

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042421.D
 Acq On : 19 Jul 2024 22:44
 Operator : JC/MD
 Sample : P3298-10 100X
 Misc : 6.45g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB30

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: VX042421.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	38	rBV	36828	51982	7.32%	0.913%
2	1.368	43	46	56	rVB	72198	88591	12.48%	1.556%
3	1.648	88	92	102	rVB	49048	67840	9.56%	1.192%
4	2.294	192	198	210	rBV	147501	228474	32.19%	4.013%
5	2.575	242	244	246	rBV	209	165	0.02%	0.003%
6	2.642	253	255	258	rVB2	155	180	0.03%	0.003%
7	2.678	258	261	262	rVB	133	122	0.02%	0.002%
8	2.697	262	264	265	rBV	331	285	0.04%	0.005%
9	2.782	274	278	285	rVB3	797	1611	0.23%	0.028%
10	2.843	285	288	289	rBV2	128	138	0.02%	0.002%
11	2.947	296	305	314	rBV2	2268	5264	0.74%	0.092%
12	3.026	316	318	321	rVB2	154	155	0.02%	0.003%
13	3.264	356	357	359	rBV	147	128	0.02%	0.002%
14	3.593	409	411	413	rBV2	117	110	0.02%	0.002%
15	3.721	430	432	433	rBV	186	107	0.02%	0.002%
16	3.892	458	460	462	rBV	155	136	0.02%	0.002%
17	3.977	472	474	478	rBV2	115	149	0.02%	0.003%
18	4.105	492	495	496	rBV2	130	112	0.02%	0.002%
19	4.135	498	500	501	rVB	211	127	0.02%	0.002%
20	4.160	501	504	507	rBV2	169	271	0.04%	0.005%
