

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035173.D
 Acq On : 19 Apr 2023 16:38
 Operator : JC/MD
 Sample : 02397-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM7

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: VX035173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	29779	28848	1.54%	0.201%
2	1.258	24	28	40	rBV	96663	241294	12.90%	1.680%
3	1.368	42	46	54	rVV	222728	248002	13.26%	1.727%
4	1.672	92	96	106	rBV	160428	202245	10.81%	1.408%
5	2.306	194	200	211	rVB	403120	615842	32.92%	4.288%
6	2.514	231	234	238	rVB2	1219	1794	0.10%	0.012%
7	2.636	250	254	257	rVB2	512	734	0.04%	0.005%
8	2.666	257	259	261	rBV2	297	214	0.01%	0.001%
9	2.721	261	268	272	rBV5	1286	3023	0.16%	0.021%
10	3.014	312	316	318	rBV2	403	629	0.03%	0.004%
11	3.093	325	329	330	rBV2	1136	1488	0.08%	0.010%
12	3.440	381	386	392	rVB5	1561	3445	0.18%	0.024%
13	3.550	399	404	405	rVB3	241	271	0.01%	0.002%
14	3.605	410	413	414	rBV2	443	466	0.02%	0.003%
15	3.666	420	423	426	rBV4	840	940	0.05%	0.007%
16	3.818	445	448	451	rBV3	341	399	0.02%	0.003%
17	3.849	451	453	458	rVV3	195	327	0.02%	0.002%
18	3.959	467	471	476	rVB3	623	1053	0.06%	0.007%
19	4.001	476	478	480	rBV2	251	248	0.01%	0.002%
20	4.105	492	495	497	rVV2	247	241	0.01%	0.002%
