

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035129.D
 Acq On : 18 Apr 2023 17:37
 Operator : JC/MD
 Sample : 02378-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ8

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\SFAMXML041823WMA.M

Title : VOC Analysis

Signal : TIC: VX035129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	25	29	42	rBV	37661	125056	8.29%	1.053%
2	1.368	43	46	56	rVB	178825	196917	13.05%	1.658%
3	1.672	92	96	107	rVB	121417	160812	10.66%	1.354%
4	2.306	194	200	210	rBV	338511	531301	35.22%	4.474%
5	2.514	230	234	239	rVB2	1230	2215	0.15%	0.019%
6	2.794	273	280	285	rBV4	1201	2502	0.17%	0.021%
7	2.940	296	304	313	rBV	30742	68597	4.55%	0.578%
8	3.087	326	328	333	rVB3	392	430	0.03%	0.004%
9	3.331	364	368	370	rBV	527	610	0.04%	0.005%
10	3.440	384	386	387	rBV2	252	202	0.01%	0.002%
11	3.477	390	392	395	rVV2	228	295	0.02%	0.002%
12	3.501	395	396	402	rVV2	292	497	0.03%	0.004%
13	3.550	402	404	406	rVV2	263	208	0.01%	0.002%
14	3.721	430	432	435	rBV	138	144	0.01%	0.001%
15	3.898	460	461	464	rVB	478	369	0.02%	0.003%
16	3.928	464	466	467	rBV2	144	138	0.01%	0.001%
17	3.946	467	469	470	rBV	256	184	0.01%	0.002%
18	3.989	474	476	479	rBV2	239	342	0.02%	0.003%
19	4.026	479	482	485	rVV2	272	304	0.02%	0.003%
