

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042474.D
 Acq On : 23 Jul 2024 16:07
 Operator : JC/MD
 Sample : P3264-12ME
 Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL8ME

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: VX042474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	21	25	27	rBV	27625	32449	5.14%	0.631%
2	1.367	43	46	62	rVB	23137	64588	10.23%	1.257%
3	2.276	189	195	211	rBV	91652	178067	28.19%	3.464%
4	2.721	260	268	273	rBV	6631	13395	2.12%	0.261%
5	2.946	298	305	316	rVB	3015	7504	1.19%	0.146%
6	3.093	327	329	331	rVV	181	162	0.03%	0.003%
7	3.129	333	335	340	rVB3	202	278	0.04%	0.005%
8	3.270	356	358	361	rVV2	195	128	0.02%	0.002%
9	3.416	380	382	384	rVV	170	127	0.02%	0.002%
10	3.526	398	400	404	rVB2	126	124	0.02%	0.002%
11	3.849	450	453	454	rBV2	118	138	0.02%	0.003%
12	3.904	459	462	463	rBV2	139	130	0.02%	0.003%
13	3.995	471	477	482	rBV2	188	482	0.08%	0.009%
14	4.160	500	504	507	rBV2	87	146	0.02%	0.003%
15	4.489	550	558	578	rBV	38339	136384	21.59%	2.653%
16	5.056	640	651	666	rBV	76839	241232	38.19%	4.693%
17	5.263	683	685	690	rVB2	208	213	0.03%	0.004%
18	5.355	699	700	702	rBV	185	153	0.02%	0.003%
19	5.556	729	733	735	rBV2	171	244	0.04%	0.005%
20	5.623	739	744	745	rBV2	107	164	0.03%	0.003%
21	5.763	764	767	770	rBV2	136	159	0.03%	0.003%
22	5.854	778	782	784	rBV2	86	156	0.02%	0.003%
23	5.964	788	800	821	rBV2	218437	631600	100.00%	12.288%
24	6.306	854	856	860	rVB	176	208	0.03%	0.004%
25	6.373	863	867	868	rBV	418	462	0.07%	0.009%
26	6.501	887	888	890	rBV	175	135	0.02%	0.003%
27	6.556	896	897	901	rVB2	168	154	0.02%	0.003%
28	6.604	902	905	908	rVB2	158	180	0.03%	0.004%
29	6.659	912	914	915	rVB	191	129	0.02%	0.003%
30	6.671	915	916	918	rBV2	232	198	0.03%	0.004%
31	6.757	922	930	949	rBV	209771	505718	80.07%	9.839%
32	7.116	983	989	998	rVB4	1174	2660	0.42%	0.052%
33	7.220	1001	1006	1007	rBV2	460	703	0.11%	0.014%
34	7.305	1012	1020	1041	rBV	125520	284489	45.04%	5.535%
35	7.555	1060	1061	1063	rBV	179	129	0.02%	0.003%
36	7.732	1088	1090	1093	rVB	170	153	0.02%	0.003%