21	4.129	497	499	500	rVV	329	216	0.01%	0.002%
22	4.202	508	511	513	rBV	244	300	0.02%	0.002%
23	4.251	517	519	524	rVB2	188	263	0.01%	0.002%
24	4.312	526	529	532	rVB2	337	399	0.02%	0.003%
25	4.465	545	554	573	rBV	115632	359825	19.23%	2.505%
26	4.763	601	603	605	rBV2	348	319	0.02%	0.002%
27	5.056	638	651	668	rBV	230515	713927	38.16%	4.971%
28	5.379	702	704	705	rBV	417	390	0.02%	0.003%
29	5.434	711	713	714	rVB	394	215	0.01%	0.001%
30	5.550	727	732	733	rBV3	1120	1668	0.09%	0.012%
31	5.659	748	750	752	rVB2	445	391	0.02%	0.003%
32	5.678	752	753	758	rBV2	344	509	0.03%	0.004%
33	5.812	773	775	776	rBV2	411	348	0.02%	0.002%
34	5.830	776	778	779	rVB	385	208	0.01%	0.001%
35	5.970	788	801	808	rBV2	621319	1870783	100.00%	13.025%
36	6.275	850	851	854	rVB	447	285	0.02%	0.002%

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

37	6.354	860	864	866	rBV2	229	369	0.02%	0.003%
38	6.519	889	891	892	rBV2	253	221	0.01%	0.002%
39	6.592	901	903	905	rBV2	212	204	0.01%	0.001%
40	6.665	913	915	917	rBV	412	218	0.01%	0.002%
41	6.696	917	920	921	rBV	204	201	0.01%	0.001%
42	6.757	921	930	946	rBV	451432	1093487	58.45%	7.613%
43	7.019	971	973	975	rBV2	358	313	0.02%	0.002%
44	7.068	979	981	984	rBV3	352	348	0.02%	0.002%
45	7.116	984	989	998	rBV7	1269	3166	0.17%	0.022%