20	4.074	489	490	492	rVV	276	135	0.01%	0.001%
21	4.093	492	493	497	rVV	290	211	0.01%	0.002%
22	4.208	510	512	514	rVB2	319	269	0.02%	0.002%
23	4.239	514	517	519	rBV2	271	251	0.02%	0.002%
24	4.391	540	542	544	rBV	249	183	0.01%	0.002%
25	4.458	544	553	566	rBV	92152	281312	18.65%	2.369%
26	4.934	629	631	632	rBV3	280	246	0.02%	0.002%
27	5.056	638	651	669	rBV	184047	576598	38.22%	4.856%
28	5.281	686	688	689	rBV	242	137	0.01%	0.001%
29	5.391	700	706	707	rBV3	1053	1651	0.11%	0.014%
30	5.659	747	750	752	rVB	328	333	0.02%	0.003%
31	5.690	752	755	757	rBV	417	409	0.03%	0.003%
32	5.757	761	766	768	rBV	253	450	0.03%	0.004%
33	5.775	768	769	772	rVB	278	189	0.01%	0.002%
34	5.970	788	801	819	rBV2	507986	1508640	100.00%	12.705%
35	6.293	852	854	855	rBV	281	131	0.01%	0.001%
36	6.348	861	863	865	rBV	248	211	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

37	6.440	876	878	881	rVV	275	254	0.02%	0.002%
38	6.482	881	885	888	rVB2	377	600	0.04%	0.005%
39	6.513	888	890	892	rBV	221	210	0.01%	0.002%
40	6.550	894	896	901	rVV	457	578	0.04%	0.005%
41	6.586	901	902	905	rVB2	265	138	0.01%	0.001%
42	6.690	917	919	921	rBV	188	182	0.01%	0.002%
43	6.763	921	931	949	rBV	494272	1202088	79.68%	10.124%
44	7.116	983	989	1002	rVB7	2526	6691	0.44%	0.056%
45	7.305	1011	1020	1032	rBV	303856	674242	44.69%	5.678%
