

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035179.D
 Acq On : 19 Apr 2023 18:57
 Operator : JC/MD
 Sample : 02378-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ5

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: VX035179.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	47793	166440	12.31%	1.546%
2	1.368	43	46	62	rVB	160970	187948	13.90%	1.746%
3	1.672	92	96	108	rVB	118763	152445	11.28%	1.416%
4	2.306	194	200	209	rBV	299895	471979	34.92%	4.384%
5	2.623	249	252	253	rBV2	292	350	0.03%	0.003%
6	2.678	259	261	265	rVB3	350	365	0.03%	0.003%
7	2.715	265	267	269	rBV	309	369	0.03%	0.003%
8	2.794	275	280	286	rVB2	1143	2213	0.16%	0.021%
9	2.940	296	304	314	rBV	24236	56794	4.20%	0.527%
10	3.044	318	321	322	rBV2	212	236	0.02%	0.002%
11	3.142	334	337	340	rBV2	163	209	0.02%	0.002%
12	3.257	355	356	359	rBV	173	209	0.02%	0.002%
13	3.337	367	369	372	rVB2	227	265	0.02%	0.002%
14	3.373	372	375	376	rBV	377	292	0.02%	0.003%
15	3.471	389	391	394	rBV	247	227	0.02%	0.002%
16	3.544	401	403	407	rVB2	463	538	0.04%	0.005%
17	3.635	416	418	420	rBV	284	249	0.02%	0.002%
18	3.709	426	430	432	rVB2	290	290	0.02%	0.003%
19	3.763	437	439	441	rBV3	246	207	0.02%	0.002%
20	3.861	453	455	457	rBV2	187	236	0.02%	0.002%
21	4.026	481	482	487	rBV3	230	308	0.02%	0.003%
22	4.202	508	511	512	rVV2	292	243	0.02%	0.002%
23	4.221	512	514	517	rVV2	242	254	0.02%	0.002%
24	4.263	519	521	524	rVB2	194	212	0.02%	0.002%
25	4.465	545	554	567	rBV	75774	242583	17.95%	2.253%
26	4.684	589	590	595	rVB3	816	719	0.05%	0.007%
27	4.922	626	629	630	rVB3	287	222	0.02%	0.002%
28	5.056	638	651	670	rBV	169149	520067	38.47%	4.830%
29	5.190	670	673	676	rBV3	346	482	0.04%	0.004%
30	5.294	688	690	691	rBV	323	210	0.02%	0.002%
31	5.348	697	699	701	rBV	271	235	0.02%	0.002%
32	5.379	701	704	705	rBV2	551	532	0.04%	0.005%
33	5.562	727	734	739	rBV6	1662	4591	0.34%	0.043%
34	5.745	762	764	765	rVV	282	227	0.02%	0.002%
35	5.763	765	767	770	rVV	274	252	0.02%	0.002%
36	5.970	789	801	826	rBV2	459807	1351712	100.00%	12.554%

