

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042420.D
 Acq On : 19 Jul 2024 22:20
 Operator : JC/MD
 Sample : P3238-06ME
 Misc : 5.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BE9ME

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: VX042420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	27	rBV	25614	31267	4.41%	0.560%
2	1.374	43	47	62	rVB	35245	89721	12.65%	1.608%
3	2.282	189	196	213	rBV	87620	170305	24.02%	3.052%
4	2.721	263	268	273	rBV2	3971	7808	1.10%	0.140%
5	2.947	296	305	318	rBV	7048	18710	2.64%	0.335%
6	3.062	322	324	326	rVB	254	180	0.03%	0.003%
7	3.148	336	338	340	rBV	297	198	0.03%	0.004%
8	3.251	352	355	359	rVB2	151	192	0.03%	0.003%
9	3.386	376	377	379	rBV	231	113	0.02%	0.002%
10	3.520	397	399	402	rVB2	139	117	0.02%	0.002%
11	3.556	402	405	407	rVB2	131	153	0.02%	0.003%
12	3.605	410	413	414	rBV2	115	136	0.02%	0.002%
13	3.727	428	433	434	rBV	126	157	0.02%	0.003%
14	3.940	465	468	470	rBV2	152	181	0.03%	0.003%
15	4.117	494	497	498	rBV2	147	136	0.02%	0.002%
16	4.148	500	502	504	rVV2	161	132	0.02%	0.002%
17	4.172	504	506	509	rVV	132	142	0.02%	0.003%
18	4.355	535	536	538	rBV	222	138	0.02%	0.002%
19	4.489	547	558	580	rBV	36735	142242	20.06%	2.549%
20	4.971	636	637	639	rBV	258	169	0.02%	0.003%