46	7.458	1043	1045	1046	rBV2	245	262	0.02%	0.002%
47	7.482	1046	1049	1051	rVV3	883	1098	0.07%	0.009%
48	7.586	1065	1066	1068	rBV2	307	189	0.01%	0.002%
49	7.659	1077	1078	1080	rBV	224	179	0.01%	0.002%
50	7.830	1104	1106	1108	rBV	177	211	0.01%	0.002%
51	7.872	1111	1113	1114	rBV	178	158	0.01%	0.001%
52	7.933	1121	1123	1124	rBV	581	422	0.03%	0.004%
53	8.007	1134	1135	1138	rBV2	310	360	0.02%	0.003%
54	8.324	1180	1187	1200	rBV	171587	286630	19.00%	2.414%
55	8.647	1234	1240	1254	rBV	791420	1244556	82.50%	10.481%
56	8.897	1280	1281	1282	rBV	262	161	0.01%	0.001%
57	8.952	1284	1290	1304	rVV	116406	179844	11.92%	1.515%
58	9.147	1320	1322	1327	rVB2	466	650	0.04%	0.005%
59	9.201	1329	1331	1332	rBV	202	131	0.01%	0.001%
60	9.281	1339	1344	1346	rBV	1685	2055	0.14%	0.017%
61	9.384	1356	1361	1381	rBV	436185	625850	41.48%	5.271%
62	9.707	1412	1414	1421	rVB2	477	656	0.04%	0.006%
63	9.781	1424	1426	1428	rVB2	314	220	0.01%	0.002%
64	9.927	1448	1450	1451	rVB	453	271	0.02%	0.002%
65	9.945	1451	1453	1454	rBV	347	295	0.02%	0.002%
66	10.055	1465	1471	1472	rBV	1031547	1299304	86.12%	10.942%
67	10.299	1509	1511	1516	rBV3	820	1132	0.08%	0.010%
68	10.366	1520	1522	1523	rBV	248	180	0.01%	0.002%
69	10.640	1564	1567	1568	rBV2	495	494	0.03%	0.004%
