

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042418.D
 Acq On : 19 Jul 2024 21:34
 Operator : JC/MD
 Sample : P3238-04ME
 Misc : 3.97g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BE7ME

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: VX042418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	27	rBV	25499	31844	5.34%	0.769%
2	1.368	43	46	49	rBV	21838	33458	5.61%	0.807%
3	2.276	189	195	210	rBV	76263	140862	23.60%	3.400%
4	2.691	261	263	264	rBV2	242	153	0.03%	0.004%
5	2.721	264	268	272	rVB4	485	775	0.13%	0.019%
6	2.782	273	278	282	rBV3	1971	3149	0.53%	0.076%
7	2.947	296	305	317	rBV	10237	27427	4.60%	0.662%
8	3.148	336	338	340	rVB2	193	189	0.03%	0.005%
9	3.178	340	343	344	rBV	141	157	0.03%	0.004%
10	3.258	354	356	358	rBV2	150	142	0.02%	0.003%
11	3.416	380	382	385	rBV2	153	179	0.03%	0.004%
12	3.489	391	394	396	rBV2	163	140	0.02%	0.003%
13	3.727	432	433	435	rBV	247	130	0.02%	0.003%
14	3.873	455	457	459	rBV	171	125	0.02%	0.003%
15	3.983	473	475	477	rBV2	149	165	0.03%	0.004%
16	4.166	503	505	507	rVB	214	150	0.03%	0.004%
17	4.245	515	518	520	rBV2	120	143	0.02%	0.003%
18	4.282	523	524	527	rBV	222	186	0.03%	0.004%
19	4.306	527	528	532	rVB	242	205	0.03%	0.005%
20	4.495	550	559	579	rBV	24079	87545	14.67%	2.113%
21	5.056	640	651	668	rBV	56226	173121	29.01%	4.178%
22	5.233	678	680	681	rVB	264	163	0.03%	0.004%
23	5.343	696	698	701	rVB2	158	133	0.02%	0.003%
24	5.367	701	702	704	rBV2	256	208	0.03%	0.005%
25	5.513	724	726	727	rVV	207	146	0.02%	0.004%
26	5.538	727	730	731	rVV2	268	273	0.05%	0.007%
27	5.556	731	733	738	rVV3	494	614	0.10%	0.015%
28	5.617	742	743	747	rVB2	140	148	0.02%	0.004%
29	5.964	789	800	818	rBV2	166144	471146	78.95%	11.371%
30	6.190	835	837	839	rBV2	357	356	0.06%	0.009%
31	6.385	862	869	873	rBV3	503	1091	0.18%	0.026%
32	6.477	883	884	890	rVB2	241	283	0.05%	0.007%
33	6.556	893	897	899	rVV2	312	365	0.06%	0.009%
34	6.599	902	904	908	rVV	162	201	0.03%	0.005%
35	6.757	918	930	948	rBV	213108	517600	86.74%	12.492%
36	7.105	984	987	994	rBV5	587	1105	0.19%	0.027%

