
98	14.505	2196	2201	2203	rBV3	242	326	0.06%	0.008%
99	14.780	2245	2246	2247	rBV	177	104	0.02%	0.003%
100	15.706	2395	2398	2400	rBV2	334	485	0.09%	0.012%

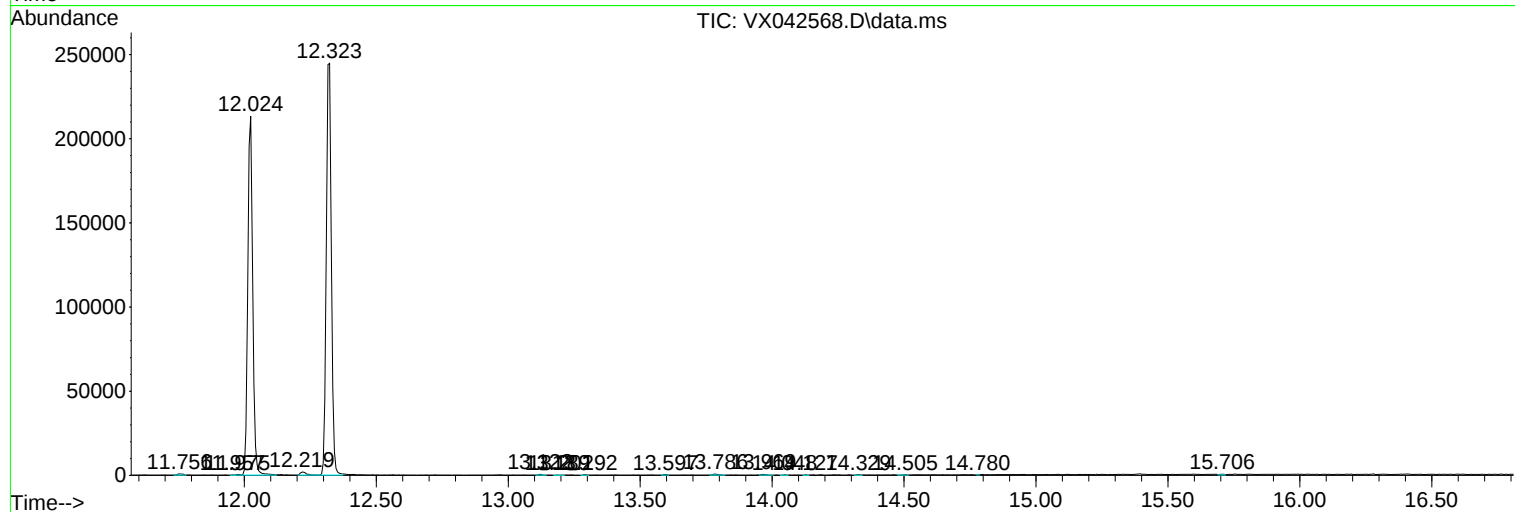
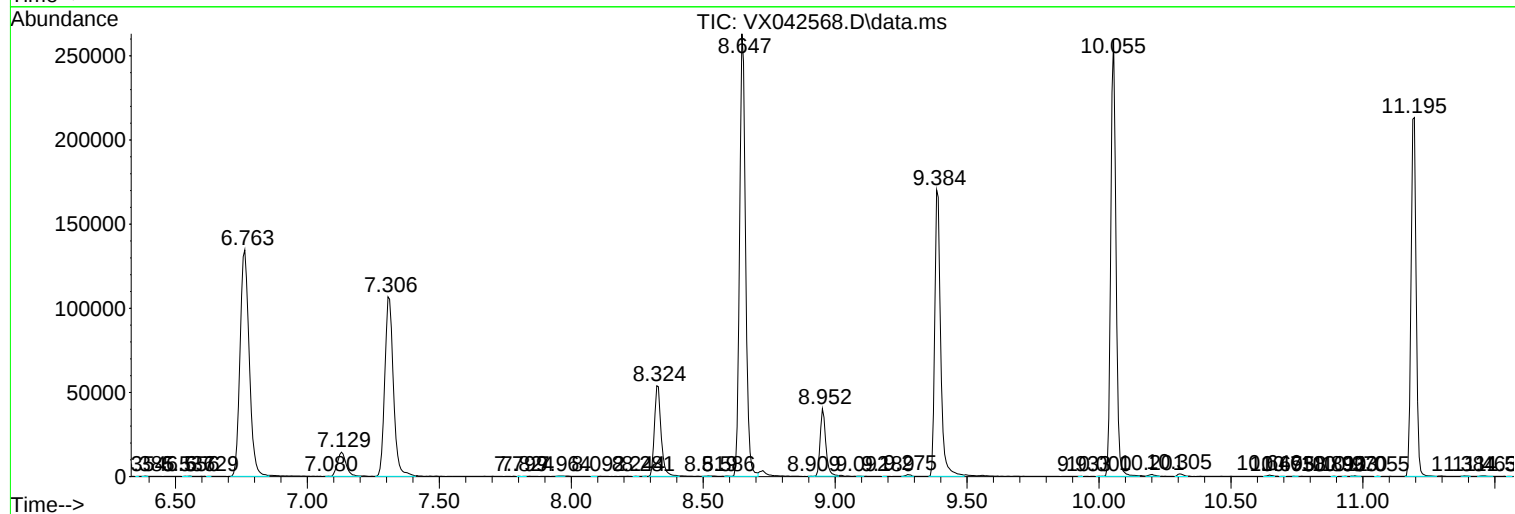
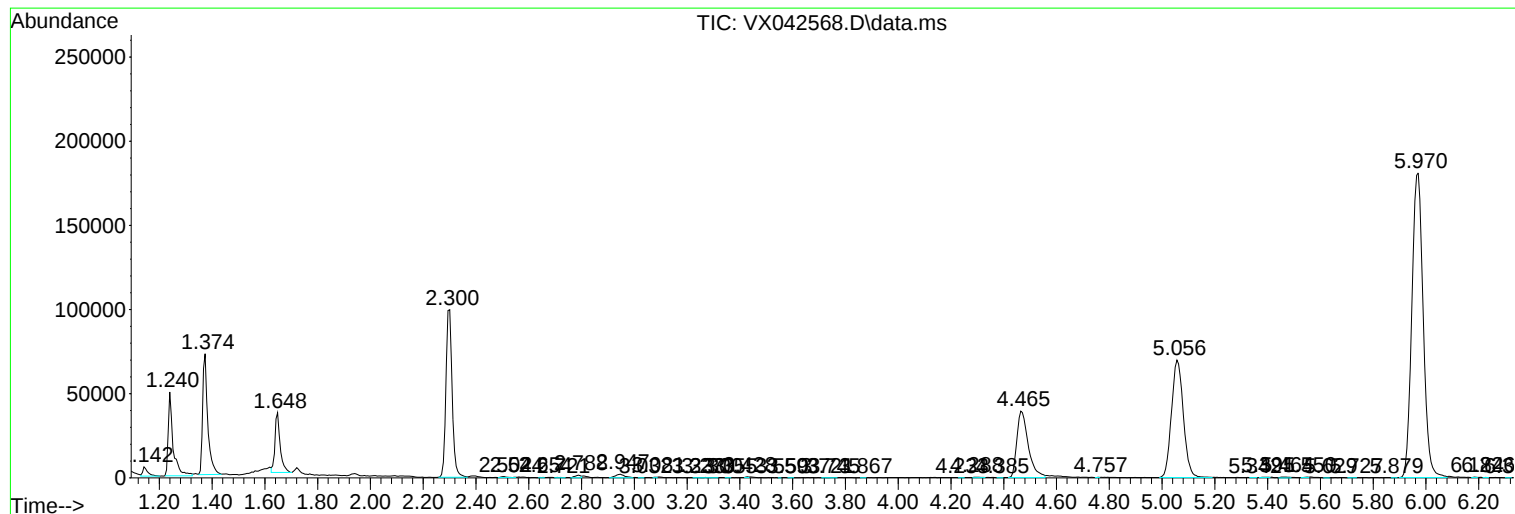
Sum of corrected areas: 3968536

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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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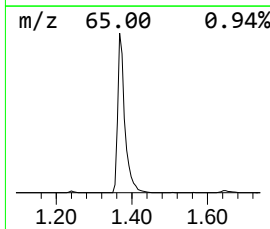