70	10.963	1616	1620	1622	rBV2	609	768	0.05%	0.006%
71	11.189	1652	1657	1669	rBV	493269	645754	42.80%	5.438%
72	11.317	1674	1678	1682	rVB4	1694	2577	0.17%	0.022%
73	11.372	1682	1687	1689	rBV3	828	1342	0.09%	0.011%
74	11.415	1692	1694	1695	rBV	299	155	0.01%	0.001%
75	11.451	1698	1700	1704	rVB	736	661	0.04%	0.006%
76	11.677	1736	1737	1739	rBV	233	188	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

77	11.756	1748	1750	1753	rVB	468	496	0.03%	0.004%
78	11.853	1764	1766	1768	rVB2	373	250	0.02%	0.002%
79	11.896	1772	1773	1775	rVB2	270	185	0.01%	0.002%
80	11.927	1775	1778	1780	rBV2	363	374	0.02%	0.003%
81	11.969	1780	1785	1788	rBV3	1188	1551	0.10%	0.013%
82	12.024	1788	1794	1805	rBV	963230	1229224	81.48%	10.352%
83	12.219	1823	1826	1832	rBV4	1479	2395	0.16%	0.020%
84	12.317	1837	1842	1849	rBV	751654	989237	65.57%	8.331%
85	12.555	1879	1881	1883	rBV	402	224	0.01%	0.002%
86	12.725	1907	1909	1910	rVB	387	219	0.01%	0.002%
87	12.762	1910	1915	1919	rBV3	871	1188	0.08%	0.010%
88	12.878	1932	1934	1936	rVB2	430	256	0.02%	0.002%
89	13.079	1966	1967	1969	rVB	357	175	0.01%	0.001%
90	13.115	1972	1973	1975	rVB2	589	338	0.02%	0.003%
91	13.213	1988	1989	1990	rBV	330	147	0.01%	0.001%
92	13.250	1993	1995	2000	rBV2	239	332	0.02%	0.003%
