

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042473.D
 Acq On : 23 Jul 2024 15:44
 Operator : JC/MD
 Sample : P3264-11ME
 Misc : 5.18g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL4ME

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: VX042473.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	21	25	27	rBV	29532	34319	5.35%	0.666%
2	1.368	43	46	50	rBV	23070	40109	6.25%	0.778%
3	1.557	69	77	80	rBV2	3446	7977	1.24%	0.155%
4	1.648	86	92	98	rBV2	15835	39480	6.15%	0.766%
5	2.276	189	195	211	rBV	74971	146579	22.83%	2.843%
6	2.538	237	238	240	rBV2	258	177	0.03%	0.003%
7	2.660	257	258	260	rBV	269	272	0.04%	0.005%
8	2.721	261	268	274	rBV	10575	21562	3.36%	0.418%
9	2.947	298	305	318	rVB	3239	8305	1.29%	0.161%
10	3.325	363	367	370	rVB2	130	179	0.03%	0.003%
11	3.410	378	381	384	rBV2	151	195	0.03%	0.004%
12	3.831	445	450	451	rBV2	168	291	0.05%	0.006%
13	3.892	458	460	463	rVB2	149	184	0.03%	0.004%
14	4.251	517	519	522	rVB	168	165	0.03%	0.003%
15	4.489	549	558	575	rBV	39259	134479	20.95%	2.608%
16	5.056	639	651	668	rBV	78546	245409	38.22%	4.759%
17	5.269	685	686	689	rBV2	196	166	0.03%	0.003%
18	5.404	704	708	712	rVB2	294	443	0.07%	0.009%
19	5.458	714	717	719	rBV3	149	154	0.02%	0.003%
20	5.544	727	731	732	rBV2	176	239	0.04%	0.005%
21	5.678	748	753	756	rVB2	129	217	0.03%	0.004%
22	5.964	788	800	831	rBV2	220471	642030	100.00%	12.451%
23	6.196	837	838	840	rBV	193	160	0.02%	0.003%
24	6.385	867	869	876	rVB2	393	626	0.10%	0.012%
25	6.550	892	896	897	rBV	163	226	0.04%	0.004%
26	6.757	920	930	953	rBV	202054	494942	77.09%	9.599%
27	7.111	983	988	989	rBV2	1104	1428	0.22%	0.028%
28	7.220	1003	1006	1008	rVV3	516	734	0.11%	0.014%
29	7.306	1012	1020	1040	rVB	126927	287562	44.79%	5.577%
30	7.489	1045	1050	1051	rBV4	203	239	0.04%	0.005%
31	7.678	1076	1081	1082	rBV2	136	217	0.03%	0.004%
32	7.732	1087	1090	1092	rVB	257	252	0.04%	0.005%
33	7.903	1115	1118	1120	rBV2	153	180	0.03%	0.003%
34	7.964	1123	1128	1130	rBV2	734	1164	0.18%	0.023%
35	8.116	1152	1153	1156	rBV2	198	166	0.03%	0.003%
36	8.324	1181	1187	1202	rBV	67529	120173	18.72%	2.331%