46	7.238	1006	1009	1010	rBV2	302	298	0.02%	0.002%
47	7.305	1011	1020	1037	rVV	375478	838824	44.84%	5.840%
48	7.488	1047	1050	1054	rVB4	934	1283	0.07%	0.009%
49	7.641	1074	1075	1078	rBV2	204	204	0.01%	0.001%
50	7.732	1089	1090	1094	rBV2	308	235	0.01%	0.002%
51	7.946	1119	1125	1137	rVV3	1607	3800	0.20%	0.026%
52	8.031	1137	1139	1140	rVB	491	274	0.01%	0.002%
53	8.159	1158	1160	1163	rVB2	202	224	0.01%	0.002%
54	8.189	1163	1165	1168	rBV	269	230	0.01%	0.002%
55	8.226	1168	1171	1173	rBV2	253	230	0.01%	0.002%
56	8.244	1173	1174	1179	rVB2	310	297	0.02%	0.002%
57	8.324	1179	1187	1203	rBV	222098	372611	19.92%	2.594%
58	8.647	1233	1240	1250	rBV	957975	1496677	80.00%	10.421%
59	8.952	1284	1290	1302	rBV	154709	233922	12.50%	1.629%
60	9.238	1335	1337	1339	rBV2	309	201	0.01%	0.001%
61	9.269	1339	1342	1348	rBV4	1144	1579	0.08%	0.011%
62	9.317	1348	1350	1352	rVB2	272	219	0.01%	0.002%
63	9.384	1356	1361	1380	rBV	561410	797417	42.62%	5.552%
64	9.775	1423	1425	1426	rBV	351	274	0.01%	0.002%
65	9.884	1441	1443	1450	rVB2	303	535	0.03%	0.004%
66	9.939	1450	1452	1455	rBV2	281	390	0.02%	0.003%
67	10.055	1465	1471	1473	rBV	950869	1322758	70.71%	9.210%
68	10.232	1498	1500	1503	rBV4	334	280	0.01%	0.002%
69	10.305	1509	1512	1515	rVB2	329	454	0.02%	0.003%
