

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042419.D
 Acq On : 19 Jul 2024 21:57
 Operator : JC/MD
 Sample : P3298-09 100X
 Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB29

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: VX042419.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	37	rBV	40648	56221	8.03%	0.988%
2	1.368	43	46	56	rVB	69255	87465	12.50%	1.537%
3	1.648	88	92	103	rVB	47534	66663	9.53%	1.171%
4	2.221	184	186	188	rVB3	206	170	0.02%	0.003%
5	2.294	192	198	208	rVV	118263	186493	26.65%	3.277%
6	2.392	212	214	221	rVB3	780	1154	0.16%	0.020%
7	2.477	226	228	229	rBV2	206	145	0.02%	0.003%
8	2.495	229	231	232	rBV	326	202	0.03%	0.004%
9	2.581	242	245	248	rBV2	101	163	0.02%	0.003%
10	2.715	263	267	269	rVB3	216	297	0.04%	0.005%
11	2.788	273	279	283	rBV3	821	1573	0.22%	0.028%
12	2.947	296	305	314	rBB	2702	6317	0.90%	0.111%
13	3.160	336	340	342	rBV2	125	161	0.02%	0.003%
14	3.270	354	358	362	rBV2	136	212	0.03%	0.004%
15	3.355	370	372	375	rVB2	153	184	0.03%	0.003%
16	3.507	394	397	398	rVV2	149	132	0.02%	0.002%
17	3.782	440	442	445	rBV2	180	194	0.03%	0.003%
18	3.873	455	457	458	rBV	177	122	0.02%	0.002%
19	3.898	458	461	462	rBV2	158	163	0.02%	0.003%
20	3.940	465	468	470	rBV	170	214	0.03%	0.004%