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

37	7.214	1000	1005	1006	rBV2	441	599	0.10%	0.014%
38	7.306	1012	1020	1039	rBV	90093	204588	34.28%	4.937%
39	7.537	1057	1058	1061	rBV	174	130	0.02%	0.003%
40	7.623	1069	1072	1075	rVV2	171	211	0.04%	0.005%
41	8.171	1160	1162	1165	rVV2	153	124	0.02%	0.003%
42	8.275	1176	1179	1182	rBV2	150	226	0.04%	0.005%
43	8.324	1182	1187	1202	rVV	47948	82740	13.87%	1.997%
44	8.647	1232	1240	1256	rBV	236605	381529	63.93%	9.208%
45	8.879	1275	1278	1280	rBV2	286	305	0.05%	0.007%
46	8.952	1285	1290	1300	rBV	32478	53092	8.90%	1.281%
47	9.250	1337	1339	1340	rBV	136	139	0.02%	0.003%
48	9.275	1340	1343	1347	rVB4	1668	2254	0.38%	0.054%
49	9.336	1350	1353	1357	rBV2	144	217	0.04%	0.005%
50	9.397	1357	1363	1384	rBV	93465	198607	33.28%	4.793%
51	9.671	1404	1408	1409	rBV2	182	197	0.03%	0.005%
52	9.708	1410	1414	1419	rVV	1646	2404	0.40%	0.058%
53	9.799	1428	1429	1433	rBV2	281	310	0.05%	0.007%
54	9.842	1433	1436	1439	rVV2	153	237	0.04%	0.006%
55	9.885	1442	1443	1445	rVV	238	138	0.02%	0.003%
56	9.903	1445	1446	1449	rVV2	153	167	0.03%	0.004%
57	9.933	1449	1451	1452	rVV	186	144	0.02%	0.003%
58	10.055	1465	1471	1491	rBV	431373	596747	100.00%	14.402%
59	10.311	1509	1513	1517	rVB2	333	476	0.08%	0.011%
60	10.415	1528	1530	1533	rBV2	162	181	0.03%	0.004%
61	10.451	1533	1536	1540	rBV2	185	280	0.05%	0.007%
62	10.653	1565	1569	1571	rVV3	133	193	0.03%	0.005%
63	10.769	1587	1588	1591	rVB2	178	125	0.02%	0.003%
64	10.817	1594	1596	1597	rBV	192	136	0.02%	0.003%
65	10.964	1618	1620	1621	rBV2	182	145	0.02%	0.003%
66	11.195	1652	1658	1668	rBV	166533	225541	37.80%	5.443%
67	11.311	1675	1677	1680	rVB3	278	179	0.03%	0.004%
68	11.457	1698	1701	1702	rBV2	339	187	0.03%	0.005%
69	11.506	1708	1709	1712	rBV	187	166	0.03%	0.004%
70	11.634	1727	1730	1735	rBV2	198	326	0.05%	0.008%
71	11.701	1740	1741	1744	rVB	184	125	0.02%	0.003%
72	11.744	1744	1748	1752	rBV3	555	744	0.12%	0.018%
73	11.933	1776	1779	1781	rVB	418	369	0.06%	0.009%
74	11.976	1784	1786	1788	rBV2	218	193	0.03%	0.005%
75	12.024	1788	1794	1805	rBV	439188	556291	93.22%	13.425%
76	12.250	1829	1831	1833	rBV	171	137	0.02%	0.003%

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Integration Parameters: LSCINT.P

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	12.323	1837	1843	1854	rBV	249010	331692	55.58%	8.005%
78	12.573	1882	1884	1889	rBV3	187	225	0.04%	0.005%
79	12.768	1912	1916	1920	rVB3	434	652	0.11%	0.016%
80	12.847	1926	1929	1930	rBV2	258	238	0.04%	0.006%
81	12.927	1939	1942	1944	rBV2	156	178	0.03%	0.004%
82	13.036	1958	1960	1963	rVB2	261	200	0.03%	0.005%
83	13.085	1963	1968	1969	rBV	218	239	0.04%	0.006%
84	13.103	1969	1971	1973	rVV2	202	161	0.03%	0.004%
85	13.152	1977	1979	1982	rVB2	153	137	0.02%	0.003%
86	13.219	1988	1990	1992	rVB	251	183	0.03%	0.004%
87	13.238	1992	1993	1996	rBV2	203	174	0.03%	0.004%
88	13.451	2026	2028	2031	rVB2	224	231	0.04%	0.006%
89	13.518	2038	2039	2042	rBV	146	125	0.02%	0.003%
90	13.603	2049	2053	2054	rBV2	276	352	0.06%	0.008%
91	13.689	2065	2067	2069	rBV2	240	289	0.05%	0.007%
92	13.792	2080	2084	2088	rBV2	543	845	0.14%	0.020%
93	13.829	2088	2090	2091	rVB	256	142	0.02%	0.003%
94	13.969	2110	2113	2116	rBV	281	361	0.06%	0.009%
95	14.067	2126	2129	2130	rBV2	152	141	0.02%	0.003%
96	14.128	2136	2139	2143	rBV3	751	1111	0.19%	0.027%
97	14.311	2167	2169	2172	rBV2	169	174	0.03%	0.004%
98	14.378	2179	2180	2182	rBV2	182	144	0.02%	0.003%
99	14.621	2216	2220	2221	rBV3	261	319	0.05%	0.008%
100	15.097	2296	2298	2300	rVB2	405	286	0.05%	0.007%