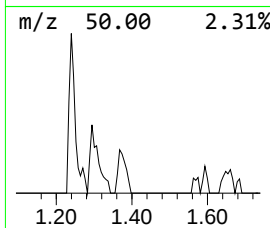
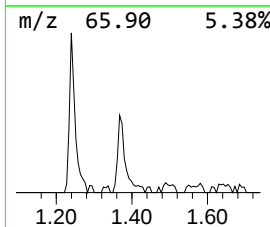
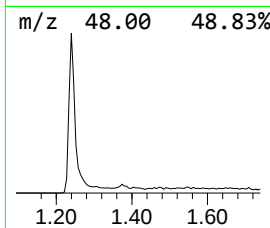
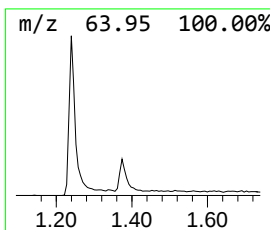
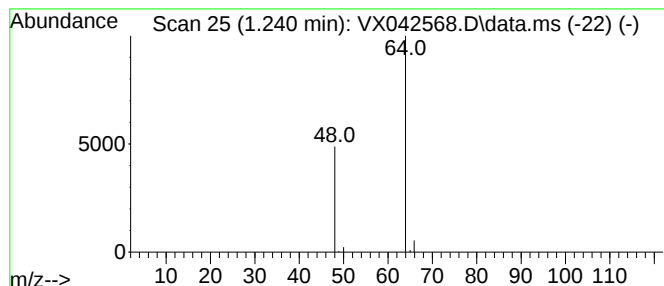
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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.
1.240	9.95 ug/L	64037	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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	1.240	9.9	ug/L	64037	1	6.763	321792	50.0