21	3.989	475	476	478	rVV	205	144	0.02%	0.003%
22	4.026	480	482	483	rVB	202	115	0.02%	0.002%
23	4.074	486	490	491	rBV	146	135	0.02%	0.002%
24	4.324	529	531	535	rBV2	159	191	0.03%	0.003%
25	4.465	546	554	570	rBV	49885	151957	21.71%	2.670%
26	4.922	627	629	631	rVB	249	187	0.03%	0.003%
27	5.056	639	651	667	rBV	86766	265706	37.97%	4.669%
28	5.385	702	705	706	rBV	351	368	0.05%	0.006%
29	5.471	717	719	722	rVB	148	135	0.02%	0.002%
30	5.544	727	731	732	rBV2	396	436	0.06%	0.008%
31	5.623	742	744	748	rVB	144	172	0.02%	0.003%
32	5.660	748	750	753	rVB2	149	158	0.02%	0.003%
33	5.690	753	755	757	rBV	206	171	0.02%	0.003%
34	5.964	787	800	823	rBV2	239937	699817	100.00%	12.296%
35	6.391	867	870	872	rVB3	299	273	0.04%	0.005%
36	6.470	882	883	886	rVB2	179	158	0.02%	0.003%

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 Title : VOC Analysis

37	6.501	886	888	890	rBV	256	175	0.03%	0.003%
38	6.531	890	893	894	rBV2	124	114	0.02%	0.002%
39	6.757	922	930	949	rBV	228760	557740	79.70%	9.800%
40	6.897	951	953	957	rVB2	460	511	0.07%	0.009%
41	7.013	970	972	974	rBV2	192	177	0.03%	0.003%
42	7.123	984	990	999	rBV6	1632	3742	0.53%	0.066%
43	7.214	1001	1005	1012	rVB4	457	1124	0.16%	0.020%
44	7.306	1012	1020	1044	rBV	139890	310945	44.43%	5.463%