21	4.349	532	535	538	rVB2	156	181	0.03%	0.003%
22	4.465	544	554	572	rBV	49584	153668	21.65%	2.699%
23	4.788	604	607	614	rBV3	215	522	0.07%	0.009%
24	4.904	624	626	629	rBV	152	116	0.02%	0.002%
25	4.971	635	637	639	rBV2	153	153	0.02%	0.003%
26	5.056	639	651	671	rBV2	89106	273405	38.52%	4.802%
27	5.391	703	706	709	rBV3	323	496	0.07%	0.009%
28	5.495	720	723	724	rBV	229	201	0.03%	0.004%
29	5.513	724	726	728	rBV2	154	133	0.02%	0.002%
30	5.538	728	730	731	rBV	176	139	0.02%	0.002%
31	5.647	745	748	750	rBV2	201	258	0.04%	0.005%
32	5.800	771	773	777	rBV2	76	103	0.01%	0.002%
33	5.964	789	800	823	rBV2	242257	709716	100.00%	12.466%
34	6.263	847	849	850	rVB2	245	149	0.02%	0.003%
35	6.367	864	866	869	rBV2	252	300	0.04%	0.005%
36	6.470	880	883	884	rBV2	98	111	0.02%	0.002%

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 Title : VOC Analysis

37	6.623	905	908	910	rBV2	180	188	0.03%	0.003%
38	6.672	914	916	918	rVB	158	124	0.02%	0.002%
39	6.757	921	930	950	rBV	220079	531696	74.92%	9.339%
40	7.068	979	981	983	rBV2	148	136	0.02%	0.002%
41	7.117	983	989	998	rVB7	1693	4714	0.66%	0.083%
42	7.208	1000	1004	1005	rBV3	413	443	0.06%	0.008%
43	7.306	1012	1020	1038	rBV	141798	314501	44.31%	5.524%
44	7.458	1043	1045	1047	rBV2	214	190	0.03%	0.003%
45	7.952	1122	1126	1127	rBV2	562	705	0.10%	0.012%
