

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042575.D
 Acq On : 25 Jul 2024 18:31
 Operator : JC/MD
 Sample : P3334-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20H0

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: VX042575.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	5688	7688	1.69%	0.230%
2	1.240	22	25	35	rBV	33671	43349	9.53%	1.296%
3	1.368	43	46	57	rVB	33194	42748	9.40%	1.278%
4	1.648	89	92	100	rVB	30092	37824	8.31%	1.131%
5	2.209	182	184	185	rVB	240	128	0.03%	0.004%
6	2.227	185	187	188	rVV	155	122	0.03%	0.004%
7	2.300	192	199	210	rVV	76145	122262	26.88%	3.656%
8	2.386	210	213	222	rVB	1256	2556	0.56%	0.076%
9	2.501	230	232	235	rBV	343	446	0.10%	0.013%
10	2.569	238	243	249	rBV2	839	1689	0.37%	0.051%
11	2.672	258	260	262	rBV2	89	85	0.02%	0.003%
12	2.745	271	272	273	rBV	160	82	0.02%	0.002%
13	2.794	273	280	281	rBV3	1066	1853	0.41%	0.055%
14	2.947	298	305	311	rBV	2406	4923	1.08%	0.147%
15	3.020	315	317	318	rVB	148	84	0.02%	0.003%
16	3.081	324	327	328	rBV	179	177	0.04%	0.005%
17	3.093	328	329	332	rVB2	388	277	0.06%	0.008%
18	3.306	361	364	365	rBV	151	158	0.03%	0.005%
19	3.355	369	372	373	rVB	145	108	0.02%	0.003%
20	3.379	373	376	378	rVB2	136	144	0.03%	0.004%
21	3.440	380	386	391	rVB2	475	841	0.18%	0.025%
22	3.483	391	393	395	rBV	126	124	0.03%	0.004%
23	3.514	395	398	402	rVB2	112	157	0.03%	0.005%
24	3.642	417	419	420	rBV	106	80	0.02%	0.002%
25	3.666	420	423	426	rVB2	129	182	0.04%	0.005%
26	3.709	428	430	432	rVB	136	99	0.02%	0.003%
27	3.757	436	438	439	rBV	93	88	0.02%	0.003%
28	3.818	446	448	451	rVB	102	113	0.02%	0.003%
29	3.861	451	455	456	rBV	153	170	0.04%	0.005%
30	3.891	458	460	462	rBV	125	146	0.03%	0.004%
31	3.946	468	469	470	rBV	149	95	0.02%	0.003%
32	4.032	481	483	484	rBV2	131	106	0.02%	0.003%
33	4.093	491	493	499	rVB2	129	193	0.04%	0.006%
34	4.276	519	523	524	rBV2	264	200	0.04%	0.006%
35	4.465	545	554	569	rBV	36485	107409	23.61%	3.212%
36	4.812	609	611	612	rBV	119	117	0.03%	0.003%