45	7.458	1044	1045	1047	rBV	238	123	0.02%	0.002%
46	7.647	1075	1076	1078	rBV	185	141	0.02%	0.002%
47	7.732	1086	1090	1091	rBV2	117	137	0.02%	0.002%
48	7.866	1110	1112	1114	rVB	182	130	0.02%	0.002%
49	7.903	1116	1118	1119	rBV2	185	170	0.02%	0.003%
50	7.958	1123	1127	1129	rBV3	673	849	0.12%	0.015%
51	8.025	1136	1138	1141	rVB2	168	206	0.03%	0.004%
52	8.324	1181	1187	1201	rBV	74944	128467	18.36%	2.257%
53	8.519	1213	1219	1222	rBV4	489	1081	0.15%	0.019%
54	8.647	1233	1240	1252	rBV	362219	566833	81.00%	9.960%
55	8.952	1285	1290	1303	rBV	55163	83525	11.94%	1.468%
56	9.110	1314	1316	1319	rVB	180	163	0.02%	0.003%
57	9.159	1321	1324	1326	rBV2	110	143	0.02%	0.003%
58	9.275	1338	1343	1350	rBV	42022	61347	8.77%	1.078%
59	9.384	1356	1361	1376	rBV	220951	329661	47.11%	5.792%
60	9.701	1410	1413	1418	rVB2	950	1388	0.20%	0.024%
61	9.762	1421	1423	1425	rVB2	213	158	0.02%	0.003%
62	9.951	1452	1454	1457	rVB2	150	162	0.02%	0.003%
63	10.055	1465	1471	1490	rBV	462554	651142	93.04%	11.441%
64	10.275	1505	1507	1509	rVB2	175	152	0.02%	0.003%
65	10.305	1509	1512	1519	rBV4	569	1048	0.15%	0.018%
66	10.500	1543	1544	1546	rBV	177	143	0.02%	0.003%
67	10.646	1566	1568	1573	rVV2	265	302	0.04%	0.005%
68	10.707	1575	1578	1582	rBV2	191	208	0.03%	0.004%