93	13.524	2038	2040	2041	rBV2	277	201	0.01%	0.002%
94	13.591	2048	2051	2055	rVB4	1227	1354	0.09%	0.011%
95	13.682	2065	2066	2069	rVB2	282	242	0.02%	0.002%
96	13.786	2080	2083	2085	rVB2	676	650	0.04%	0.005%
97	13.865	2094	2096	2097	rBV	335	261	0.02%	0.002%
98	13.908	2101	2103	2104	rBV	234	181	0.01%	0.002%
99	14.146	2141	2142	2143	rVB	378	138	0.01%	0.001%
100	14.536	2204	2206	2207	rBV2	301	146	0.01%	0.001%

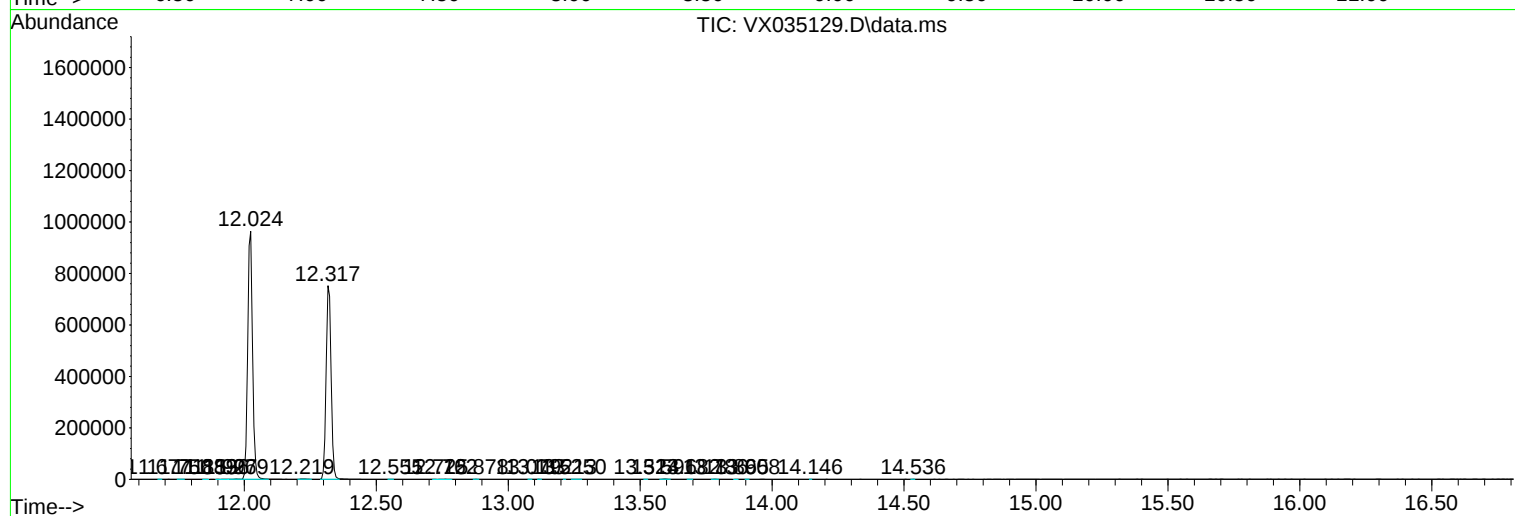
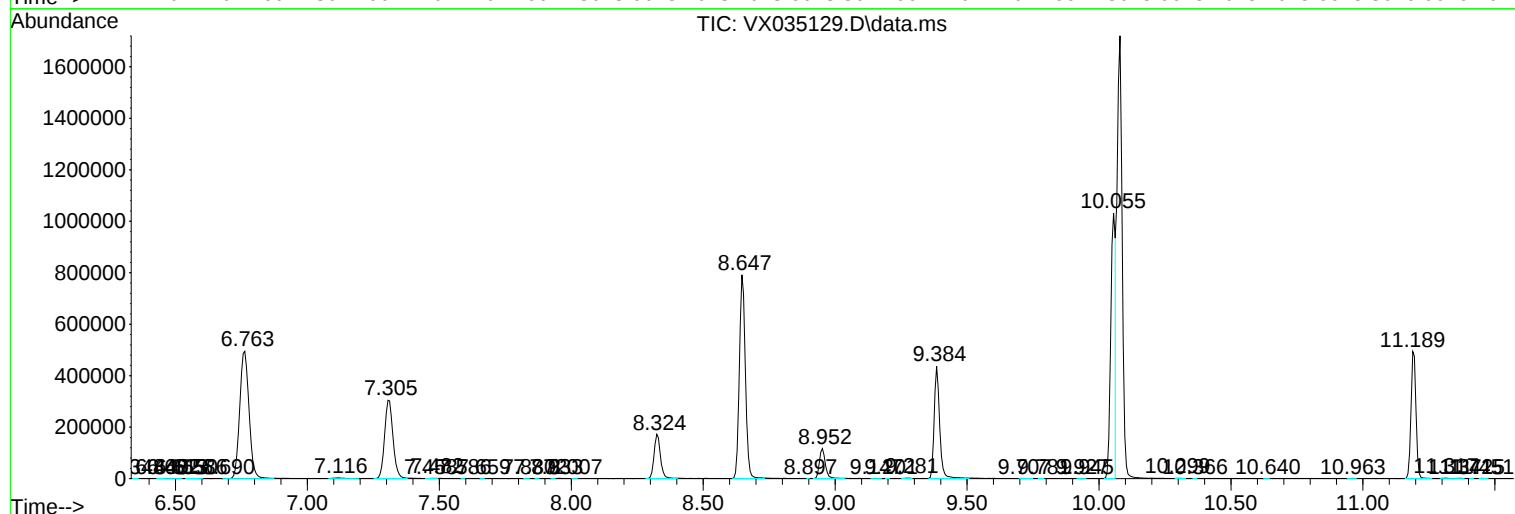
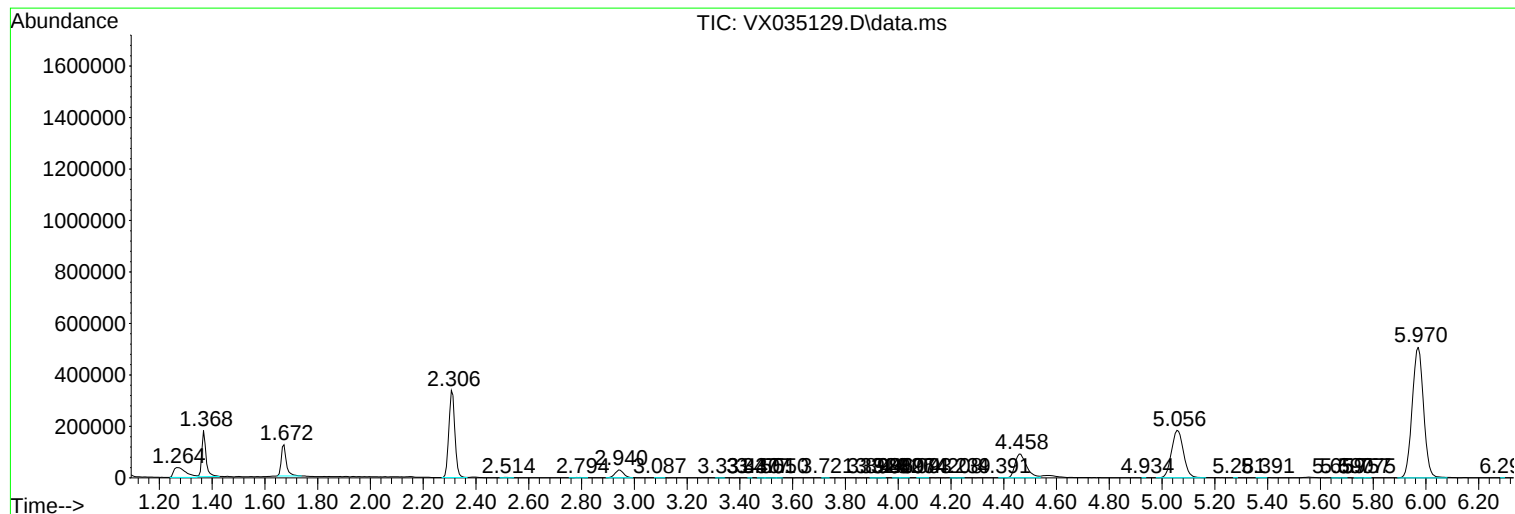
Sum of corrected areas: 11873979

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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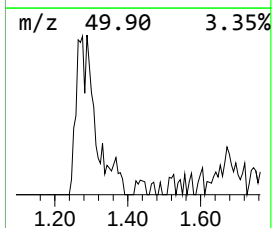
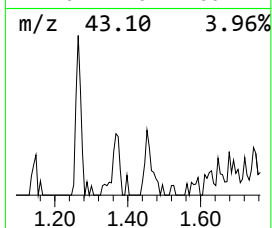
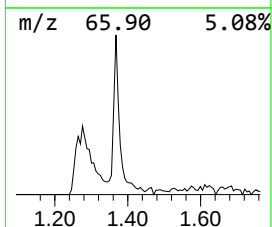
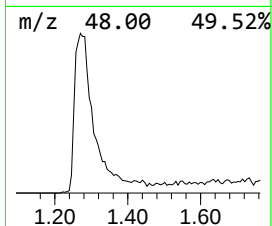
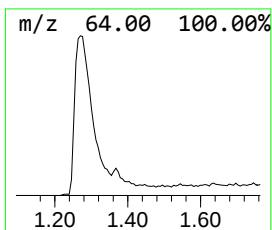
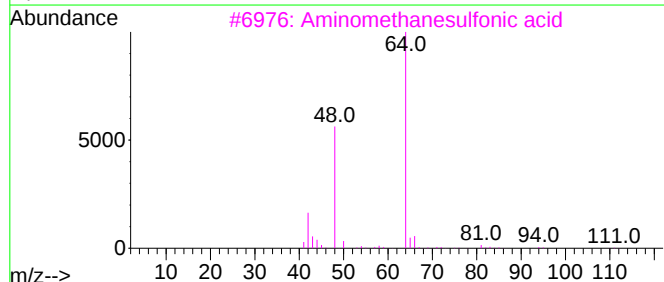
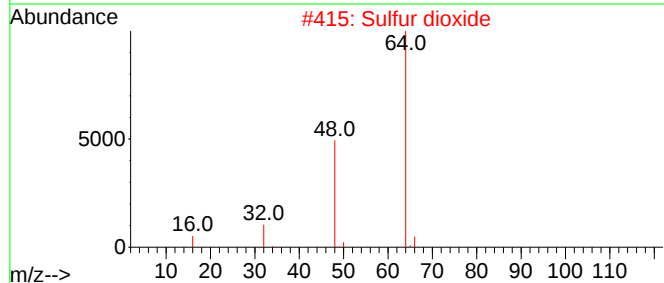
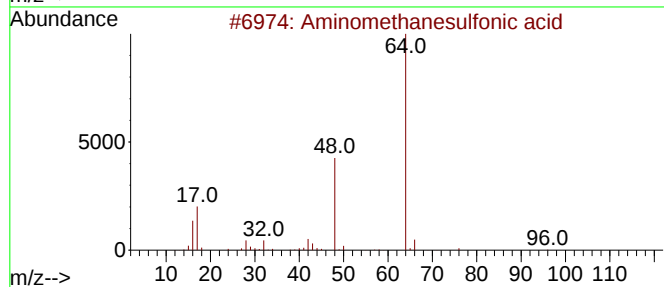
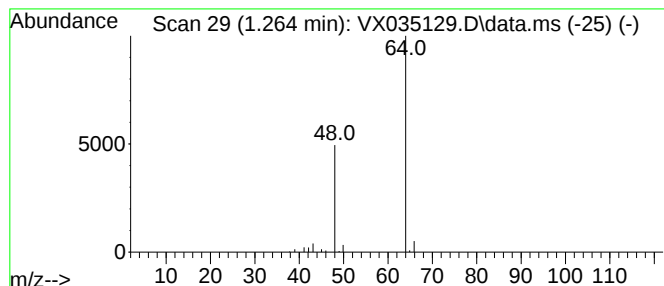
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.20 ug/L	125056	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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
Aminomethanesul...	1.264	5.2	ug/L	125056	1	6.763	1202090	50.0