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Integrator: RTE

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 Title : VOC Analysis

37	7.769	1093	1096	1097	rBV	157	172	0.03%	0.003%
38	7.872	1110	1113	1116	rVB	144	164	0.03%	0.003%
39	7.964	1123	1128	1135	rBV4	780	1808	0.29%	0.035%
40	8.086	1146	1148	1149	rBV2	198	156	0.02%	0.003%
41	8.116	1151	1153	1155	rBV2	151	137	0.02%	0.003%
42	8.232	1168	1172	1173	rBV2	115	165	0.03%	0.003%
43	8.324	1182	1187	1201	rBV	66303	117044	18.53%	2.277%
44	8.647	1234	1240	1250	rBV	313225	501246	79.36%	9.752%
45	8.909	1281	1283	1285	rBV	173	177	0.03%	0.003%
46	8.951	1285	1290	1305	rVV	47349	76628	12.13%	1.491%
47	9.189	1327	1329	1332	rVB	177	161	0.03%	0.003%
48	9.275	1339	1343	1352	rVB2	6059	9539	1.51%	0.186%
49	9.390	1357	1362	1381	rBV	158476	318492	50.43%	6.197%
50	9.646	1403	1404	1406	rVB2	439	256	0.04%	0.005%
51	9.671	1406	1408	1411	rBV3	247	303	0.05%	0.006%
52	9.714	1411	1415	1422	rVB4	969	1896	0.30%	0.037%
53	9.768	1422	1424	1426	rBV2	166	198	0.03%	0.004%
54	9.896	1442	1445	1448	rVV2	186	157	0.02%	0.003%
55	9.921	1448	1449	1452	rVB2	189	164	0.03%	0.003%
56	9.945	1452	1453	1456	rBV	144	156	0.02%	0.003%
57	10.055	1465	1471	1483	rBV	417692	589544	93.34%	11.470%
58	10.305	1509	1512	1518	rVB3	707	1268	0.20%	0.025%
59	10.372	1521	1523	1525	rBV2	144	139	0.02%	0.003%
60	10.512	1542	1546	1548	rVB	167	158	0.03%	0.003%
61	10.646	1564	1568	1576	rVV4	406	790	0.13%	0.015%
62	10.707	1576	1578	1581	rVV	134	122	0.02%	0.002%
63	10.750	1583	1585	1587	rVV2	172	133	0.02%	0.003%
64	10.982	1618	1623	1625	rBV3	559	874	0.14%	0.017%
65	11.195	1652	1658	1666	rBV	254931	336825	53.33%	6.553%
66	11.311	1675	1677	1680	rVB2	369	454	0.07%	0.009%
67	11.451	1698	1700	1703	rBV2	130	147	0.02%	0.003%
68	11.640	1727	1731	1733	rBV2	227	341	0.05%	0.007%
69	11.756	1747	1750	1755	rVB3	580	776	0.12%	0.015%
70	11.841	1762	1764	1767	rBV	130	146	0.02%	0.003%
71	11.927	1776	1778	1781	rVB2	194	186	0.03%	0.004%
72	12.024	1788	1794	1803	rBV	450461	557478	88.26%	10.846%
73	12.219	1822	1826	1835	rBV	7797	11220	1.78%	0.218%
74	12.323	1837	1843	1859	rBV	360440	474853	75.18%	9.239%
75	12.506	1872	1873	1878	rBV2	156	209	0.03%	0.004%
76	12.548	1878	1880	1881	rVB	304	212	0.03%	0.004%

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Instrument :
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 ClientSampleId :
 A4CL8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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

77	12.561	1881	1882	1886	rBV	202	186	0.03%	0.004%
78	12.640	1893	1895	1897	rVB2	204	185	0.03%	0.004%
79	12.762	1911	1915	1920	rVV3	808	1277	0.20%	0.025%
80	12.872	1929	1933	1938	rBV2	2954	4189	0.66%	0.082%
81	13.036	1958	1960	1965	rVB2	379	556	0.09%	0.011%
82	13.073	1965	1966	1969	rVB	178	140	0.02%	0.003%
83	13.103	1969	1971	1972	rBV	223	150	0.02%	0.003%
84	13.170	1977	1982	1984	rBV	144	266	0.04%	0.005%
85	13.402	2017	2020	2027	rVV2	3205	4377	0.69%	0.085%
86	13.457	2027	2029	2033	rVV	149	132	0.02%	0.003%
87	13.597	2050	2052	2056	rBV3	246	279	0.04%	0.005%
88	13.688	2063	2067	2072	rVB3	922	1426	0.23%	0.028%
89	13.786	2078	2083	2089	rBV	1524	2344	0.37%	0.046%
90	13.963	2110	2112	2114	rBV3	400	301	0.05%	0.006%
91	14.127	2135	2139	2144	rVB	2434	2883	0.46%	0.056%
92	14.207	2150	2152	2153	rBV2	200	143	0.02%	0.003%
93	14.316	2168	2170	2172	rBV2	236	203	0.03%	0.004%
94	14.396	2181	2183	2186	rBV2	352	415	0.07%	0.008%
95	14.432	2186	2189	2193	rVV	1176	1436	0.23%	0.028%
96	14.548	2198	2208	2220	rBV5	1491	4859	0.77%	0.095%
97	14.646	2221	2224	2227	rBV3	661	825	0.13%	0.016%
98	14.786	2244	2247	2249	rVB3	592	668	0.11%	0.013%
99	14.883	2260	2263	2267	rBV3	784	1231	0.19%	0.024%
100	15.389	2343	2346	2352	rVB5	1974	3100	0.49%	0.060%