69	10.848	1599	1601	1604	rBV	131	127	0.02%	0.002%
70	10.963	1619	1620	1624	rBV2	97	128	0.02%	0.002%
71	11.031	1630	1631	1633	rBV2	152	131	0.02%	0.002%
72	11.104	1640	1643	1648	rVB3	247	278	0.04%	0.005%
73	11.189	1652	1657	1671	rBV	279563	358771	51.27%	6.304%
74	11.390	1686	1690	1692	rVB2	99	120	0.02%	0.002%
75	11.433	1695	1697	1700	rVB2	166	153	0.02%	0.003%
76	11.463	1700	1702	1703	rBV	180	121	0.02%	0.002%

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 Title : VOC Analysis

77	11.622	1726	1728	1733	rBV3	100	156	0.02%	0.003%
78	11.756	1748	1750	1753	rVB2	180	179	0.03%	0.003%
79	11.811	1756	1759	1761	rBV2	127	147	0.02%	0.003%
80	11.847	1761	1765	1768	rVB2	142	253	0.04%	0.004%
81	11.908	1773	1775	1778	rBV2	228	192	0.03%	0.003%
82	11.969	1783	1785	1788	rBV3	260	225	0.03%	0.004%
83	12.024	1788	1794	1804	rBV	455164	595348	85.07%	10.461%
84	12.317	1837	1842	1857	rBV	387845	498565	71.24%	8.760%
85	12.652	1895	1897	1899	rBV2	116	119	0.02%	0.002%
86	12.762	1911	1915	1917	rVB2	415	537	0.08%	0.009%
87	13.042	1958	1961	1962	rBV3	170	185	0.03%	0.003%
88	13.323	2005	2007	2011	rBB	155	147	0.02%	0.003%
89	13.524	2037	2040	2041	rBV	199	174	0.02%	0.003%
90	13.597	2049	2052	2053	rBV	208	184	0.03%	0.003%