21	5.056	639	651	667	rBV	85871	266945	37.65%	4.784%
22	5.263	683	685	687	rVB2	176	150	0.02%	0.003%
23	5.318	693	694	698	rBV	174	172	0.02%	0.003%
24	5.385	701	705	708	rBV3	296	523	0.07%	0.009%
25	5.544	730	731	734	rBV3	217	259	0.04%	0.005%
26	5.617	740	743	744	rBV2	143	142	0.02%	0.003%
27	5.672	751	752	755	rBV	163	145	0.02%	0.003%
28	5.720	758	760	762	rBV2	151	147	0.02%	0.003%
29	5.775	767	769	770	rBV	176	122	0.02%	0.002%
30	5.800	770	773	776	rBV2	129	179	0.03%	0.003%
31	5.842	778	780	783	rBV	250	199	0.03%	0.004%
32	5.958	789	799	828	rBV2	245263	709026	100.00%	12.706%
33	6.226	842	843	847	rVB	249	225	0.03%	0.004%
34	6.257	847	848	851	rBV	174	146	0.02%	0.003%
35	6.306	854	856	857	rBV	185	120	0.02%	0.002%
36	6.373	866	867	868	rBV	203	115	0.02%	0.002%

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 Title : VOC Analysis

37	6.397	869	871	872	rVB2	338	195	0.03%	0.003%
38	6.495	886	887	890	rVV	220	128	0.02%	0.002%
39	6.556	893	897	900	rVB2	206	307	0.04%	0.006%
40	6.598	900	904	905	rBV2	128	164	0.02%	0.003%
41	6.757	920	930	948	rBV	228800	556464	78.48%	9.972%
42	7.117	984	989	995	rVB5	1014	2324	0.33%	0.042%
43	7.214	1001	1005	1008	rBV3	628	874	0.12%	0.016%
44	7.306	1012	1020	1040	rVV	139292	310773	43.83%	5.569%
