

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035137.D
 Acq On : 18 Apr 2023 21:05
 Operator : JC/MD
 Sample : 02397-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COML3

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: VX035137.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	24	29	43	rBV	50232	165778	7.99%	1.122%
2	1.367	43	46	63	rVB	264245	292611	14.10%	1.980%
3	1.672	92	96	115	rVB	180400	246929	11.90%	1.671%
4	2.306	194	200	211	rBV	466089	729196	35.13%	4.934%
5	2.513	230	234	239	rVB2	1414	2187	0.11%	0.015%
6	2.788	275	279	286	rVB5	1277	2254	0.11%	0.015%
7	2.934	299	303	304	rBV3	500	557	0.03%	0.004%
8	2.995	311	313	316	rBV2	236	280	0.01%	0.002%
9	3.160	337	340	343	rVB2	316	394	0.02%	0.003%
10	3.184	343	344	347	rBV2	318	357	0.02%	0.002%
11	3.282	357	360	361	rBV2	185	195	0.01%	0.001%
12	3.477	390	392	396	rBV2	325	395	0.02%	0.003%
13	3.513	396	398	400	rVB	418	316	0.02%	0.002%
14	3.538	400	402	405	rBV2	292	267	0.01%	0.002%
15	3.568	405	407	409	rBV	208	200	0.01%	0.001%
16	3.593	409	411	413	rVV	336	215	0.01%	0.001%
17	3.647	418	420	425	rVB2	204	268	0.01%	0.002%
18	3.721	430	432	434	rVB	203	200	0.01%	0.001%
19	3.751	434	437	439	rBV	216	204	0.01%	0.001%
20	3.861	453	455	458	rVB	265	199	0.01%	0.001%
21	4.233	513	516	518	rVB3	562	644	0.03%	0.004%
22	4.275	520	523	525	rBV2	288	386	0.02%	0.003%
23	4.312	527	529	530	rBV	345	244	0.01%	0.002%
24	4.373	537	539	541	rVB	272	197	0.01%	0.001%
25	4.464	544	554	581	rBV	127536	396485	19.10%	2.683%
26	4.751	598	601	602	rBV2	364	337	0.02%	0.002%