91	13.774	2078	2081	2082	rBV2	228	275	0.04%	0.005%
92	13.993	2115	2117	2119	rBV2	226	172	0.02%	0.003%
93	14.030	2121	2123	2126	rBV2	155	151	0.02%	0.003%
94	14.128	2135	2139	2143	rBV	868	1261	0.18%	0.022%
95	14.487	2196	2198	2199	rBV2	235	167	0.02%	0.003%
96	14.695	2229	2232	2233	rBV2	223	181	0.03%	0.003%
97	14.743	2238	2240	2242	rBV2	320	301	0.04%	0.005%
98	15.133	2302	2304	2305	rBV	378	162	0.02%	0.003%
99	15.389	2343	2346	2352	rVB5	1070	1517	0.22%	0.027%
100	15.554	2371	2373	2375	rBV2	462	366	0.05%	0.006%

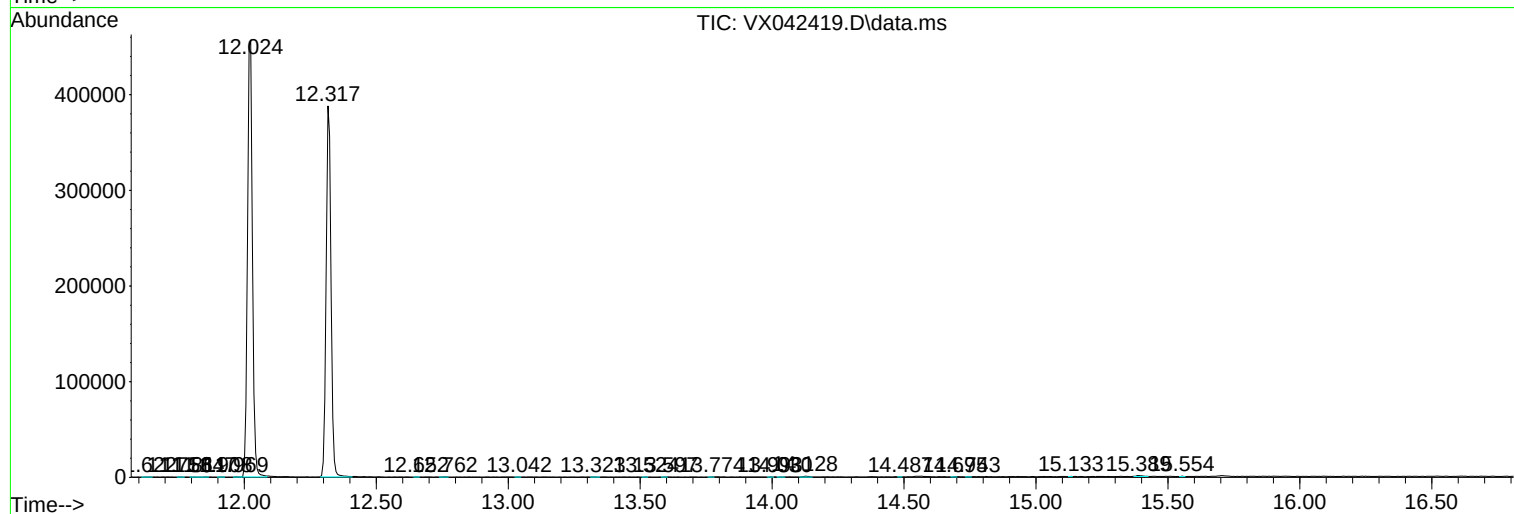
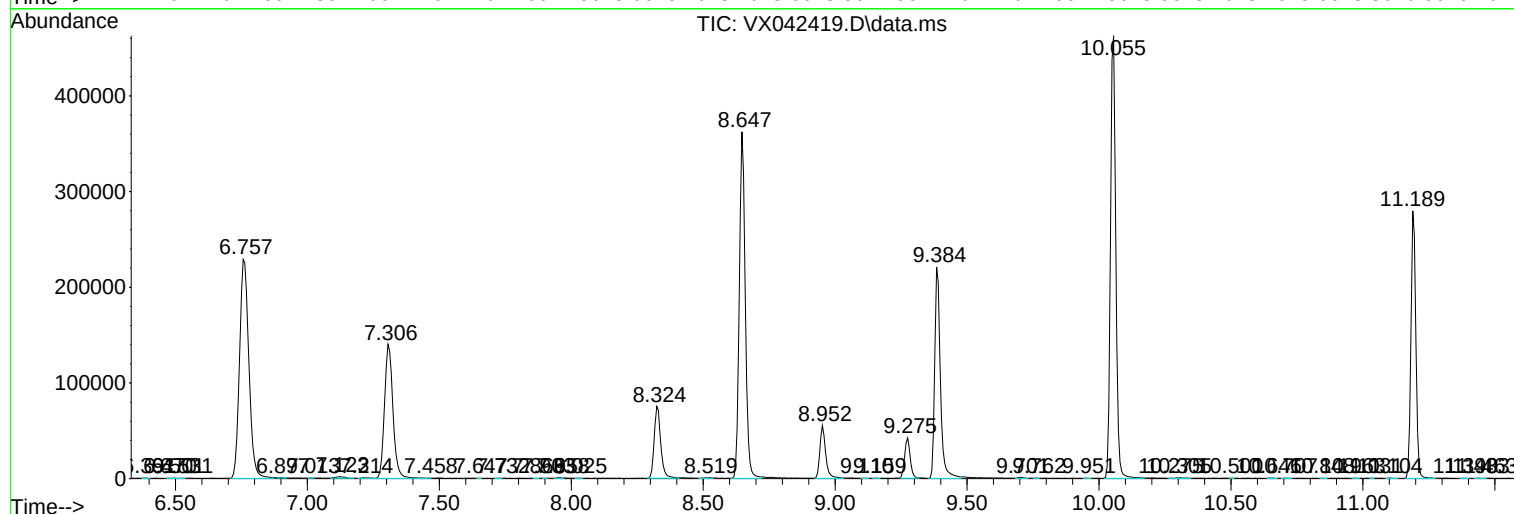
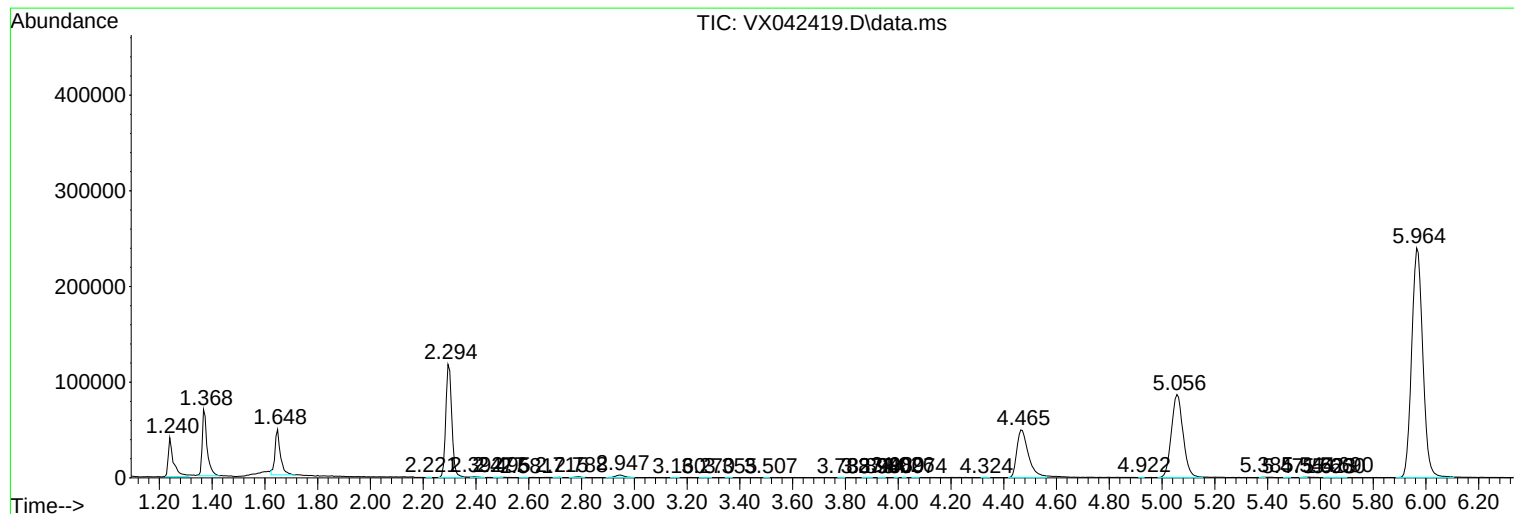
Sum of corrected areas: 5691368

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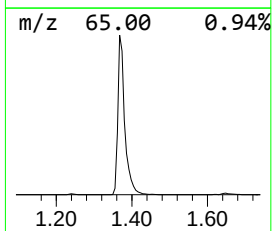
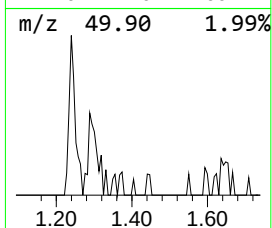
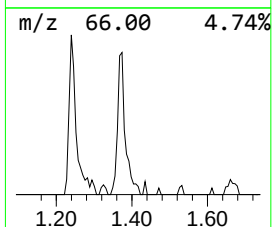
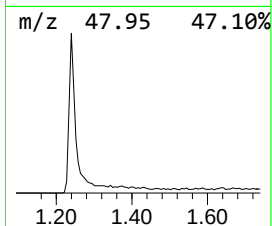
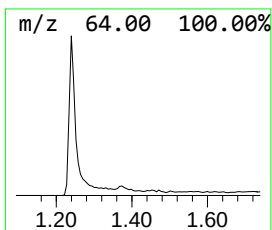
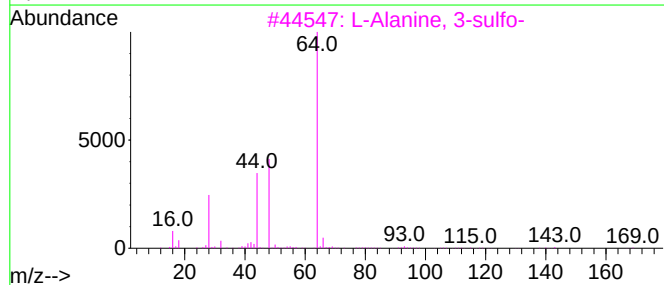
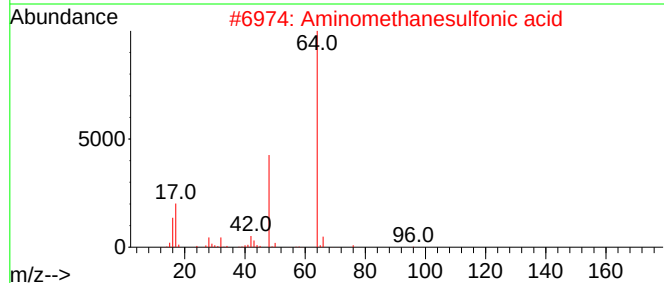
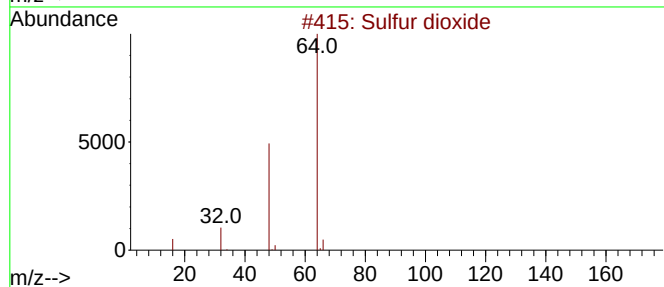
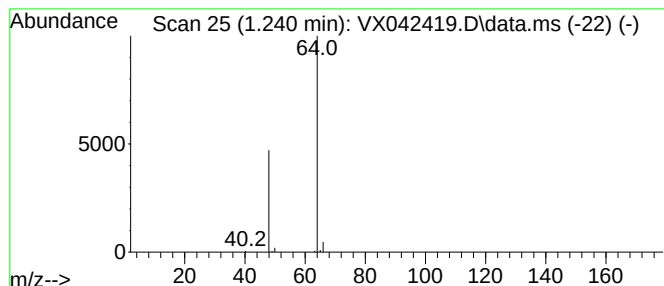
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	5.04 ug/L	56221	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	5.0	ug/L	56221	1	6.757	557740	50.0