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 Title : VOC Analysis

37	5.062	640	652	672	rBV	58936	184363	40.53%	5.513%
38	5.294	688	690	693	rVB	113	118	0.03%	0.004%
39	5.330	693	696	697	rBV	130	156	0.03%	0.005%
40	5.373	701	703	704	rBV2	220	194	0.04%	0.006%
41	5.458	713	717	718	rBV	260	378	0.08%	0.011%
42	5.556	732	733	739	rVB2	217	207	0.05%	0.006%
43	5.727	759	761	763	rBV2	128	144	0.03%	0.004%
44	5.964	789	800	822	rBV2	152372	454914	100.00%	13.604%
45	6.233	842	844	847	rVV	184	238	0.05%	0.007%
46	6.281	850	852	857	rVB	183	189	0.04%	0.006%
47	6.440	874	878	881	rBV	131	216	0.05%	0.006%
48	6.763	922	931	950	rBV	126430	302849	66.57%	9.056%
49	7.129	984	991	1004	rBV2	22006	50976	11.21%	1.524%
50	7.220	1004	1006	1010	rVB2	545	584	0.13%	0.017%
51	7.306	1012	1020	1038	rBV	91118	207126	45.53%	6.194%
52	7.494	1048	1051	1055	rBV2	181	268	0.06%	0.008%
53	7.812	1101	1103	1104	rBV	132	100	0.02%	0.003%
54	7.860	1108	1111	1113	rBV2	131	173	0.04%	0.005%
55	7.958	1122	1127	1129	rBV3	532	644	0.14%	0.019%
56	8.086	1146	1148	1151	rBV2	109	126	0.03%	0.004%
57	8.324	1182	1187	1201	rBV	42825	75071	16.50%	2.245%
58	8.458	1208	1209	1211	rVB2	158	99	0.02%	0.003%
59	8.513	1216	1218	1219	rBV	266	185	0.04%	0.006%
60	8.647	1234	1240	1249	rBV	212977	336208	73.91%	10.054%
61	8.891	1279	1280	1281	rBV	145	92	0.02%	0.003%
62	8.952	1285	1290	1301	rVV	30794	47320	10.40%	1.415%
63	9.281	1340	1344	1347	rBV	904	988	0.22%	0.030%
64	9.336	1350	1353	1356	rBV2	91	108	0.02%	0.003%
65	9.384	1356	1361	1380	rBV	149700	235752	51.82%	7.050%
66	10.055	1465	1471	1484	rBV	238237	327758	72.05%	9.801%
67	10.195	1492	1494	1500	rVB2	947	1251	0.27%	0.037%
68	10.305	1508	1512	1519	rVB2	1670	2741	0.60%	0.082%
69	10.360	1519	1521	1526	rVB2	145	162	0.04%	0.005%
70	10.500	1542	1544	1545	rBV2	100	88	0.02%	0.003%
71	10.555	1552	1553	1557	rVB2	168	140	0.03%	0.004%
72	10.646	1565	1568	1573	rVB2	844	1180	0.26%	0.035%
73	10.799	1592	1593	1597	rBB	111	94	0.02%	0.003%
74	10.963	1617	1620	1623	rBV2	203	272	0.06%	0.008%
75	11.189	1652	1657	1671	rBV	193012	256378	56.36%	7.667%
76	11.390	1686	1690	1692	rVV	267	290	0.06%	0.009%

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 Title : VOC Analysis

77	11.433	1696	1697	1698	rBV	159	91	0.02%	0.003%
78	11.451	1698	1700	1705	rVB2	353	407	0.09%	0.012%
79	11.622	1725	1728	1731	rBV3	273	388	0.09%	0.012%
80	11.756	1747	1750	1756	rVB	670	848	0.19%	0.025%
81	11.872	1766	1769	1770	rBV2	150	183	0.04%	0.005%
82	12.024	1789	1794	1803	rBV	167353	220564	48.48%	6.596%
83	12.219	1822	1826	1833	rBV	4746	6682	1.47%	0.200%
84	12.317	1837	1842	1852	rBV	185807	245723	54.02%	7.348%
85	12.506	1871	1873	1874	rVB	210	107	0.02%	0.003%
86	12.579	1882	1885	1886	rBV	162	170	0.04%	0.005%
87	12.762	1912	1915	1916	rBV	127	129	0.03%	0.004%
88	13.030	1958	1959	1961	rBV	97	106	0.02%	0.003%
89	13.286	1999	2001	2003	rBV2	231	205	0.05%	0.006%
90	13.463	2026	2030	2031	rBV	113	122	0.03%	0.004%
91	13.481	2031	2033	2036	rBV2	145	185	0.04%	0.006%
92	13.560	2045	2046	2047	rBV2	177	92	0.02%	0.003%
93	14.018	2120	2121	2125	rVB2	179	120	0.03%	0.004%
94	14.073	2128	2130	2131	rVB2	155	113	0.02%	0.003%
95	14.091	2131	2133	2136	rBV	140	90	0.02%	0.003%
96	14.207	2150	2152	2153	rBV	158	107	0.02%	0.003%
97	14.566	2209	2211	2213	rBV2	165	125	0.03%	0.004%
98	14.615	2217	2219	2222	rBV2	197	262	0.06%	0.008%
99	14.658	2225	2226	2227	rBV	200	85	0.02%	0.003%
100	14.761	2241	2243	2244	rBV	209	142	0.03%	0.004%