45	7.488	1047	1050	1051	rBV2	306	326	0.05%	0.006%
46	7.958	1123	1127	1131	rBV5	685	1349	0.19%	0.024%
47	8.153	1157	1159	1162	rBV2	157	187	0.03%	0.003%
48	8.324	1181	1187	1202	rBV	75720	130605	18.42%	2.340%
49	8.647	1231	1240	1249	rBV	360477	571118	80.55%	10.234%
50	8.952	1285	1290	1309	rVB	53412	84105	11.86%	1.507%
51	9.275	1340	1343	1348	rBV3	1061	1423	0.20%	0.025%
52	9.317	1348	1350	1353	rVB2	146	143	0.02%	0.003%
53	9.354	1353	1356	1357	rBV2	150	174	0.02%	0.003%
54	9.391	1357	1362	1384	rBV	158714	321402	45.33%	5.759%
55	9.628	1399	1401	1403	rBV2	332	219	0.03%	0.004%
56	9.708	1410	1414	1419	rVV2	2077	3170	0.45%	0.057%
57	9.762	1422	1423	1427	rVB	247	182	0.03%	0.003%
58	9.897	1443	1445	1451	rVB2	233	284	0.04%	0.005%
59	9.939	1451	1452	1454	rBV	214	129	0.02%	0.002%
60	10.055	1465	1471	1488	rBV	466810	638697	90.08%	11.445%
61	10.311	1509	1513	1518	rVB3	873	1491	0.21%	0.027%
62	10.488	1540	1542	1544	rBV	123	119	0.02%	0.002%
63	10.512	1544	1546	1549	rBV	153	158	0.02%	0.003%
64	10.640	1566	1567	1572	rBV3	236	308	0.04%	0.006%
65	10.756	1585	1586	1590	rBV2	158	174	0.02%	0.003%
66	10.866	1601	1604	1606	rBV	165	219	0.03%	0.004%
67	10.896	1606	1609	1612	rBV2	185	269	0.04%	0.005%
68	10.976	1619	1622	1624	rVB3	308	330	0.05%	0.006%