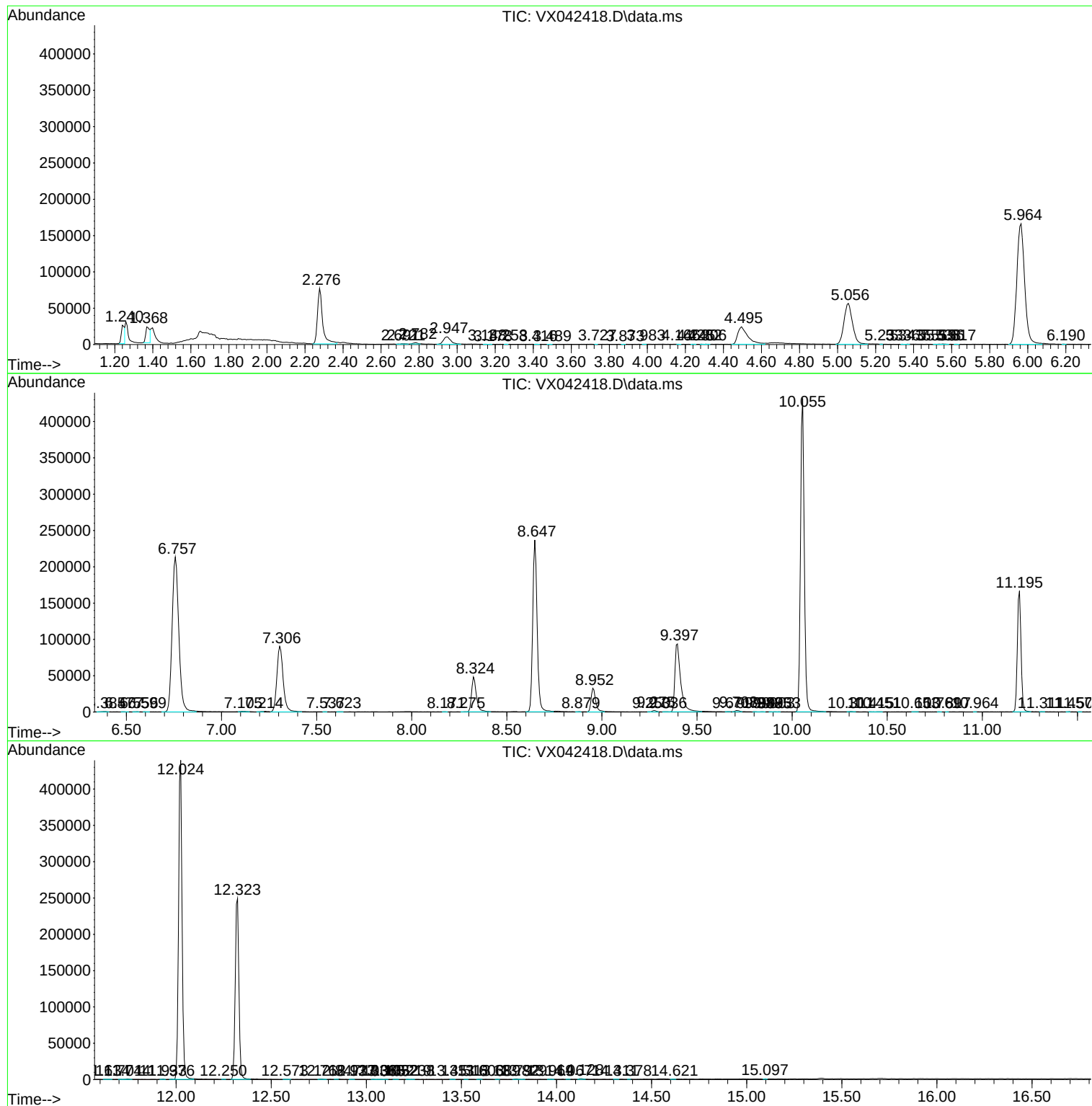
Sum of corrected areas: 4143575

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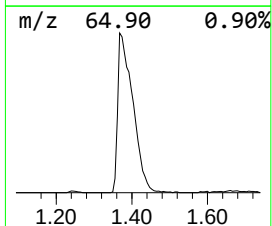
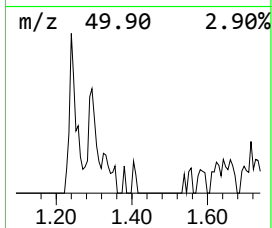
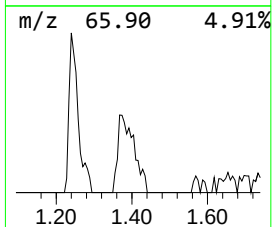
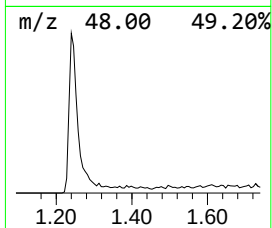
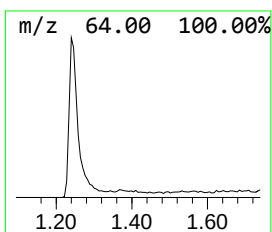
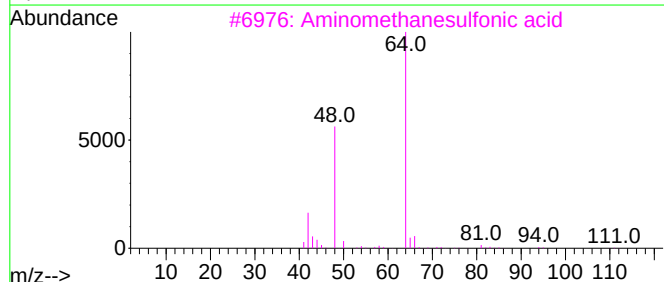