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37	8.440	1205	1206	1209	rVB2	343	233	0.04%	0.005%
38	8.519	1214	1219	1222	rBV4	560	1008	0.16%	0.020%
39	8.592	1229	1231	1232	rBV	213	172	0.03%	0.003%
40	8.647	1234	1240	1256	rVV	317322	512222	79.78%	9.934%
41	8.952	1285	1290	1306	rVV	49100	78336	12.20%	1.519%
42	9.122	1317	1318	1321	rBV	191	221	0.03%	0.004%
43	9.275	1338	1343	1352	rVB2	6326	9754	1.52%	0.189%
44	9.391	1357	1362	1381	rBV	155404	319535	49.77%	6.197%
45	9.714	1411	1415	1422	rVV5	743	1471	0.23%	0.029%
46	9.939	1449	1452	1455	rBV2	167	225	0.04%	0.004%
47	10.055	1465	1471	1488	rBV	416542	577958	90.02%	11.208%
48	10.201	1492	1495	1500	rVV2	625	1018	0.16%	0.020%
49	10.250	1500	1503	1506	rVB4	207	259	0.04%	0.005%
50	10.305	1509	1512	1518	rVB2	754	1207	0.19%	0.023%
51	10.598	1559	1560	1563	rBV	168	159	0.02%	0.003%
52	10.653	1565	1569	1571	rBV3	434	672	0.10%	0.013%
53	10.970	1617	1621	1624	rBV3	1260	1376	0.21%	0.027%
54	11.085	1637	1640	1643	rVB2	164	228	0.04%	0.004%
55	11.195	1652	1658	1667	rBV	248538	338018	52.65%	6.555%
56	11.311	1674	1677	1680	rVB3	478	647	0.10%	0.013%
57	11.463	1698	1702	1703	rVV2	360	415	0.06%	0.008%
58	11.476	1703	1704	1706	rVV2	302	289	0.05%	0.006%
59	11.494	1706	1707	1710	rVB	396	254	0.04%	0.005%
60	11.756	1742	1750	1756	rBV4	475	1267	0.20%	0.025%
61	11.933	1777	1779	1782	rBV	250	279	0.04%	0.005%
62	11.982	1782	1787	1788	rBV3	1178	1365	0.21%	0.026%
63	12.024	1788	1794	1804	rVV	416209	540770	84.23%	10.487%
64	12.219	1821	1826	1837	rBV2	10244	15532	2.42%	0.301%
65	12.317	1837	1842	1858	rVV	357126	476193	74.17%	9.235%
66	12.427	1858	1860	1863	rVV2	529	656	0.10%	0.013%
67	12.494	1867	1871	1874	rVB3	206	298	0.05%	0.006%
68	12.555	1876	1881	1882	rVB2	221	260	0.04%	0.005%
69	12.756	1910	1914	1918	rBV3	738	1242	0.19%	0.024%
70	12.872	1927	1933	1943	rBV	5586	7820	1.22%	0.152%
71	13.042	1956	1961	1963	rBV2	322	456	0.07%	0.009%
72	13.201	1984	1987	1989	rBV2	148	166	0.03%	0.003%
73	13.402	2016	2020	2026	rBV2	2475	3127	0.49%	0.061%
74	13.561	2043	2046	2049	rBV	140	230	0.04%	0.004%
75	13.597	2049	2052	2055	rVB2	251	247	0.04%	0.005%
76	13.683	2062	2066	2073	rBV	1720	2449	0.38%	0.047%

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Peak Location: TOP

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 Title : VOC Analysis

77	13.780	2078	2082	2092	rVV4	1245	2417	0.38%	0.047%
78	13.963	2108	2112	2115	rBV	248	334	0.05%	0.006%
79	14.018	2119	2121	2124	rBV3	184	268	0.04%	0.005%
80	14.134	2132	2140	2144	rBV	2286	3362	0.52%	0.065%
81	14.426	2184	2188	2194	rBV3	1178	1940	0.30%	0.038%
82	14.499	2197	2200	2201	rBV	236	219	0.03%	0.004%
83	14.554	2201	2209	2214	rBV3	1761	3815	0.59%	0.074%
84	14.646	2221	2224	2233	rBV5	420	696	0.11%	0.013%
85	14.786	2244	2247	2252	rVB2	416	564	0.09%	0.011%
86	14.884	2261	2263	2265	rBV3	295	218	0.03%	0.004%
87	14.926	2269	2270	2272	rVB2	366	186	0.03%	0.004%
88	14.993	2279	2281	2286	rVB4	268	340	0.05%	0.007%
89	15.036	2286	2288	2290	rBV2	299	237	0.04%	0.005%
90	15.182	2309	2312	2315	rVB3	286	349	0.05%	0.007%
91	15.390	2341	2346	2352	rVB4	2429	4459	0.69%	0.086%
92	15.493	2360	2363	2364	rBV3	312	375	0.06%	0.007%
93	15.579	2375	2377	2378	rBV	330	277	0.04%	0.005%
94	15.700	2394	2397	2399	rBV3	715	887	0.14%	0.017%
95	15.786	2409	2411	2414	rBV3	343	248	0.04%	0.005%
96	15.957	2434	2439	2446	rBV3	2485	3866	0.60%	0.075%
97	16.280	2488	2492	2497	rVB5	726	1464	0.23%	0.028%
98	16.334	2498	2501	2502	rBV	455	423	0.07%	0.008%
99	16.700	2559	2561	2562	rBV2	320	244	0.04%	0.005%
100	16.737	2565	2567	2568	rBV	293	226	0.04%	0.004%