70	10.409	1525	1529	1531	rBV2	351	397	0.02%	0.003%
71	10.488	1540	1542	1543	rBV	348	231	0.01%	0.002%
72	10.610	1560	1562	1563	rVB	400	234	0.01%	0.002%
73	10.634	1563	1566	1569	rBV2	349	446	0.02%	0.003%
74	10.823	1595	1597	1601	rVV2	186	214	0.01%	0.001%
75	11.055	1633	1635	1637	rBV	344	258	0.01%	0.002%
76	11.122	1644	1646	1648	rBV2	220	225	0.01%	0.002%

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 Title : VOC Analysis

77	11.189	1652	1657	1667	rVV	637247	829375	44.33%	5.775%
78	11.390	1685	1690	1692	rVB2	357	446	0.02%	0.003%
79	11.421	1692	1695	1697	rBV2	313	444	0.02%	0.003%
80	11.494	1705	1707	1708	rBV	353	200	0.01%	0.001%
81	11.634	1727	1730	1732	rBV	260	258	0.01%	0.002%
82	11.707	1740	1742	1747	rBV2	924	839	0.04%	0.006%
83	11.969	1781	1785	1789	rBV	30246	37123	1.98%	0.258%
84	12.024	1789	1794	1807	rVB2	916469	1398955	74.78%	9.740%
85	12.219	1822	1826	1833	rBV4	3476	6318	0.34%	0.044%
86	12.323	1837	1843	1854	rVV2	1009249	1515167	80.99%	10.549%
87	12.536	1876	1878	1881	rBV	255	260	0.01%	0.002%
88	12.762	1913	1915	1918	rBB3	332	352	0.02%	0.002%
89	13.115	1971	1973	1975	rVV2	479	377	0.02%	0.003%
90	13.298	1998	2003	2004	rBV2	299	461	0.02%	0.003%
91	13.554	2042	2045	2046	rBV	265	268	0.01%	0.002%
92	13.591	2046	2051	2059	rVV	55018	72962	3.90%	0.508%