27	5.062	637	652	674	rBV	262488	828902	39.93%	5.609%
28	5.379	702	704	705	rBV2	307	226	0.01%	0.002%
29	5.482	719	721	724	rVB	610	363	0.02%	0.002%
30	5.550	726	732	740	rBV4	1150	3405	0.16%	0.023%
31	5.610	740	742	744	rVB	329	221	0.01%	0.001%
32	5.702	755	757	760	rVB2	235	200	0.01%	0.001%
33	5.732	760	762	764	rVB2	236	212	0.01%	0.001%
34	5.787	767	771	773	rBV2	382	581	0.03%	0.004%
35	5.970	788	801	819	rBV2	693640	2075818	100.00%	14.046%
36	6.318	856	858	861	rVB2	384	330	0.02%	0.002%

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

37	6.476	882	884	887	rBV	235	279	0.01%	0.002%
38	6.543	891	895	896	rBV2	248	276	0.01%	0.002%
39	6.555	896	897	899	rVB2	423	230	0.01%	0.002%
40	6.763	919	931	949	rBV	471413	1141510	54.99%	7.724%
41	7.116	983	989	999	rVB3	3551	7773	0.37%	0.053%
42	7.305	1010	1020	1043	rBV	417061	929775	44.79%	6.291%
43	7.470	1045	1047	1048	rBV	669	572	0.03%	0.004%
44	7.628	1071	1073	1076	rVB2	332	364	0.02%	0.002%
45	7.689	1080	1083	1085	rBV2	357	353	0.02%	0.002%
46	7.781	1095	1098	1099	rBV	336	307	0.01%	0.002%
47	7.836	1105	1107	1108	rBV	361	302	0.01%	0.002%
48	7.945	1121	1125	1130	rVV5	1248	2341	0.11%	0.016%
49	8.159	1159	1160	1163	rVB2	312	230	0.01%	0.002%
50	8.208	1166	1168	1170	rBV	226	205	0.01%	0.001%
51	8.323	1181	1187	1200	rBV	255506	423177	20.39%	2.863%
52	8.500	1212	1216	1222	rVB5	1112	2029	0.10%	0.014%
53	8.647	1233	1240	1257	rBV	1064913	1683593	81.11%	11.392%
54	8.951	1284	1290	1299	rBV	180018	266099	12.82%	1.801%
55	9.177	1325	1327	1331	rVB2	267	293	0.01%	0.002%
56	9.274	1339	1343	1348	rVB4	1487	2028	0.10%	0.014%