46	8.104	1149	1151	1155	rBV2	159	239	0.03%	0.004%
47	8.245	1172	1174	1177	rBV	170	120	0.02%	0.002%
48	8.324	1181	1187	1201	rBV	76871	132189	18.63%	2.322%
49	8.647	1234	1240	1255	rBV	366998	578810	81.56%	10.166%
50	8.952	1285	1290	1305	rBV	54650	85367	12.03%	1.499%
51	9.086	1311	1312	1315	rVB2	136	121	0.02%	0.002%
52	9.159	1322	1324	1325	rBV	186	136	0.02%	0.002%
53	9.275	1338	1343	1356	rVB	38240	55952	7.88%	0.983%
54	9.385	1356	1361	1378	rBV	214948	330852	46.62%	5.811%
55	9.659	1404	1406	1410	rVB3	198	159	0.02%	0.003%
56	9.702	1410	1413	1417	rVV3	660	889	0.13%	0.016%
57	9.738	1417	1419	1422	rVB2	189	172	0.02%	0.003%
58	9.921	1447	1449	1450	rBV2	161	135	0.02%	0.002%
59	10.055	1465	1471	1491	rBV	444261	620266	87.40%	10.895%
60	10.269	1505	1506	1509	rBV2	212	195	0.03%	0.003%
61	10.311	1509	1513	1516	rVV3	626	897	0.13%	0.016%
62	10.342	1516	1518	1521	rVB2	128	140	0.02%	0.002%
63	10.445	1532	1535	1539	rBV	152	262	0.04%	0.005%
64	10.647	1564	1568	1572	rBV3	221	340	0.05%	0.006%
65	10.726	1579	1581	1582	rBV	226	110	0.02%	0.002%
66	10.775	1587	1589	1591	rVB2	118	102	0.01%	0.002%
67	10.836	1596	1599	1600	rVV2	125	106	0.01%	0.002%
68	10.866	1600	1604	1605	rVB2	182	199	0.03%	0.003%
69	10.927	1611	1614	1615	rBV	135	108	0.02%	0.002%