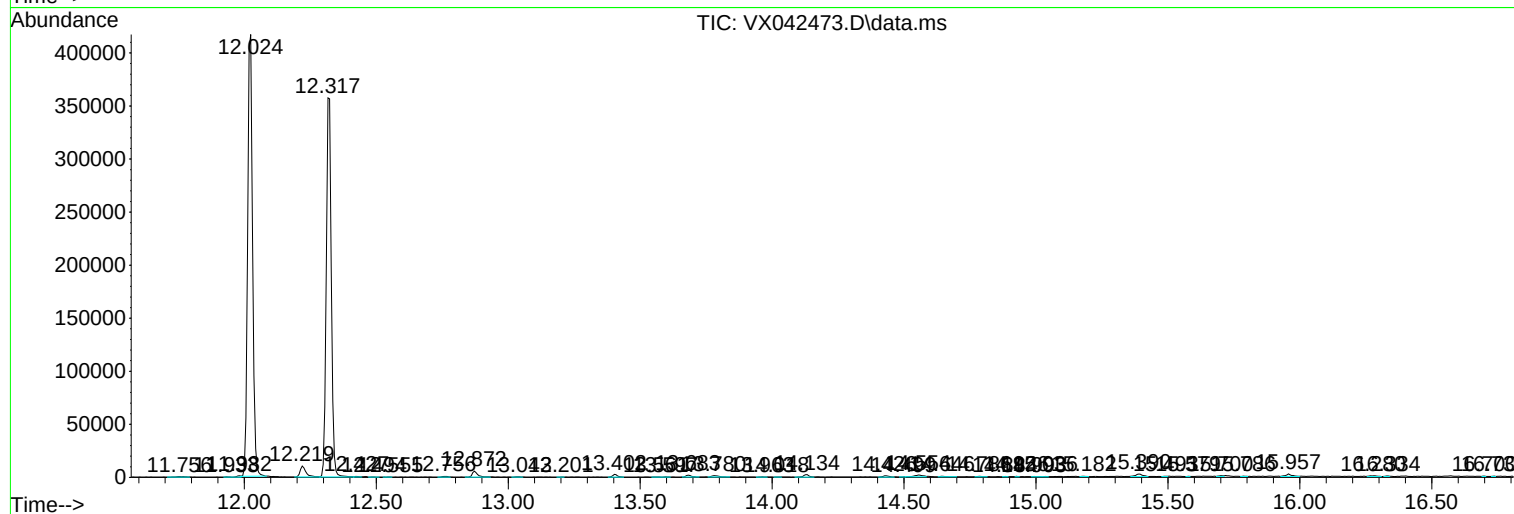
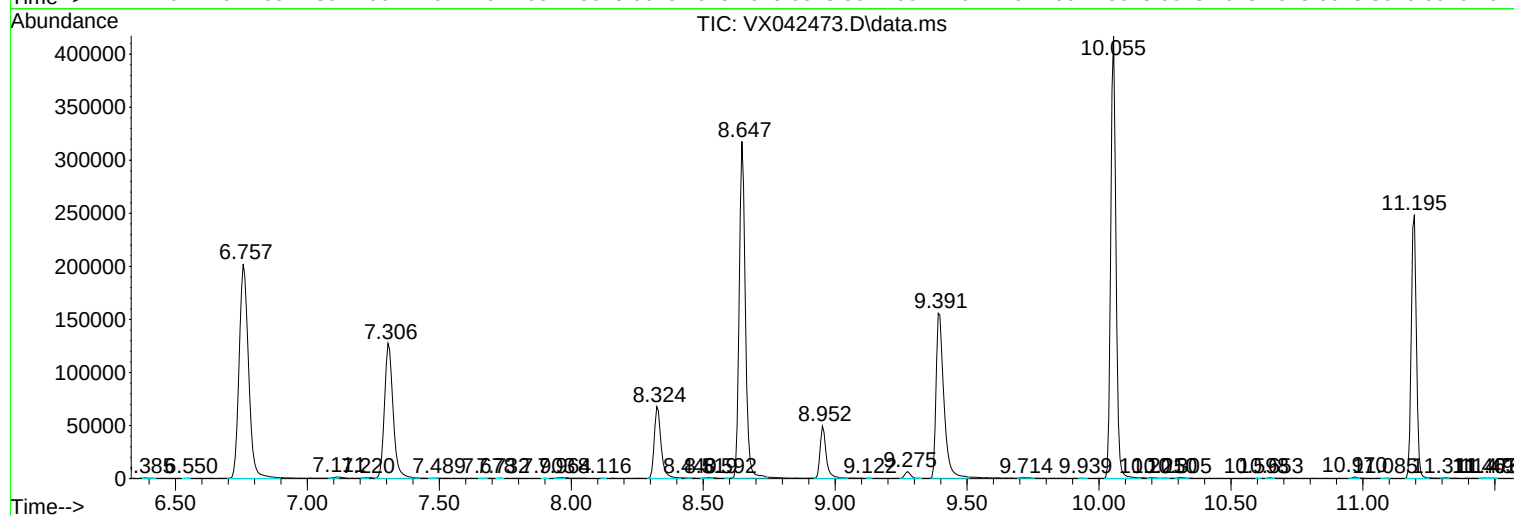