57	9.384	1356	1361	1381	rBV	606077	866556	41.75%	5.863%
58	9.671	1407	1408	1411	rBV	212	195	0.01%	0.001%
59	9.695	1411	1412	1414	rBV2	302	215	0.01%	0.001%
60	9.866	1438	1440	1444	rVB2	401	379	0.02%	0.003%
61	9.902	1444	1446	1449	rBV2	234	243	0.01%	0.002%
62	9.939	1449	1452	1454	rVV2	334	293	0.01%	0.002%
63	10.055	1465	1471	1487	rBV	926767	1276299	61.48%	8.636%
64	10.274	1506	1507	1508	rBV	353	197	0.01%	0.001%
65	10.305	1510	1512	1515	rVV2	616	844	0.04%	0.006%
66	10.646	1566	1568	1570	rBV2	461	464	0.02%	0.003%
67	10.671	1570	1572	1574	rVB	547	391	0.02%	0.003%
68	10.866	1601	1604	1605	rBV2	632	598	0.03%	0.004%
69	10.927	1612	1614	1617	rBV2	319	234	0.01%	0.002%
70	11.189	1652	1657	1672	rBV	661414	885695	42.67%	5.993%
71	11.317	1676	1678	1681	rVB2	762	632	0.03%	0.004%
72	11.634	1728	1730	1733	rVB2	427	278	0.01%	0.002%
73	11.707	1740	1742	1745	rBV2	721	709	0.03%	0.005%
74	11.756	1748	1750	1752	rBV2	636	725	0.03%	0.005%
75	11.933	1777	1779	1782	rVB2	710	591	0.03%	0.004%
76	11.969	1783	1785	1788	rBV	888	669	0.03%	0.005%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
 Title : VOC Analysis

77	12.024	1788	1794	1806	rBV	903567	1156742	55.72%	7.827%
78	12.219	1823	1826	1837	rBV2	7956	12625	0.61%	0.085%
79	12.317	1837	1842	1854	rBV	1018631	1340837	64.59%	9.073%
80	12.573	1882	1884	1885	rBV	430	264	0.01%	0.002%
81	12.591	1885	1887	1889	rVV	584	454	0.02%	0.003%
82	12.762	1913	1915	1917	rBV3	496	492	0.02%	0.003%
83	12.823	1922	1925	1927	rVV	534	534	0.03%	0.004%
84	12.859	1927	1931	1937	rVB2	4699	6495	0.31%	0.044%