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 Title : VOC Analysis

37	6.324	856	859	860	rBV2	297	266	0.02%	0.002%
38	6.354	863	864	867	rBV2	201	247	0.02%	0.002%
39	6.428	873	876	878	rBV	241	207	0.02%	0.002%
40	6.537	891	894	896	rBV3	386	488	0.04%	0.005%
41	6.610	904	906	908	rVB	312	233	0.02%	0.002%
42	6.641	908	911	913	rVB2	323	258	0.02%	0.002%
43	6.763	920	931	948	rBV	447239	1089436	80.60%	10.119%
44	7.123	983	990	995	rVB5	1862	4437	0.33%	0.041%
45	7.220	1004	1006	1011	rVB2	288	286	0.02%	0.003%
46	7.305	1011	1020	1036	rBV	271834	606582	44.88%	5.634%
47	7.476	1046	1048	1049	rBV	566	371	0.03%	0.003%
48	7.592	1065	1067	1070	rBV2	253	245	0.02%	0.002%
49	7.775	1094	1097	1100	rBV2	299	393	0.03%	0.004%
50	7.860	1108	1111	1113	rBV2	227	218	0.02%	0.002%
51	7.891	1113	1116	1120	rVB2	256	376	0.03%	0.003%
52	7.958	1120	1127	1135	rBV4	793	2041	0.15%	0.019%
53	8.208	1166	1168	1171	rBV2	291	432	0.03%	0.004%
54	8.324	1181	1187	1202	rVV	135389	222849	16.49%	2.070%
55	8.513	1215	1218	1219	rBV2	362	405	0.03%	0.004%
56	8.647	1233	1240	1252	rBV	712740	1101168	81.46%	10.227%
57	8.952	1285	1290	1302	rBV	91420	136208	10.08%	1.265%
58	9.140	1319	1321	1325	rBV3	249	229	0.02%	0.002%
59	9.214	1332	1333	1335	rVB	494	246	0.02%	0.002%
60	9.244	1335	1338	1339	rBV2	269	352	0.03%	0.003%
61	9.262	1339	1341	1342	rBV	650	418	0.03%	0.004%
62	9.384	1356	1361	1380	rBV	372229	537169	39.74%	4.989%
63	9.640	1400	1403	1404	rVB2	380	300	0.02%	0.003%
64	9.823	1431	1433	1436	rVB	415	309	0.02%	0.003%
65	9.909	1446	1447	1450	rBV	289	293	0.02%	0.003%
66	9.933	1450	1451	1454	rVB	301	262	0.02%	0.002%
67	9.970	1454	1457	1462	rVB2	292	492	0.04%	0.005%
68	10.055	1465	1471	1489	rBV	892527	1290189	95.45%	11.983%
69	10.342	1517	1518	1520	rBV	336	215	0.02%	0.002%
70	10.439	1533	1534	1537	rBV2	303	328	0.02%	0.003%
71	10.671	1570	1572	1575	rVB2	232	248	0.02%	0.002%
72	10.762	1584	1587	1588	rBV2	350	336	0.02%	0.003%
73	10.787	1589	1591	1596	rVV	345	451	0.03%	0.004%
74	10.841	1599	1600	1606	rVV3	235	405	0.03%	0.004%
75	11.189	1652	1657	1671	rVV	440753	579815	42.89%	5.385%
76	11.311	1675	1677	1681	rVB2	1023	1136	0.08%	0.011%

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 Title : VOC Analysis

77	11.354	1681	1684	1686	rBV	283	274	0.02%	0.003%
78	11.408	1691	1693	1695	rBV2	287	280	0.02%	0.003%
79	11.457	1697	1701	1702	rBV2	313	289	0.02%	0.003%
80	11.713	1741	1743	1745	rVB	347	234	0.02%	0.002%
81	11.969	1781	1785	1788	rBV2	9636	12336	0.91%	0.115%
82	12.024	1789	1794	1804	rVB	833892	1099060	81.31%	10.208%
83	12.219	1822	1826	1831	rBV5	4229	5955	0.44%	0.055%
84	12.317	1837	1842	1857	rBV	669811	888381	65.72%	8.251%
85	12.756	1910	1914	1917	rBV2	377	480	0.04%	0.004%
86	12.817	1922	1924	1927	rVB2	303	292	0.02%	0.003%
87	12.859	1929	1931	1934	rBV	341	471	0.03%	0.004%
88	13.560	2044	2046	2047	rVB2	361	234	0.02%	0.002%
89	13.591	2047	2051	2059	rBV3	5149	7468	0.55%	0.069%
90	13.713	2069	2071	2072	rBV	284	216	0.02%	0.002%
91	13.749	2076	2077	2080	rVB2	359	342	0.03%	0.003%
92	13.963	2108	2112	2116	rVV3	1248	2039	0.15%	0.019%
93	14.005	2118	2119	2122	rVB	325	246	0.02%	0.002%
94	14.097	2132	2134	2135	rBV	492	294	0.02%	0.003%
95	14.310	2167	2169	2172	rBV2	219	244	0.02%	0.002%
96	14.444	2189	2191	2194	rVB2	325	294	0.02%	0.003%
97	14.798	2247	2249	2250	rVB2	514	311	0.02%	0.003%
98	14.902	2264	2266	2268	rBV2	565	544	0.04%	0.005%
99	15.249	2321	2323	2326	rBV3	858	1198	0.09%	0.011%
100	15.475	2359	2360	2361	rBV	533	225	0.02%	0.002%

