

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042424.D
 Acq On : 19 Jul 2024 23:53
 Operator : JC/MD
 Sample : P3298-13 100X
 Misc : 3.26g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB43

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: VX042424.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	36	rBV	30735	43638	6.11%	0.789%
2	1.368	43	46	60	rVB	63331	80887	11.33%	1.462%
3	1.648	88	92	103	rVB	57305	78675	11.02%	1.422%
4	2.294	192	198	211	rBV	136864	219693	30.77%	3.972%
5	2.459	223	225	227	rBV2	183	116	0.02%	0.002%
6	2.508	229	233	236	rBV3	276	466	0.07%	0.008%
7	2.721	263	268	272	rVB3	293	488	0.07%	0.009%
8	2.788	275	279	285	rVB3	932	1721	0.24%	0.031%
9	2.861	288	291	292	rBV	110	106	0.01%	0.002%
10	2.941	297	304	315	rBV	3517	8449	1.18%	0.153%
11	3.062	323	324	328	rVB	165	171	0.02%	0.003%
12	3.593	410	411	414	rVV	209	138	0.02%	0.002%
13	3.654	419	421	423	rBV2	156	164	0.02%	0.003%
14	3.806	444	446	449	rBV2	110	130	0.02%	0.002%
15	3.837	449	451	453	rBV	113	124	0.02%	0.002%
16	3.910	461	463	465	rVB2	141	116	0.02%	0.002%
17	3.977	473	474	476	rVB2	160	108	0.02%	0.002%
18	4.129	496	499	501	rBV2	175	156	0.02%	0.003%
19	4.282	522	524	526	rBV	160	138	0.02%	0.002%
20	4.337	531	533	535	rBV	86	100	0.01%	0.002%
21	4.465	545	554	573	rBV	52762	159621	22.36%	2.886%
22	4.946	631	633	637	rVB2	142	201	0.03%	0.004%
23	5.056	637	651	667	rBV	89614	275680	38.61%	4.984%
24	5.263	684	685	690	rVB2	169	207	0.03%	0.004%
25	5.312	692	693	695	rVB	223	99	0.01%	0.002%
26	5.397	701	707	708	rBV3	389	682	0.10%	0.012%
27	5.538	729	730	731	rBV	260	180	0.03%	0.003%
28	5.879	784	786	789	rVB	176	163	0.02%	0.003%
29	5.964	789	800	821	rBV2	241411	713990	100.00%	12.908%
30	6.251	846	847	850	rVB2	240	209	0.03%	0.004%
31	6.287	851	853	855	rVB	156	127	0.02%	0.002%
32	6.434	873	877	878	rBV2	116	125	0.02%	0.002%
33	6.495	885	887	890	rVB2	124	100	0.01%	0.002%
34	6.641	910	911	914	rVB2	154	147	0.02%	0.003%
35	6.757	921	930	946	rBV	218156	528295	73.99%	9.551%
36	6.958	961	963	965	rBV	195	137	0.02%	0.002%