Sum of corrected areas: 5139806

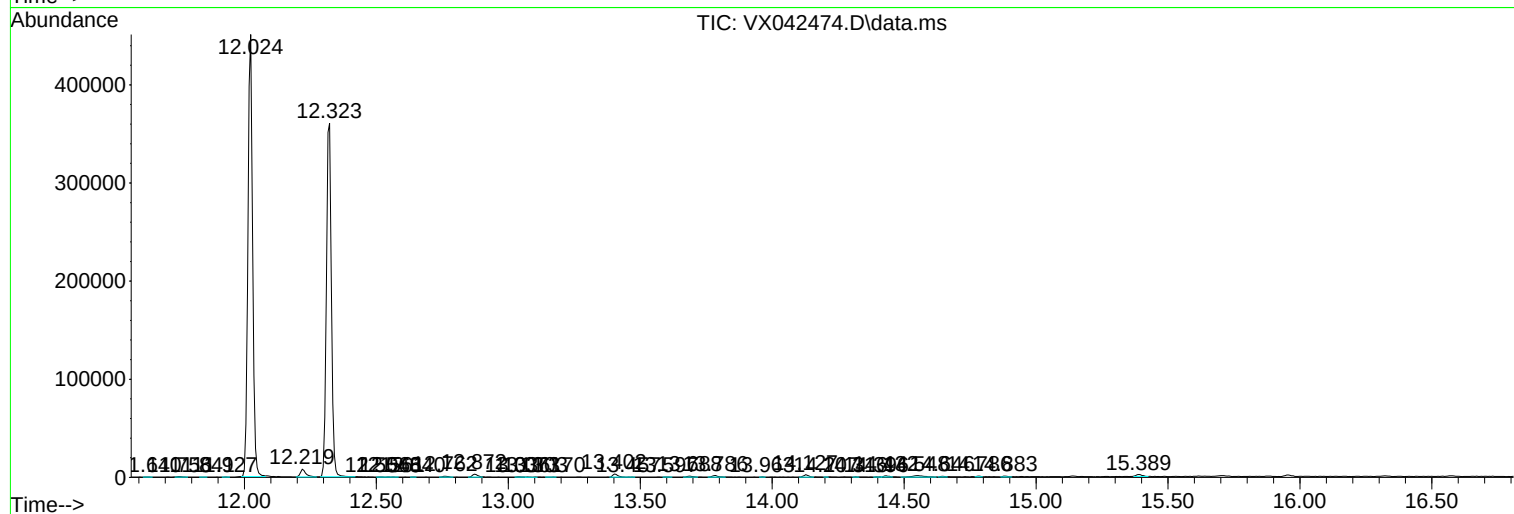
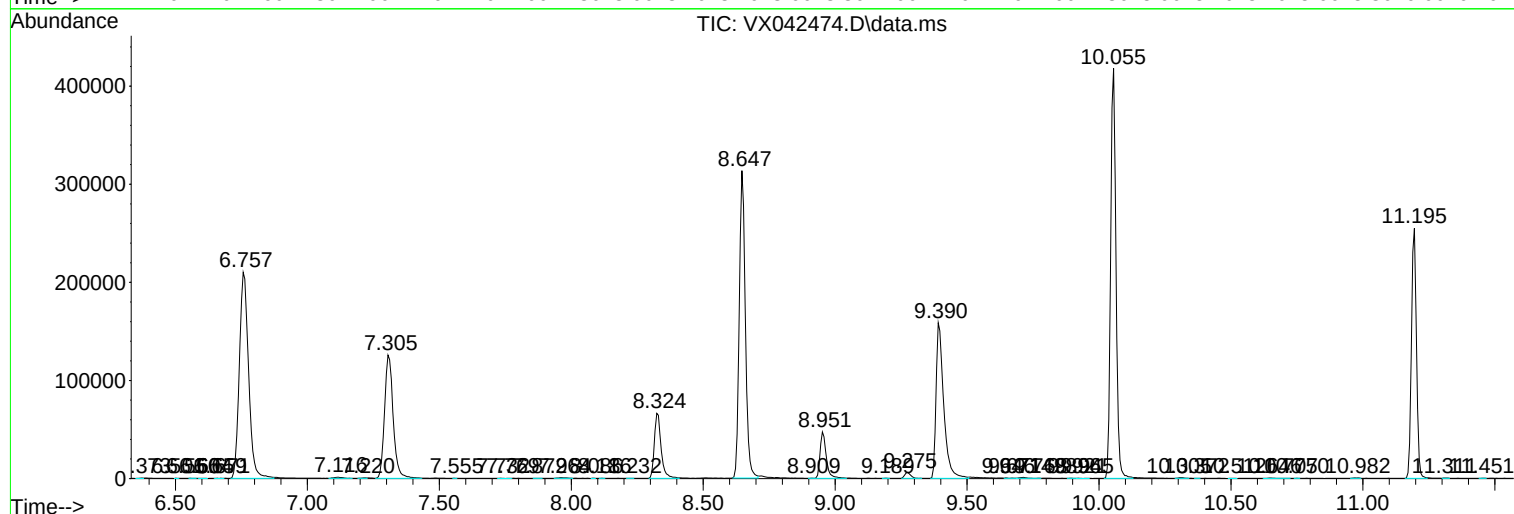