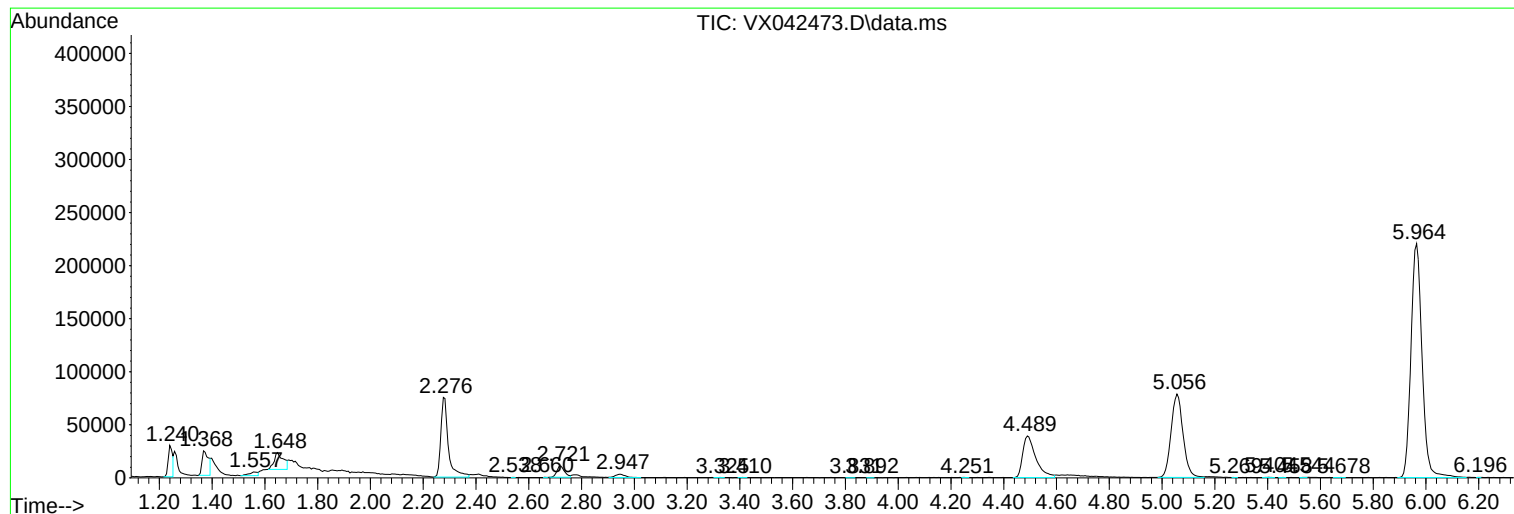
Sum of corrected areas: 5156448