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 Title : VOC Analysis

37	7.056	977	979	980	rBV	180	117	0.02%	0.002%
38	7.117	984	989	997	rVB5	1373	3351	0.47%	0.061%
39	7.208	999	1004	1006	rBV2	321	518	0.07%	0.009%
40	7.306	1011	1020	1034	rBV	143826	317192	44.43%	5.735%
41	7.745	1090	1092	1096	rVB	155	106	0.01%	0.002%
42	7.891	1115	1116	1120	rVB	218	174	0.02%	0.003%
43	7.964	1123	1128	1129	rBV3	626	959	0.13%	0.017%
44	8.062	1142	1144	1147	rBV2	129	130	0.02%	0.002%
45	8.202	1163	1167	1170	rBV2	201	258	0.04%	0.005%
46	8.324	1181	1187	1208	rBV	80680	133262	18.66%	2.409%
47	8.647	1234	1240	1256	rVV	357870	559045	78.30%	10.107%
48	8.903	1279	1282	1285	rBV2	193	229	0.03%	0.004%
49	8.952	1285	1290	1307	rBV	55716	85851	12.02%	1.552%
50	9.147	1319	1322	1325	rVB	145	180	0.03%	0.003%
51	9.171	1325	1326	1330	rVV2	121	135	0.02%	0.002%
52	9.202	1330	1331	1333	rVB2	195	137	0.02%	0.002%
53	9.226	1333	1335	1338	rBV2	130	166	0.02%	0.003%
54	9.275	1339	1343	1348	rVB2	582	858	0.12%	0.016%
55	9.384	1356	1361	1378	rBV	225825	341283	47.80%	6.170%
56	9.604	1396	1397	1398	rVB	372	136	0.02%	0.002%
57	9.702	1409	1413	1417	rVB3	1302	1798	0.25%	0.033%
58	9.823	1428	1433	1435	rVV3	148	247	0.03%	0.004%
59	9.982	1457	1459	1461	rBV	227	136	0.02%	0.002%
60	10.055	1465	1471	1490	rVV	425481	599366	83.95%	10.836%
61	10.305	1509	1512	1513	rBV2	364	326	0.05%	0.006%
62	10.415	1527	1530	1532	rVB	158	128	0.02%	0.002%
63	10.433	1532	1533	1537	rBV2	181	247	0.03%	0.004%
64	10.494	1542	1543	1547	rVV	243	166	0.02%	0.003%
65	10.707	1575	1578	1581	rBV2	91	132	0.02%	0.002%
66	10.896	1607	1609	1612	rVB	142	126	0.02%	0.002%
67	10.963	1618	1620	1623	rBV2	320	328	0.05%	0.006%
68	11.031	1630	1631	1634	rVB	171	110	0.02%	0.002%
69	11.061	1634	1636	1637	rBV2	117	111	0.02%	0.002%
70	11.189	1652	1657	1668	rBV	279665	363732	50.94%	6.576%
71	11.311	1675	1677	1678	rVB2	375	206	0.03%	0.004%
72	11.402	1690	1692	1693	rBV2	193	163	0.02%	0.003%
73	11.482	1703	1705	1710	rVB	148	215	0.03%	0.004%
74	11.543	1710	1715	1720	rBV2	170	347	0.05%	0.006%
75	11.628	1727	1729	1731	rBV	145	106	0.01%	0.002%
76	11.707	1740	1742	1745	rVV2	129	110	0.02%	0.002%

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 Title : VOC Analysis

77	11.762	1748	1751	1754	rBV2	259	253	0.04%	0.005%
78	12.018	1788	1793	1806	rBV	401820	527552	73.89%	9.538%
79	12.317	1837	1842	1850	rBV	368659	471197	65.99%	8.519%
80	12.555	1879	1881	1884	rVB	248	182	0.03%	0.003%
81	12.603	1887	1889	1894	rVB3	255	381	0.05%	0.007%
82	12.652	1894	1897	1898	rBV	153	153	0.02%	0.003%
83	12.805	1919	1922	1923	rBV2	163	169	0.02%	0.003%
84	12.981	1948	1951	1954	rVB2	117	108	0.02%	0.002%
85	13.280	1999	2000	2003	rVB	105	98	0.01%	0.002%
86	13.311	2003	2005	2007	rBV2	98	106	0.01%	0.002%
87	13.347	2009	2011	2012	rBV2	119	106	0.01%	0.002%
88	13.603	2051	2053	2055	rBV	247	185	0.03%	0.003%
89	13.676	2063	2065	2068	rVB2	182	156	0.02%	0.003%
90	13.737	2073	2075	2077	rVB	192	120	0.02%	0.002%
91	13.780	2080	2082	2084	rBV2	252	236	0.03%	0.004%
92	13.914	2102	2104	2107	rVB2	150	176	0.02%	0.003%
93	13.975	2110	2114	2116	rBV2	166	269	0.04%	0.005%
94	14.048	2123	2126	2128	rBV2	262	343	0.05%	0.006%
95	14.073	2128	2130	2131	rVV	231	161	0.02%	0.003%
96	14.097	2132	2134	2136	rVV2	301	276	0.04%	0.005%
97	14.134	2136	2140	2143	rVB2	683	945	0.13%	0.017%
98	14.219	2153	2154	2156	rBV	189	106	0.01%	0.002%
99	14.518	2202	2203	2206	rBV2	200	150	0.02%	0.003%
100	14.548	2206	2208	2209	rVV2	250	130	0.02%	0.002%