70	10.964	1618	1620	1621	rBV2	162	147	0.02%	0.003%
71	11.073	1636	1638	1641	rBV2	134	169	0.02%	0.003%
72	11.189	1652	1657	1670	rBV	275909	362700	51.10%	6.371%
73	11.567	1717	1719	1722	rBV	108	101	0.01%	0.002%
74	11.598	1722	1724	1727	rVV	144	146	0.02%	0.003%
75	11.628	1727	1729	1733	rVB2	209	293	0.04%	0.005%
76	11.713	1737	1743	1746	rBV2	206	267	0.04%	0.005%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.756	1749	1750	1753	rVV2	204	160	0.02%	0.003%
78	11.957	1780	1783	1784	rBV2	125	130	0.02%	0.002%
79	12.024	1788	1794	1806	rBV	438251	571661	80.55%	10.041%
80	12.238	1827	1829	1831	rVB	229	129	0.02%	0.002%
81	12.317	1837	1842	1852	rBV	383252	506353	71.35%	8.894%
82	12.543	1878	1879	1881	rBV2	164	116	0.02%	0.002%
83	12.689	1900	1903	1904	rBV2	172	125	0.02%	0.002%
84	12.762	1912	1915	1921	rBV4	502	871	0.12%	0.015%
85	13.036	1957	1960	1961	rBV2	200	270	0.04%	0.005%
86	13.292	1998	2002	2004	rBV	209	227	0.03%	0.004%
87	13.353	2011	2012	2016	rVB2	258	191	0.03%	0.003%
88	13.420	2021	2023	2024	rBV	148	109	0.02%	0.002%
89	13.451	2026	2028	2031	rVV2	161	106	0.01%	0.002%
90	13.518	2037	2039	2040	rBV2	192	157	0.02%	0.003%
91	13.640	2057	2059	2061	rBV	171	147	0.02%	0.003%
92	13.719	2070	2072	2075	rBV	212	229	0.03%	0.004%
93	13.780	2080	2082	2083	rBV2	264	217	0.03%	0.004%