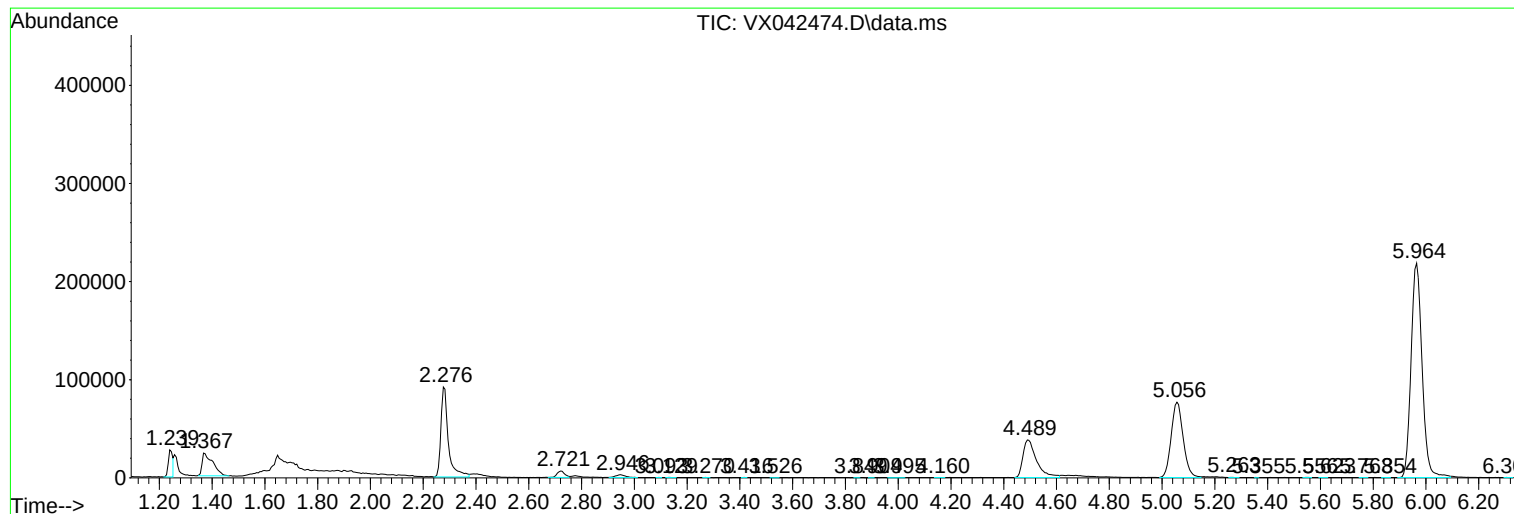
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Instrument :
MSVOA_X
ClientSampleId :
A4CL8ME