93	13.810	2086	2087	2089	rVB	402	200	0.01%	0.001%
94	13.896	2099	2101	2103	rBV	234	239	0.01%	0.002%
95	13.963	2108	2112	2118	rVV	13959	17684	0.95%	0.123%
96	14.091	2130	2133	2137	rBV3	331	516	0.03%	0.004%
97	14.152	2142	2143	2145	rBV2	366	306	0.02%	0.002%
98	14.219	2152	2154	2157	rBV2	243	279	0.01%	0.002%
99	14.707	2230	2234	2236	rBV2	362	510	0.03%	0.004%
100	15.249	2320	2323	2327	rBV5	3045	3799	0.20%	0.026%

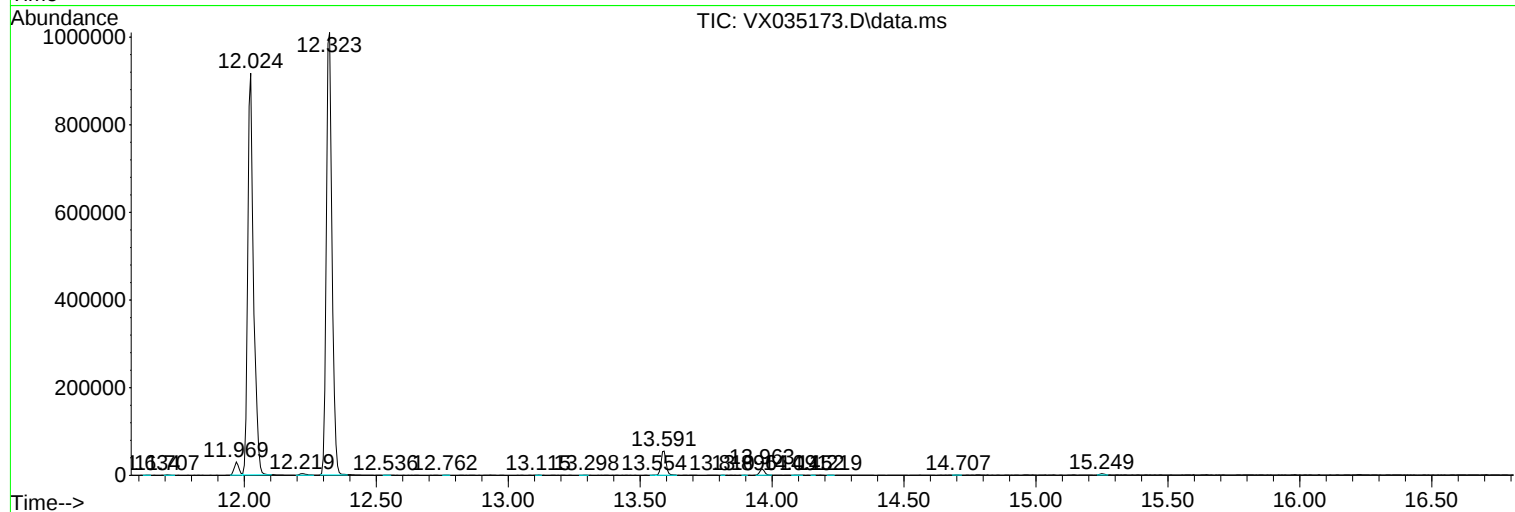
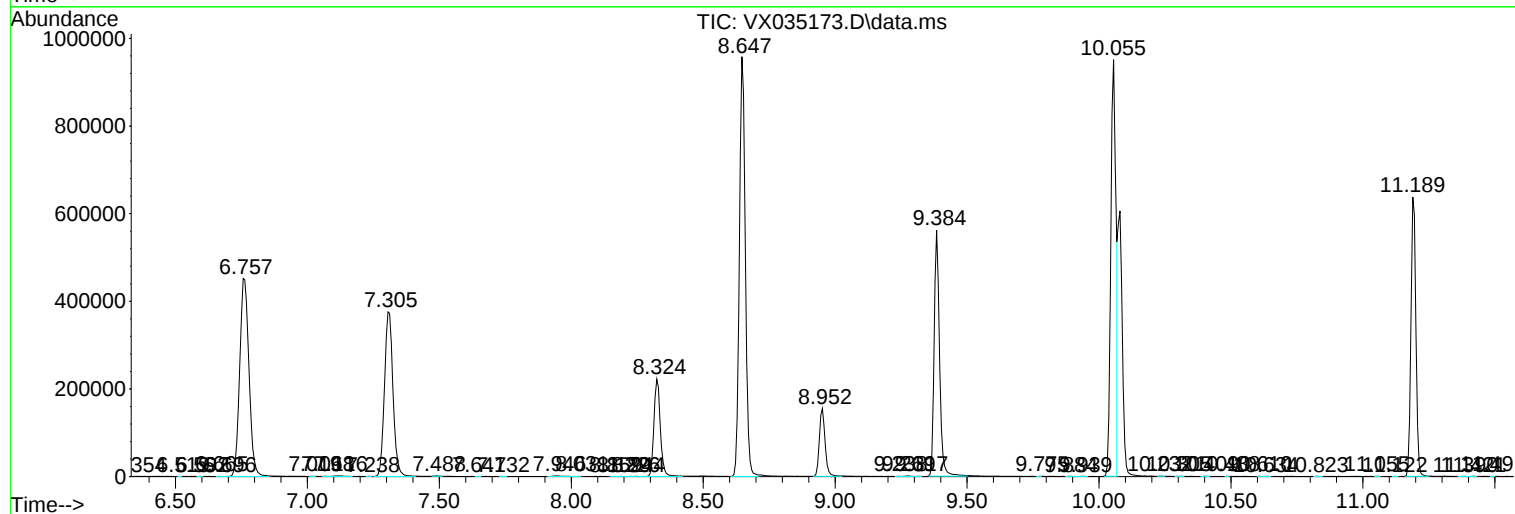
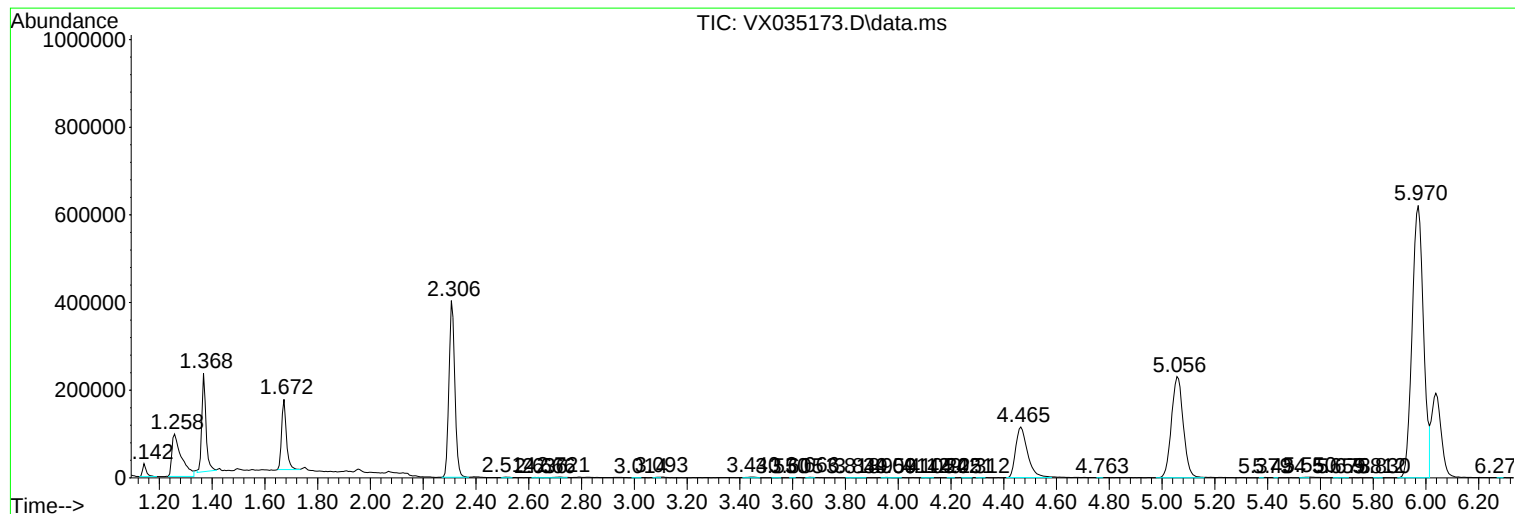
Sum of corrected areas: 14362635

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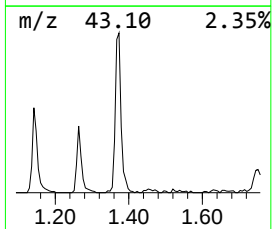
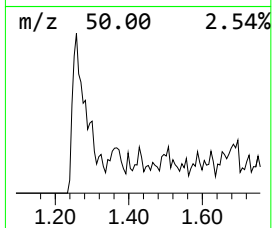
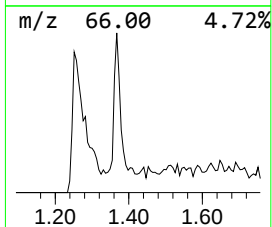
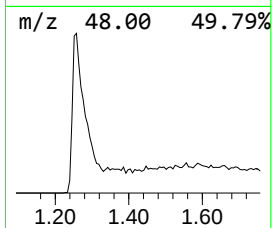
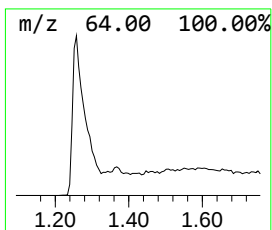
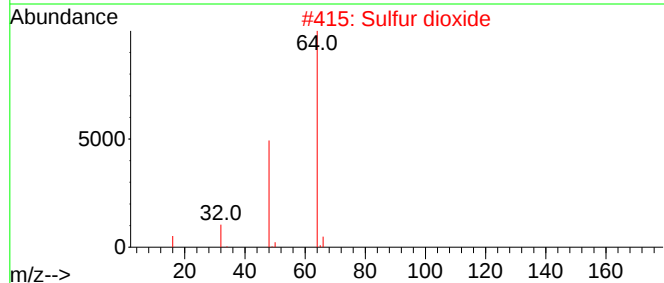
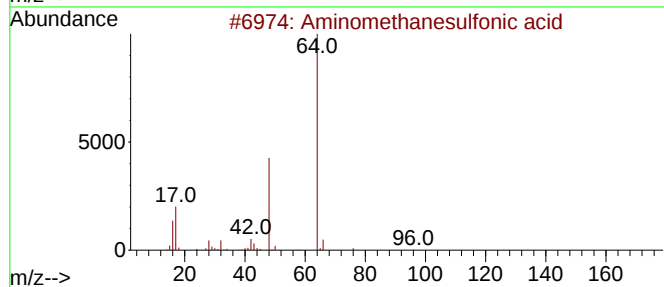
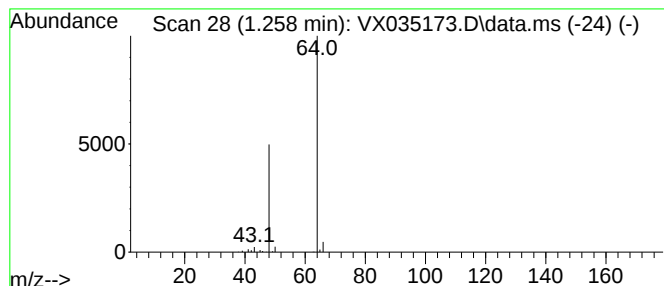
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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.
1.258	11.03 ug/L	241294	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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.258	11.0	ug/L	241294	1	6.763	1093490	50.0