Sum of corrected areas: 3344009

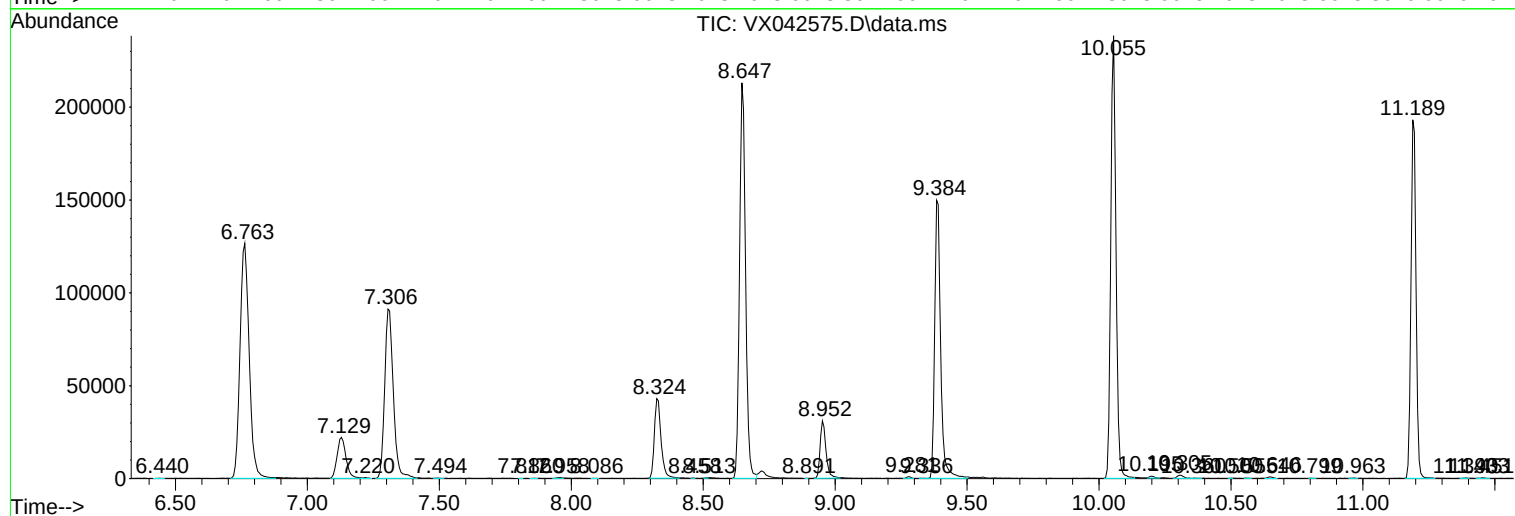
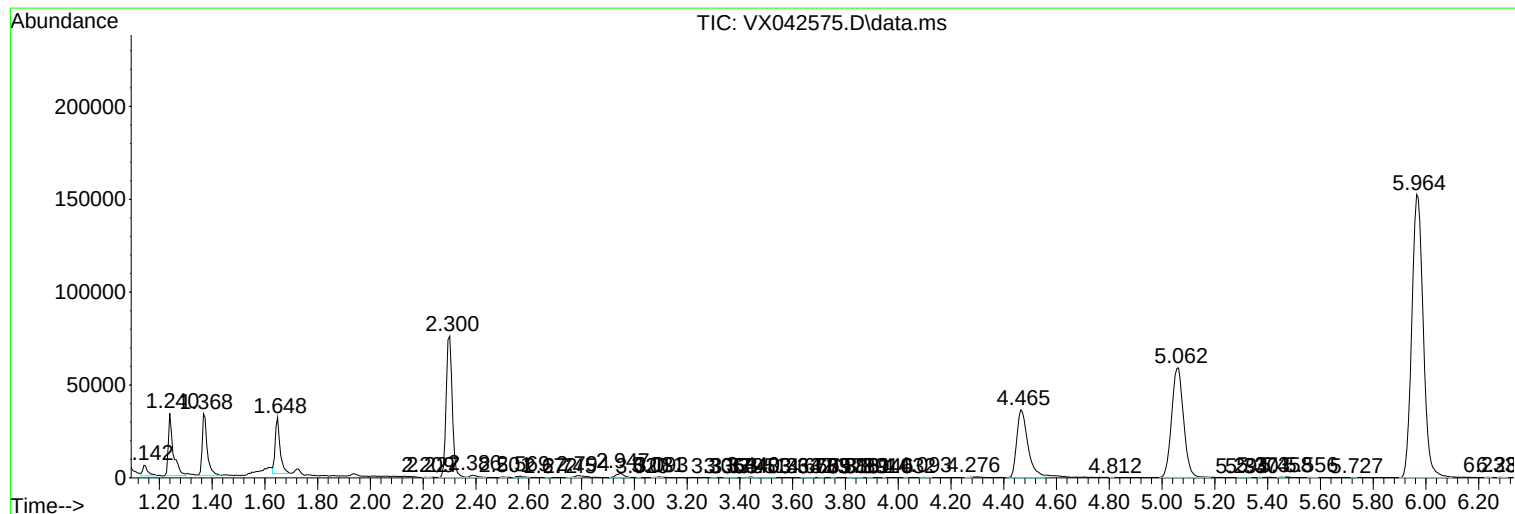
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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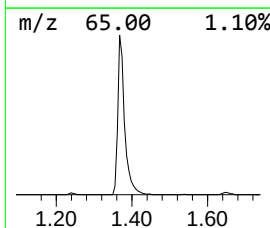
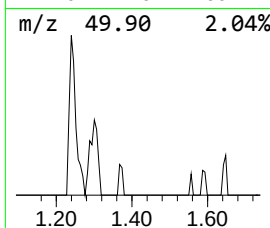
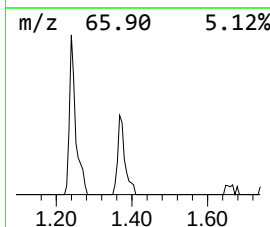
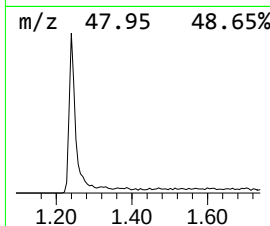