85	13.005	1953	1955	1958	rBV2	247	261	0.01%	0.002%
86	13.073	1963	1966	1969	rBV2	318	496	0.02%	0.003%
87	13.115	1969	1973	1978	rVB5	952	1577	0.08%	0.011%
88	13.158	1978	1980	1981	rBV	424	302	0.01%	0.002%
89	13.292	2000	2002	2004	rBV2	289	284	0.01%	0.002%
90	13.505	2036	2037	2039	rBV	352	235	0.01%	0.002%
91	13.591	2048	2051	2055	rVB2	1773	2049	0.10%	0.014%
92	13.786	2078	2083	2088	rBV3	1227	1874	0.09%	0.013%
93	13.963	2109	2112	2115	rBV3	1178	1398	0.07%	0.009%
94	14.048	2125	2126	2128	rBV2	469	334	0.02%	0.002%
95	14.194	2149	2150	2153	rVB	419	238	0.01%	0.002%
96	14.584	2212	2214	2216	rBV2	407	346	0.02%	0.002%
97	14.761	2241	2243	2245	rBV	483	329	0.02%	0.002%
98	14.901	2264	2266	2269	rBV3	668	458	0.02%	0.003%
99	16.017	2447	2449	2452	rBV2	660	435	0.02%	0.003%
100	16.042	2452	2453	2455	rBV2	785	506	0.02%	0.003%

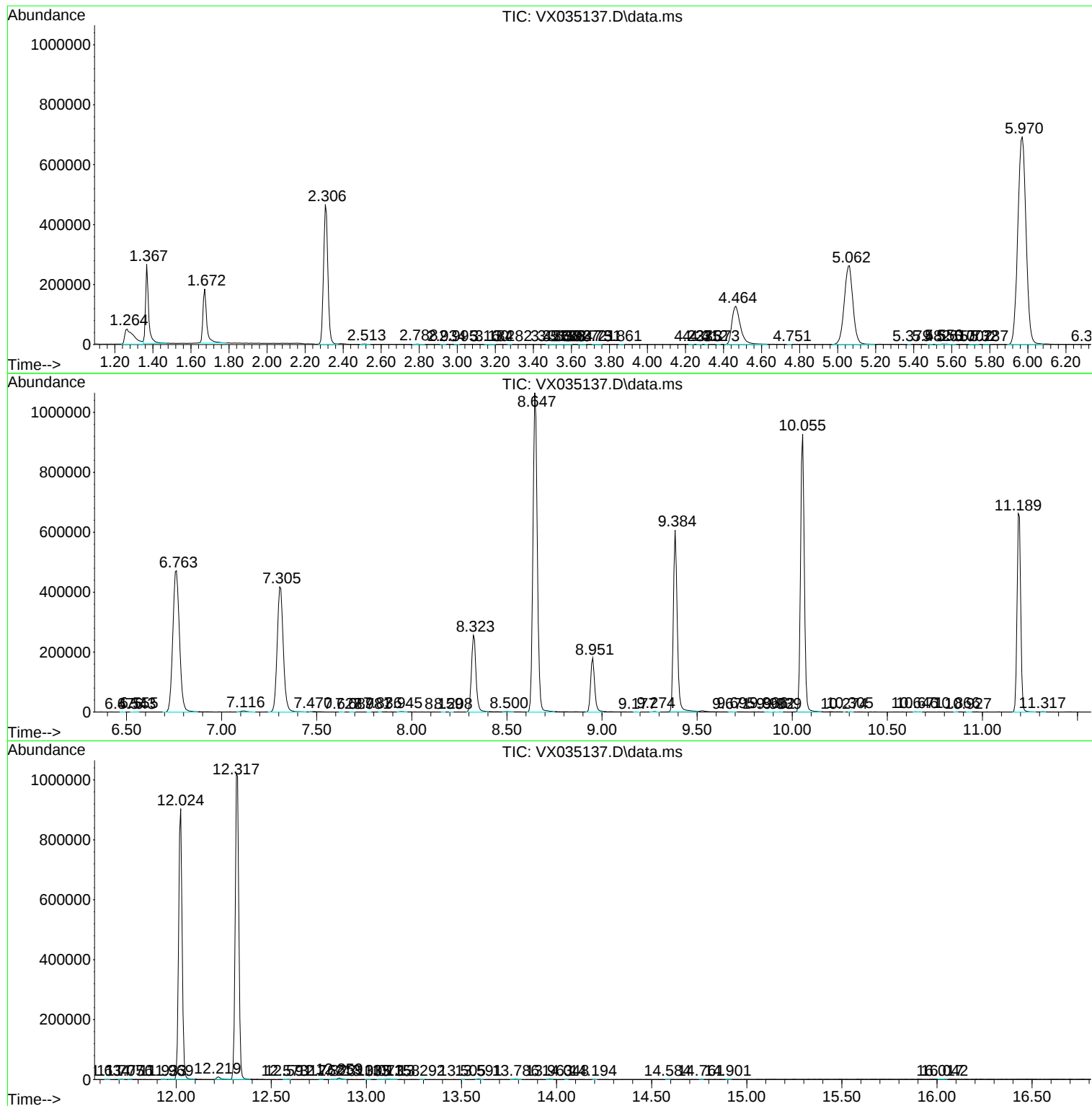
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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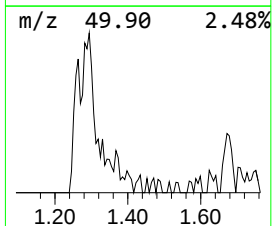
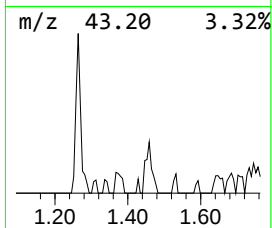
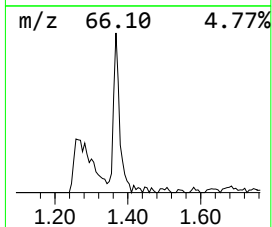
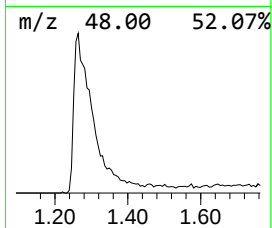
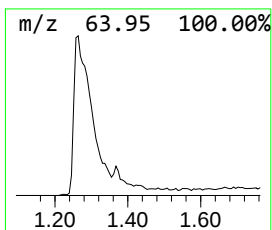
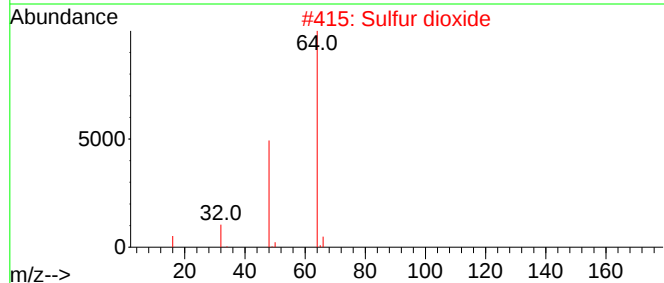
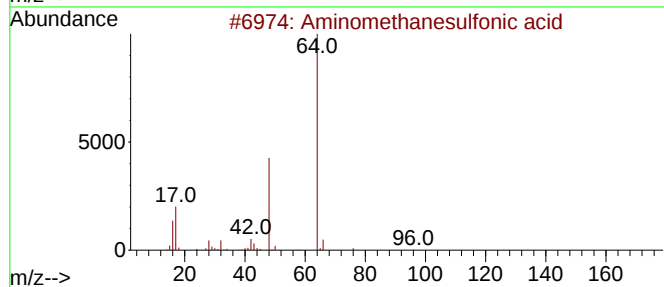
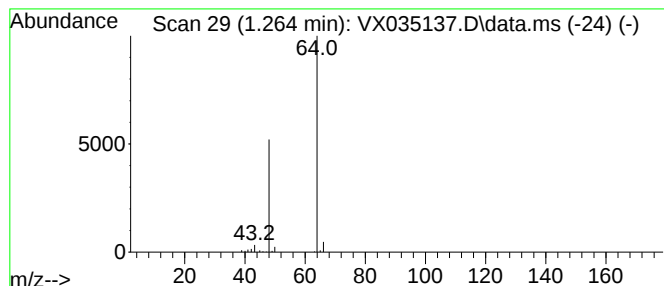
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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	7.26 ug/L	165778	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.264	7.3	ug/L	165778	1	6.763	1141510	50.0