Sum of corrected areas: 5531292

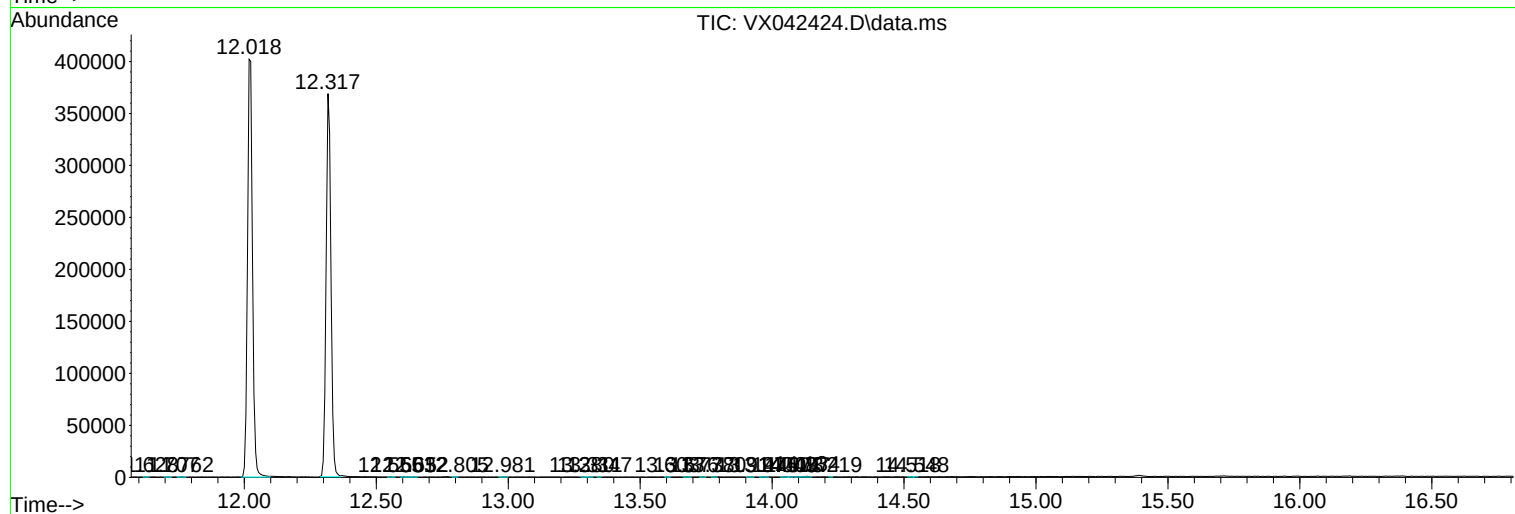
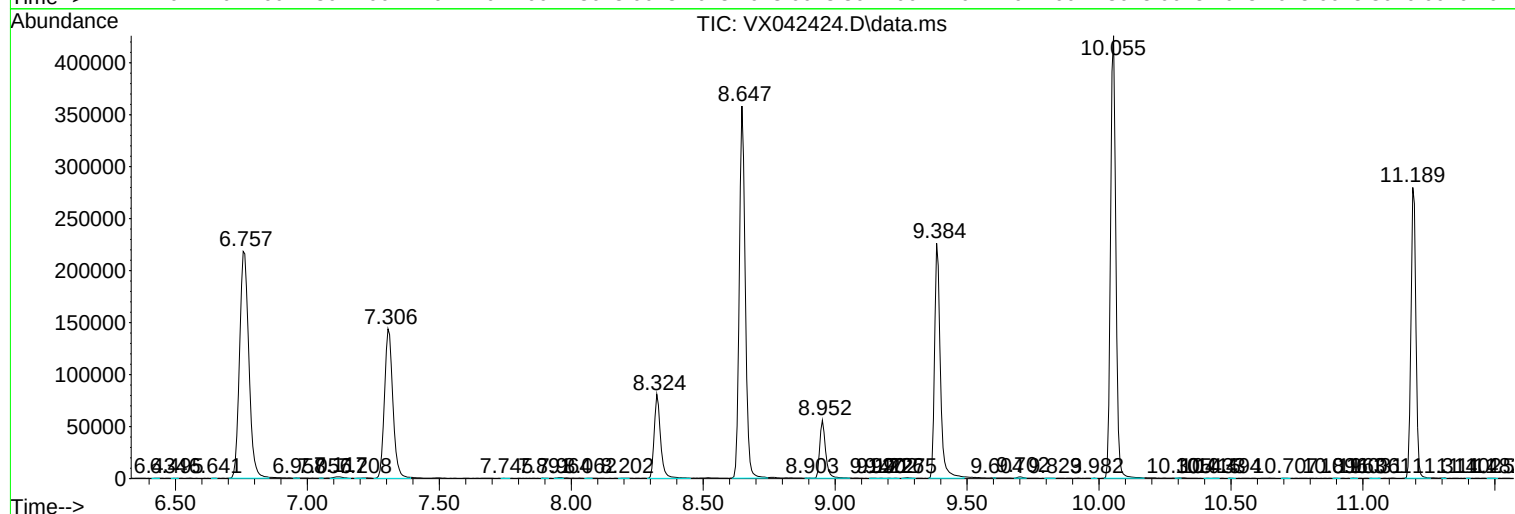
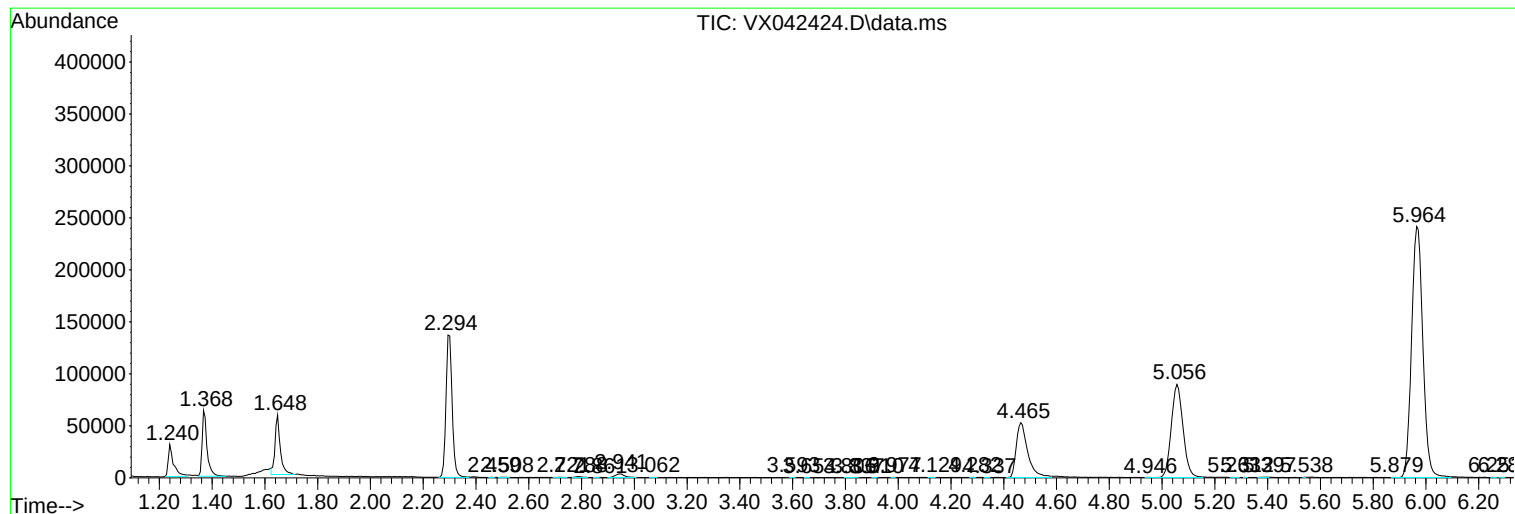
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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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