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Instrument :
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A4CL4ME

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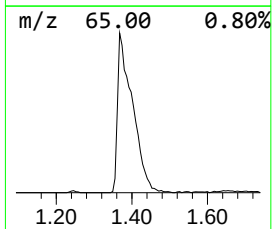
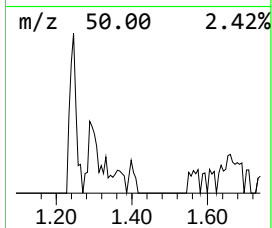
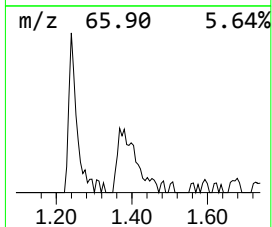
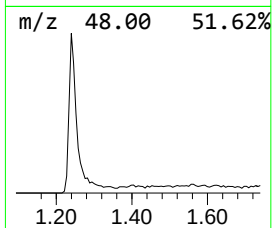
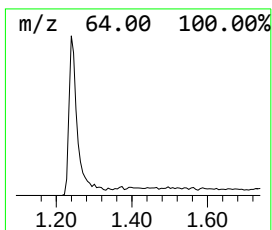
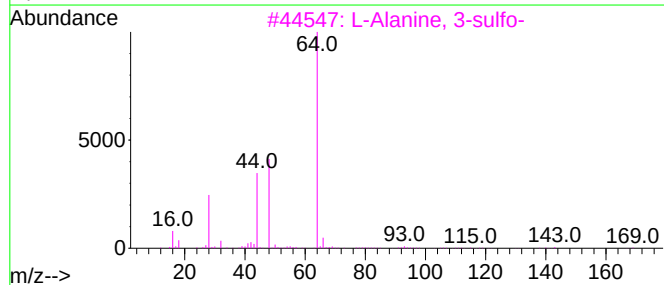
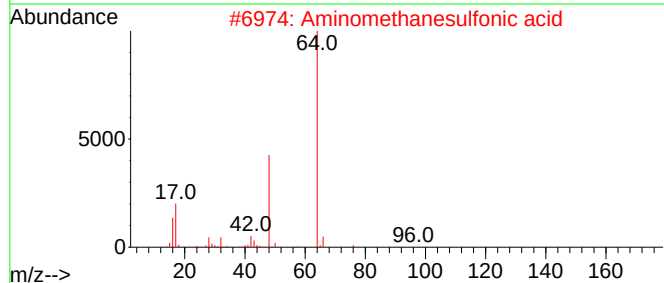
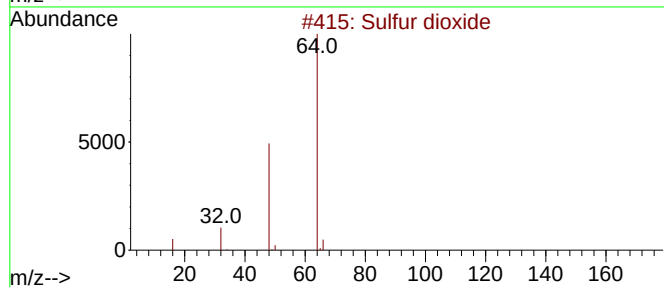
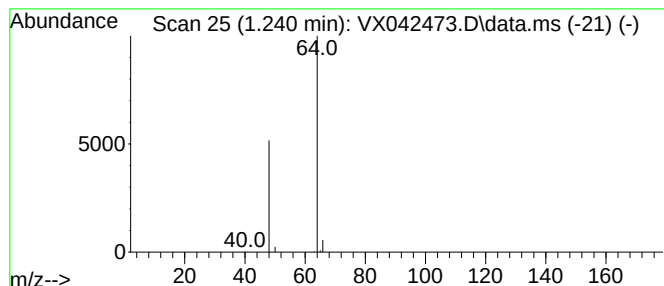
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.47 ug/L	34319	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			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	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.5	ug/L	34319	1	6.757	494942	50.0