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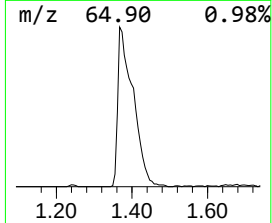
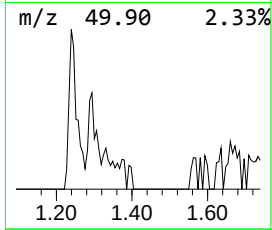
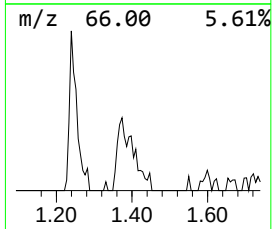
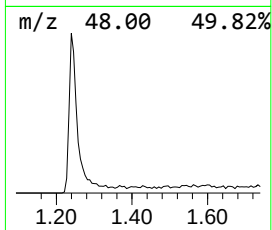
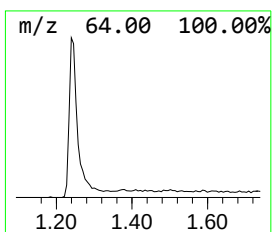
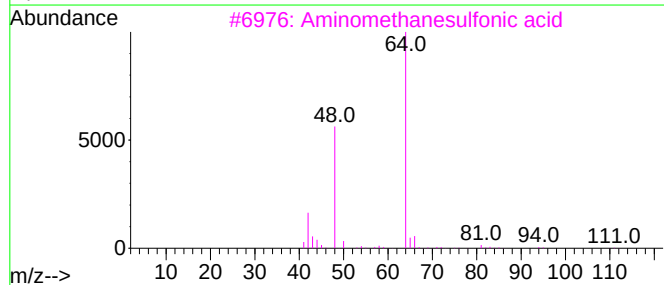
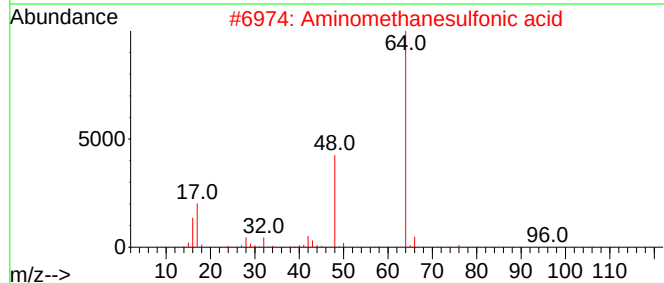
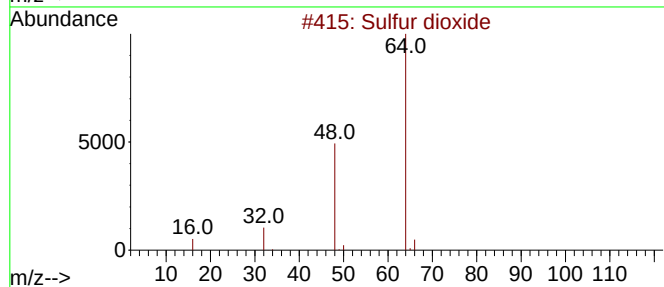
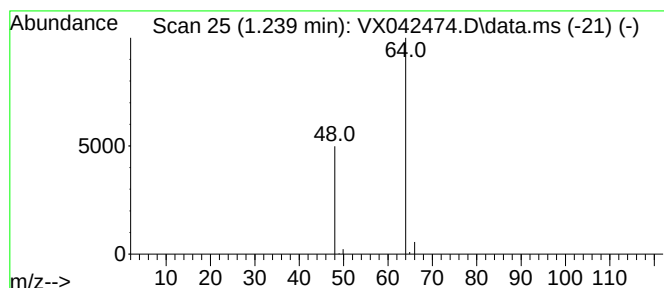
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.21 ug/L	32449	1,4-Difluorobenzene	6.757

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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	3.2	ug/L	32449	1	6.757	505718	50.0