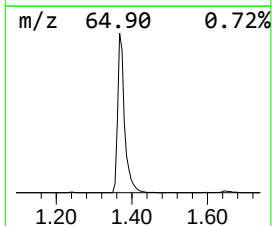
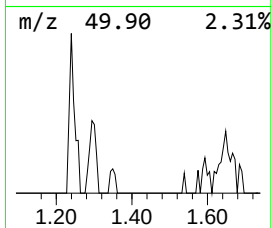
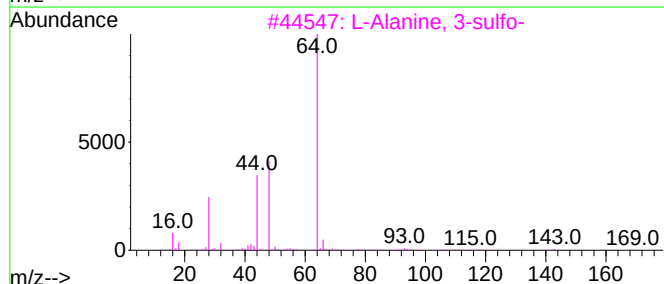
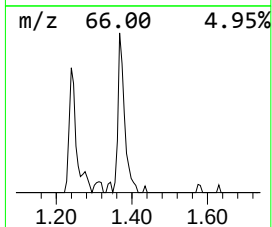
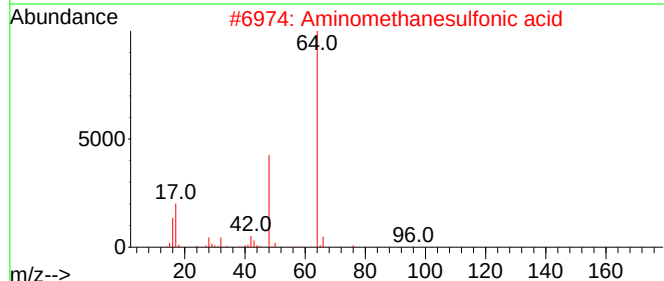
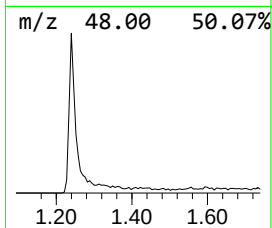
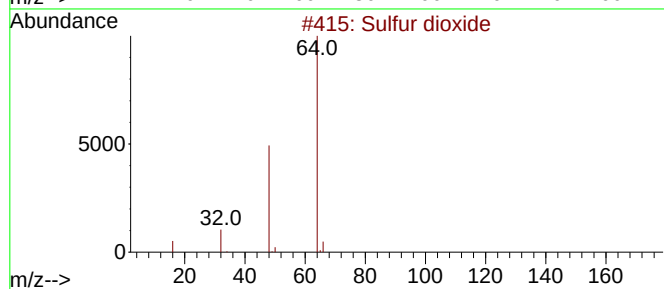
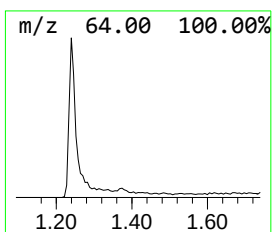
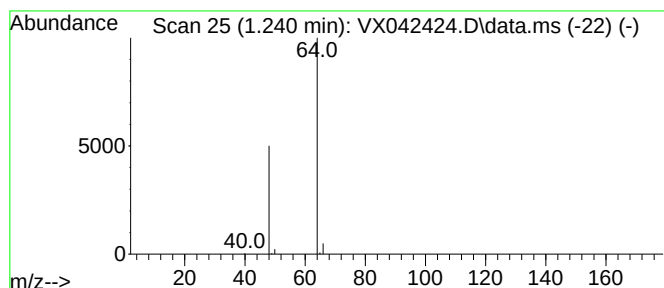
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	4.13 ug/L	43638	1,4-Difluorobenzene	6.763

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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	4.1	ug/L	43638	1	6.763	528295	50.0