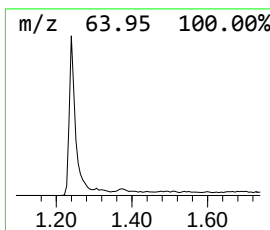
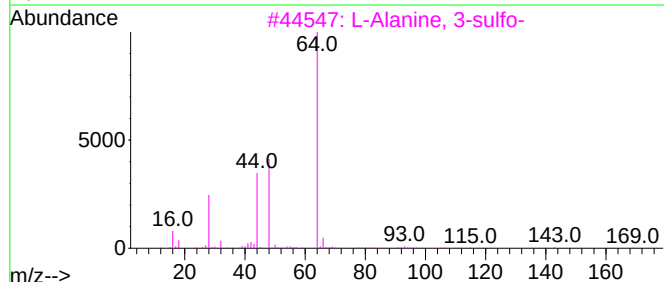
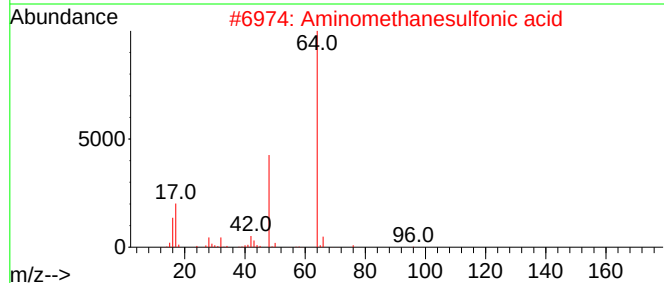
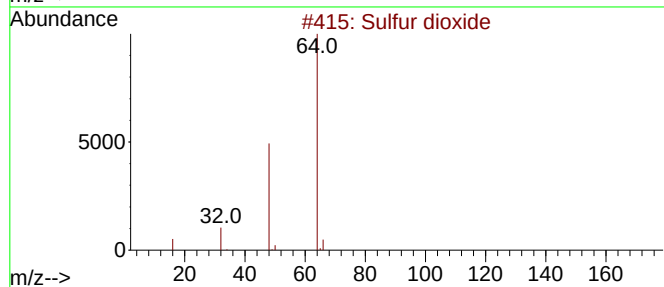
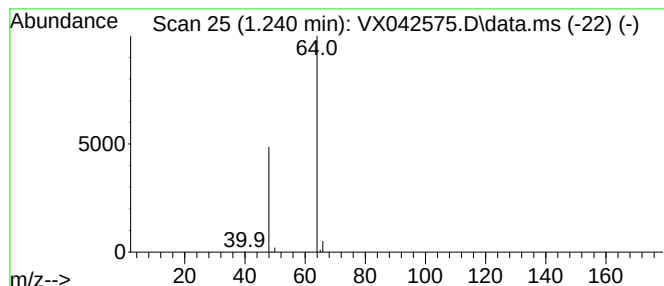
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.240	7.16 ug/L	43349	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	7.2	ug/L	43349	1	6.763	302849	50.0