Sum of corrected areas: 10766756

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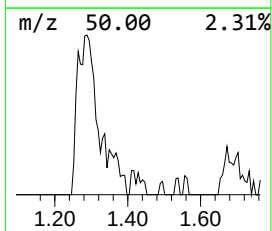
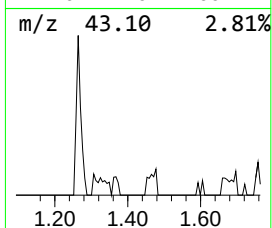
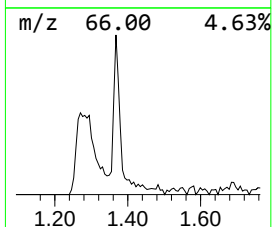
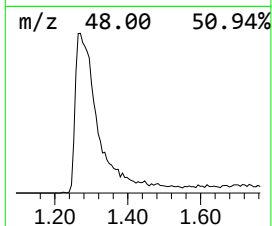
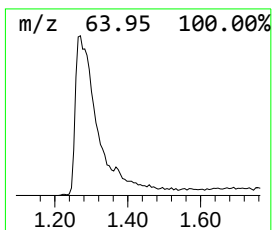
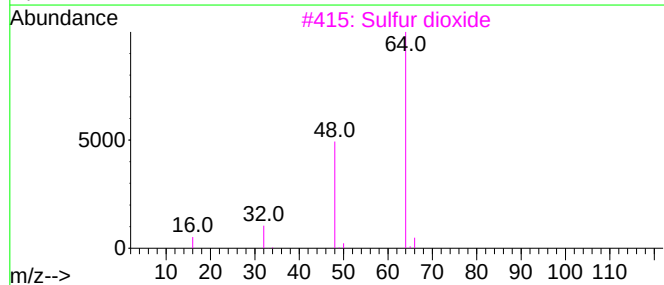
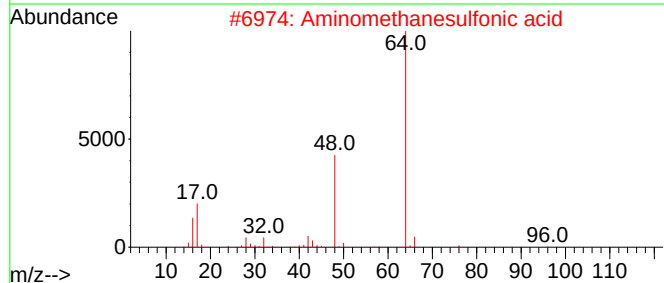
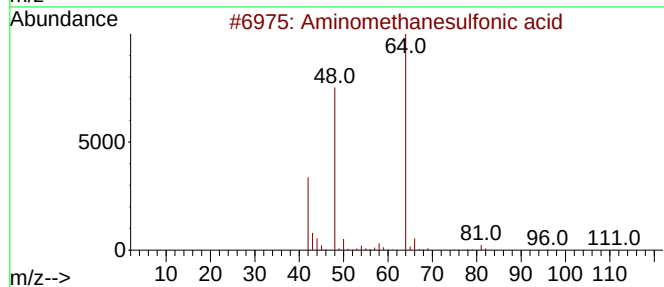
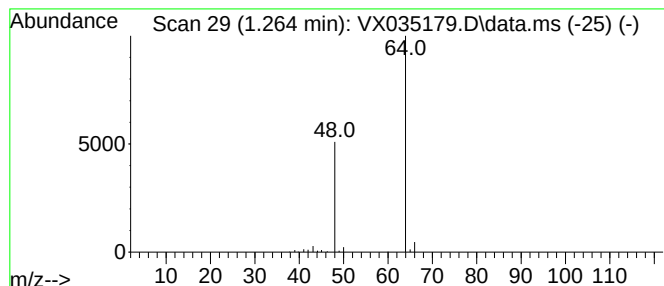
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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	7.64 ug/L	166440	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
3			Sulfur dioxide	64	O2S	007446-09-5	83
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.264	7.6	ug/L	166440	1	6.757	1089440	50.0