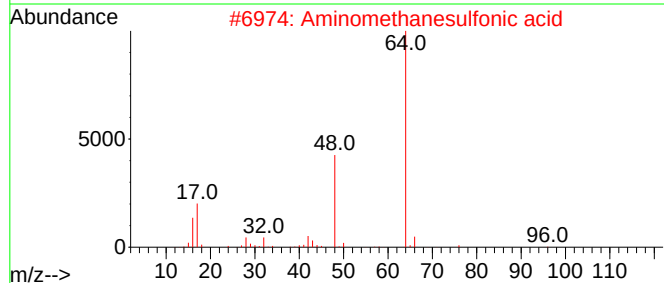
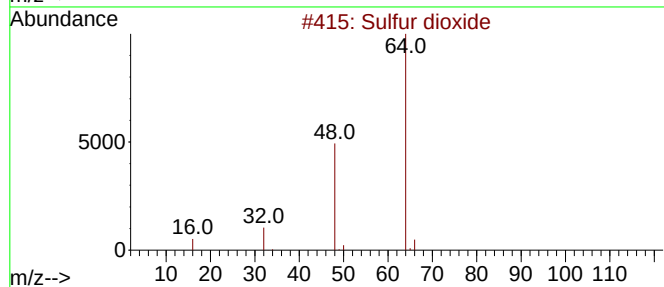
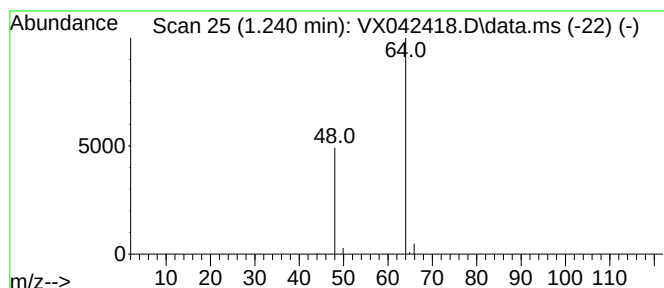
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.08 ug/L	31844	1,4-Difluorobenzene	6.757

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	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.1	ug/L	31844	1	6.757	517600	50.0