94	13.835	2089	2091	2094	rBV3	152	152	0.02%	0.003%
95	13.920	2103	2105	2108	rBV2	110	105	0.01%	0.002%
96	14.061	2126	2128	2129	rBV	243	160	0.02%	0.003%
97	14.134	2136	2140	2143	rVB	826	955	0.13%	0.017%
98	14.749	2239	2241	2242	rBV2	325	264	0.04%	0.005%
99	15.140	2304	2305	2307	rVB2	473	228	0.03%	0.004%
100	15.237	2319	2321	2323	rBV2	420	324	0.05%	0.006%

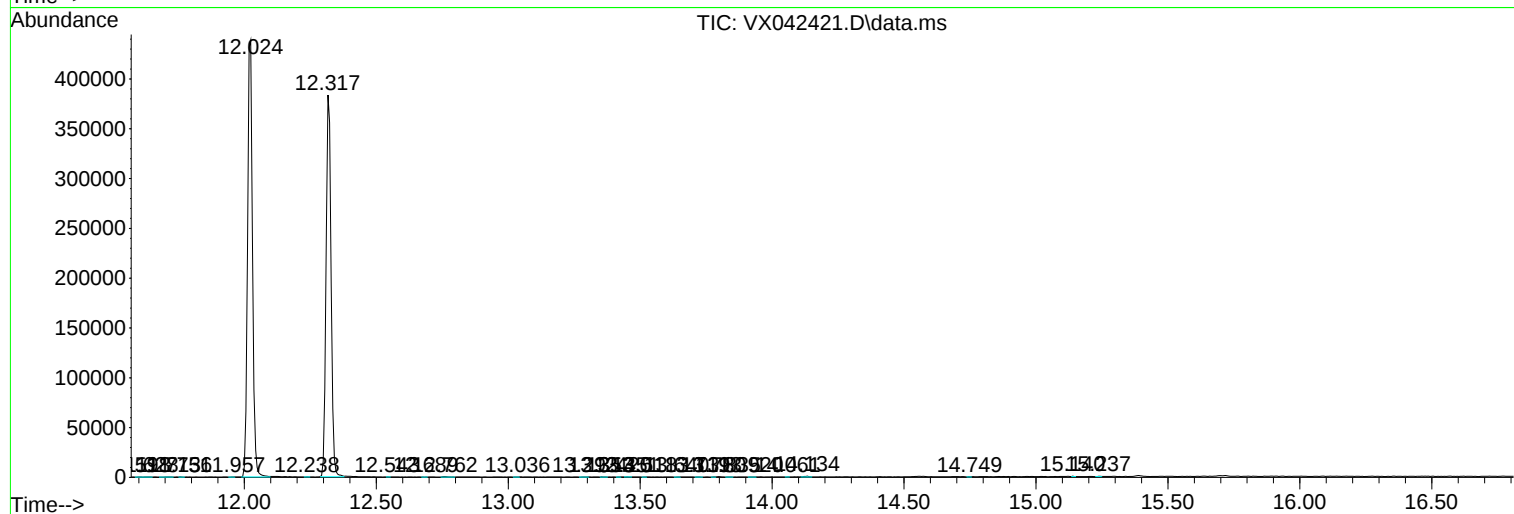
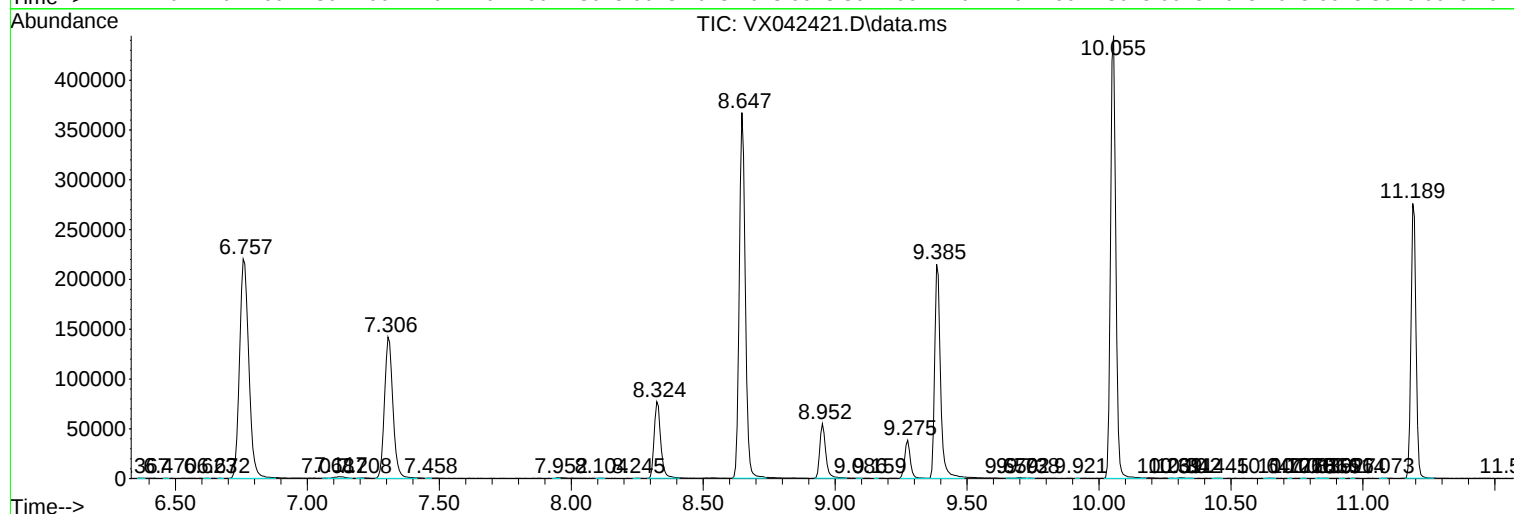
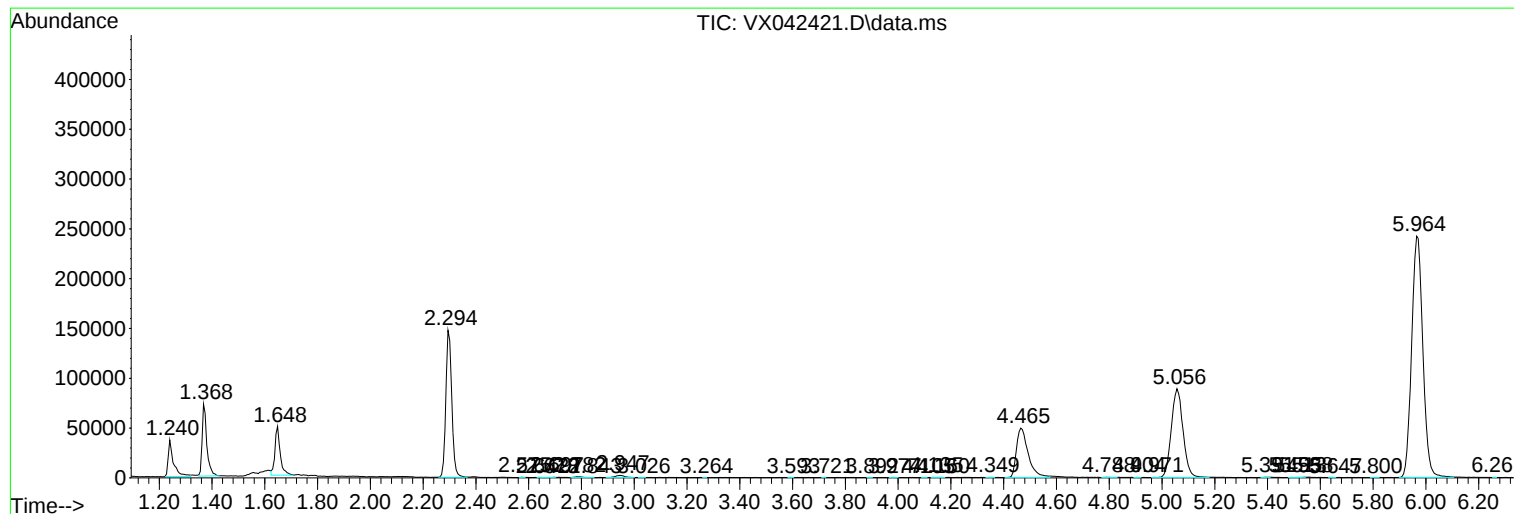
Sum of corrected areas: 5693370

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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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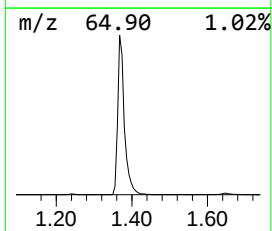
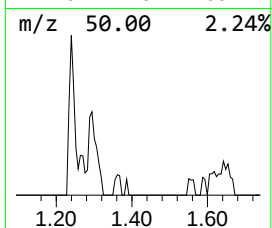
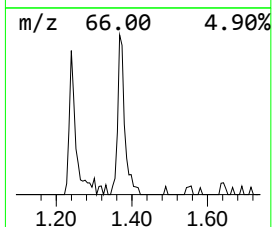
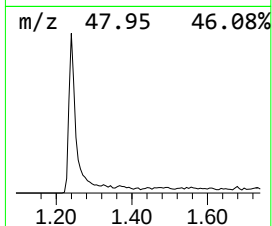
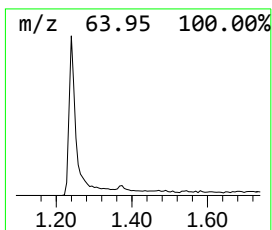
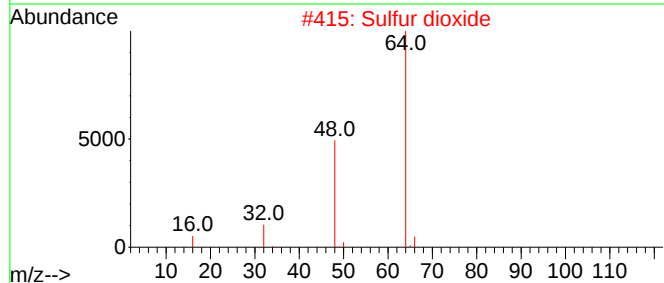
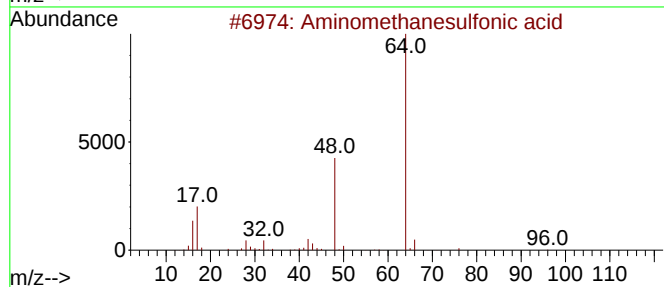
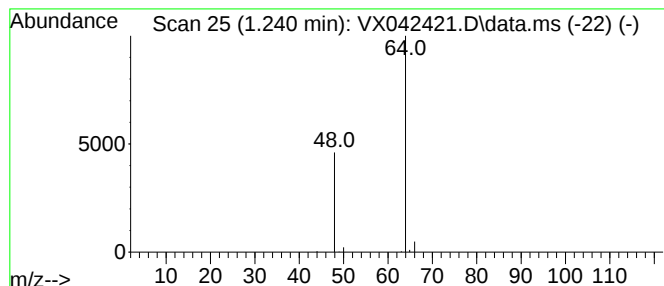
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.89 ug/L	51982	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
2			Sulfur dioxide	64	O2S	007446-09-5	9
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
Aminomethanesul...	1.240	4.9	ug/L	51982	1	6.757	531696	50.0