69	11.079	1637	1639	1640	rBV	176	117	0.02%	0.002%
70	11.195	1652	1658	1668	rBV	265342	352010	49.65%	6.308%
71	11.378	1686	1688	1690	rBV	137	142	0.02%	0.003%
72	11.396	1690	1691	1694	rVV	193	182	0.03%	0.003%
73	11.451	1699	1700	1702	rBV2	150	136	0.02%	0.002%
74	11.488	1702	1706	1708	rVB2	496	480	0.07%	0.009%
75	11.567	1717	1719	1721	rVB2	192	161	0.02%	0.003%
76	11.634	1728	1730	1732	rVB	184	139	0.02%	0.002%

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77	11.689	1737	1739	1741	rVV2	125	133	0.02%	0.002%
78	11.713	1741	1743	1745	rVV	246	265	0.04%	0.005%
79	11.750	1745	1749	1754	rVV3	774	1120	0.16%	0.020%
80	11.939	1778	1780	1781	rBV2	601	381	0.05%	0.007%
81	12.024	1788	1794	1810	rBV	472722	614781	86.71%	11.017%
82	12.207	1823	1824	1826	rBV	164	134	0.02%	0.002%
83	12.231	1826	1828	1830	rVB2	428	356	0.05%	0.006%
84	12.317	1837	1842	1854	rBV	381287	514907	72.62%	9.227%
85	12.549	1877	1880	1883	rBV2	242	331	0.05%	0.006%
86	12.756	1912	1914	1915	rBV	383	244	0.03%	0.004%
87	12.878	1930	1934	1940	rVV3	786	1047	0.15%	0.019%
88	13.042	1959	1961	1963	rVB2	219	168	0.02%	0.003%
89	13.250	1993	1995	1996	rBV	191	144	0.02%	0.003%
90	13.384	2016	2017	2019	rVV	162	149	0.02%	0.003%
91	13.414	2019	2022	2026	rVB4	439	585	0.08%	0.010%
92	13.506	2034	2037	2038	rBV2	176	176	0.02%	0.003%
93	13.524	2038	2040	2043	rBV2	146	165	0.02%	0.003%
94	13.652	2058	2061	2062	rBV	141	146	0.02%	0.003%
95	13.780	2077	2082	2088	rBV	11375	16269	2.29%	0.292%
96	14.042	2120	2125	2128	rBV2	576	712	0.10%	0.013%
97	14.134	2134	2140	2142	rBV	1092	1572	0.22%	0.028%
98	14.213	2151	2153	2157	rBV2	339	356	0.05%	0.006%
99	14.438	2185	2190	2193	rBV4	860	1358	0.19%	0.024%
100	14.646	2220	2224	2228	rBV2	2233	2946	0.42%	0.053%

Sum of corrected areas: 5580434

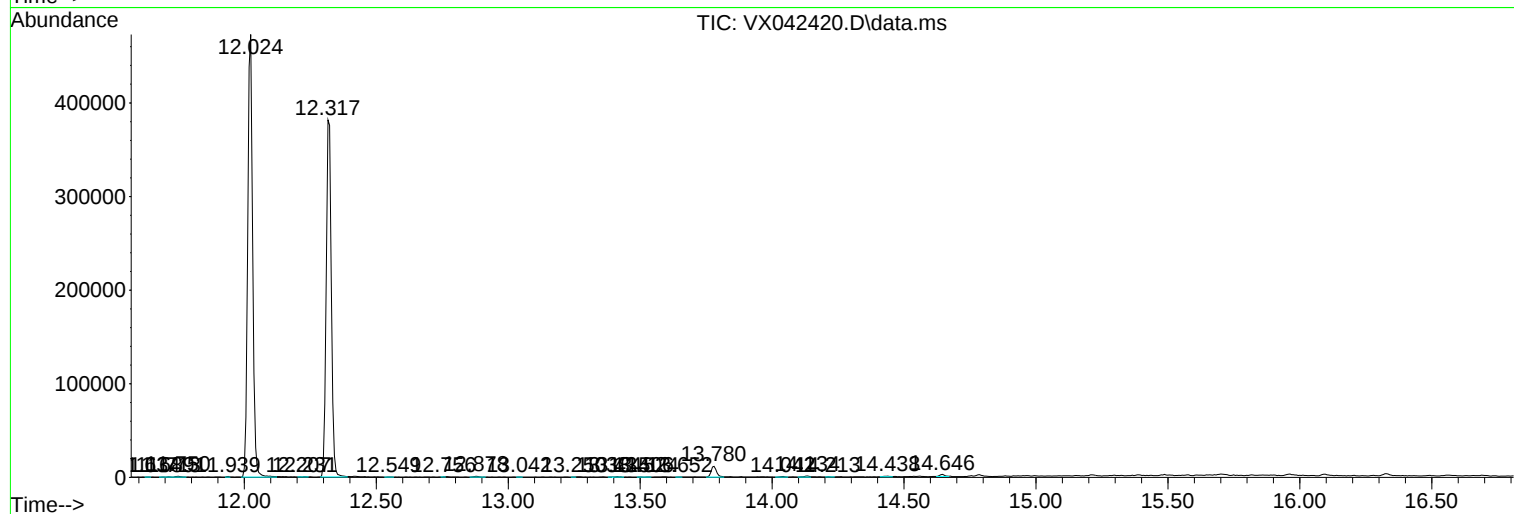
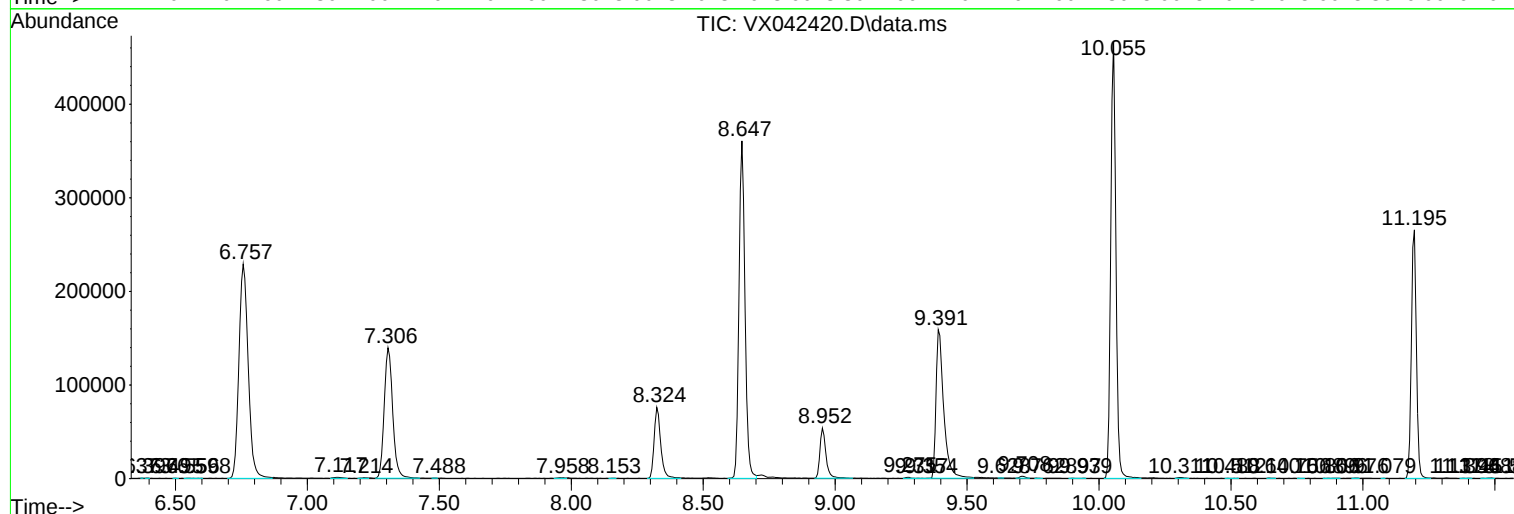
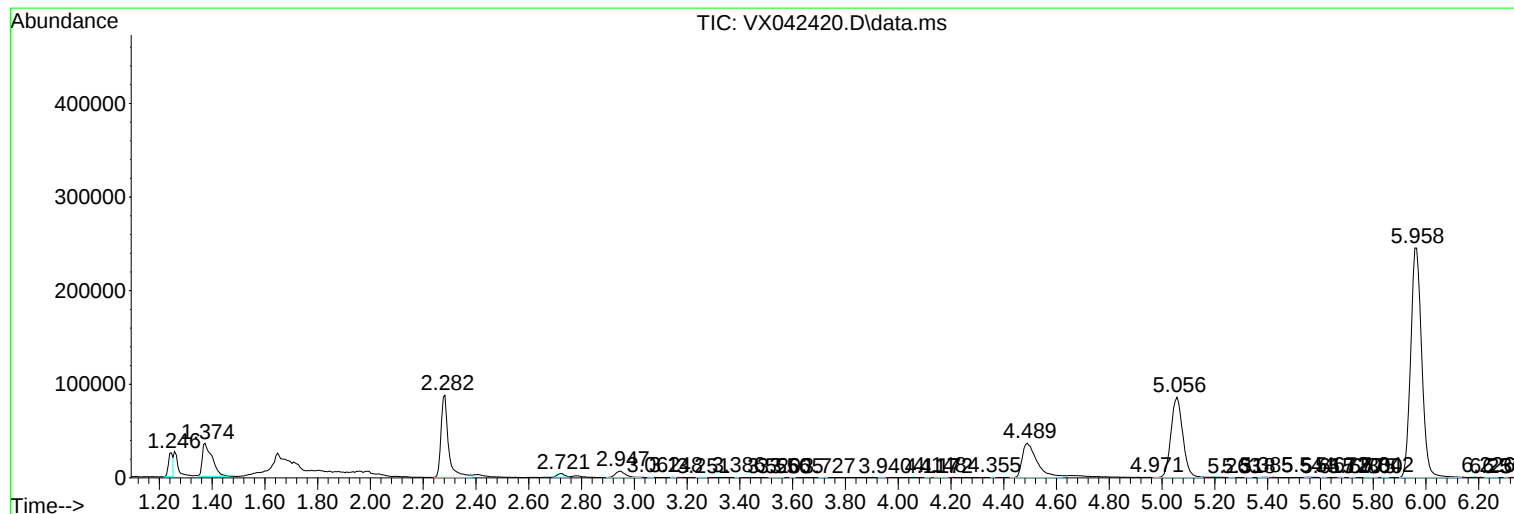
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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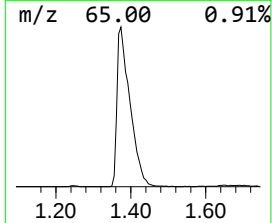
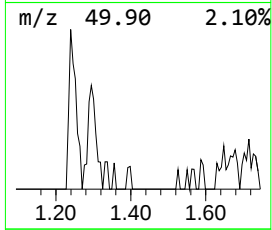
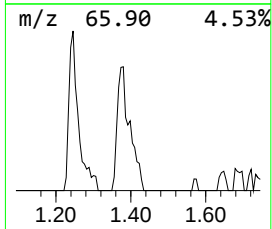
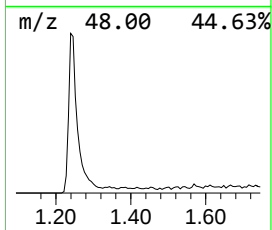
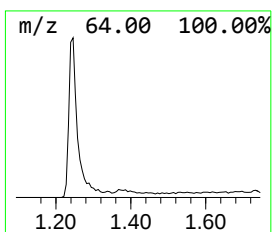
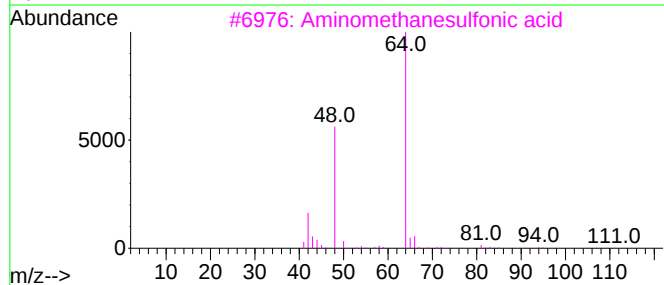
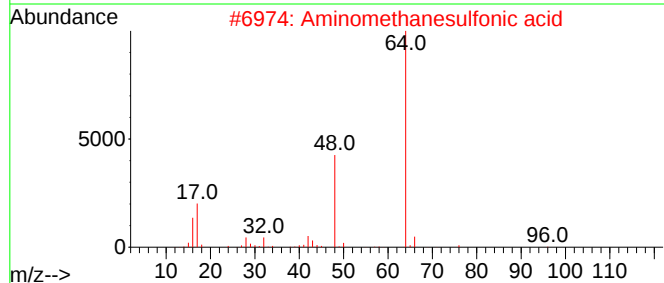
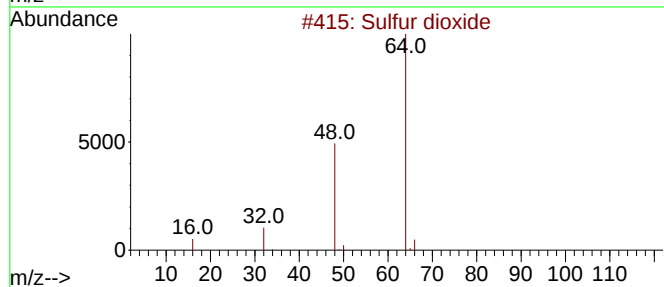
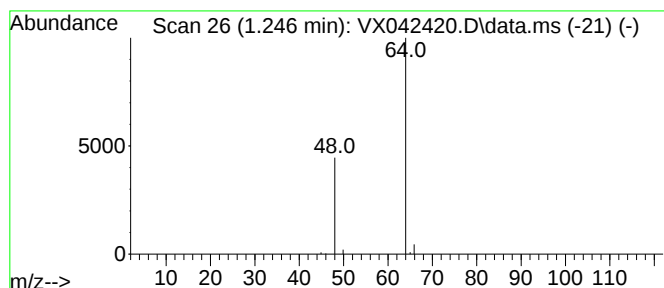
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.246	2.81 ug/L	31267	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	1.246	2.8	ug/L	31267	1	6.757	556464	50.0