

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035178.D
 Acq On : 19 Apr 2023 18:33
 Operator : JC/MD
 Sample : 02333-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMH3

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: VX035178.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	67473	212849	14.90%	1.915%
2	1.367	43	46	59	rVB	168744	194734	13.63%	1.752%
3	1.672	92	96	106	rBV	124673	163511	11.44%	1.471%
4	2.306	194	200	211	rBV	332446	513639	35.95%	4.622%
5	2.666	257	259	262	rBV2	323	303	0.02%	0.003%
6	2.782	275	278	285	rBV4	884	1779	0.12%	0.016%
7	2.916	298	300	301	rVV	195	184	0.01%	0.002%
8	2.946	301	305	311	rVB3	732	1409	0.10%	0.013%
9	2.995	311	313	315	rBV2	198	173	0.01%	0.002%
10	3.074	324	326	327	rVB2	314	185	0.01%	0.002%
11	3.093	327	329	331	rBV2	276	286	0.02%	0.003%
12	3.203	345	347	349	rVB	362	217	0.02%	0.002%
13	3.233	349	352	353	rBV	322	231	0.02%	0.002%
14	3.398	377	379	384	rVB	167	244	0.02%	0.002%
15	3.648	416	420	422	rBV2	260	271	0.02%	0.002%
16	3.800	441	445	446	rVB2	198	199	0.01%	0.002%
17	3.843	449	452	456	rVB2	214	335	0.02%	0.003%
18	4.007	476	479	481	rBV	297	243	0.02%	0.002%
19	4.050	483	486	488	rVB	374	290	0.02%	0.003%
20	4.068	488	489	492	rVB2	302	279	0.02%	0.003%
21	4.147	500	502	504	rVB2	277	245	0.02%	0.002%
22	4.190	507	509	511	rVB	260	223	0.02%	0.002%
23	4.221	511	514	516	rBV	302	437	0.03%	0.004%
24	4.471	546	555	578	rBV	78663	264789	18.53%	2.383%
25	5.062	639	652	669	rVV	177302	536808	37.57%	4.830%
26	5.379	701	704	705	rBV2	425	403	0.03%	0.004%
27	5.556	725	733	743	rVB4	1177	3492	0.24%	0.031%
28	5.678	749	753	758	rBV3	257	391	0.03%	0.004%
29	5.781	768	770	774	rBV2	131	190	0.01%	0.002%
30	5.970	788	801	820	rBV2	481882	1428816	100.00%	12.857%
31	6.324	857	859	863	rBV3	210	379	0.03%	0.003%
32	6.391	867	870	873	rBV	417	390	0.03%	0.004%
33	6.452	877	880	881	rBV2	276	223	0.02%	0.002%
34	6.543	893	895	897	rBV2	338	340	0.02%	0.003%
35	6.690	916	919	920	rBV	210	198	0.01%	0.002%
36	6.763	920	931	945	rBV	457410	1110032	77.69%	9.988%

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 Title : VOC Analysis

37	7.110	985	988	996	rVB4	1604	3868	0.27%	0.035%
38	7.305	1011	1020	1036	rBV	289779	637007	44.58%	5.732%
39	7.482	1044	1049	1050	rBV3	911	993	0.07%	0.009%
40	7.690	1081	1083	1084	rBV2	238	223	0.02%	0.002%
41	7.738	1088	1091	1092	rBV	233	216	0.02%	0.002%
42	7.952	1121	1126	1128	rBV3	643	861	0.06%	0.008%
43	8.055	1141	1143	1146	rVB	254	222	0.02%	0.002%
44	8.135	1155	1156	1158	rBV	366	233	0.02%	0.002%
45	8.324	1181	1187	1197	rBV	139131	233500	16.34%	2.101%
46	8.647	1234	1240	1257	rVV	743607	1160786	81.24%	10.445%
47	8.884	1277	1279	1281	rBV	253	190	0.01%	0.002%
48	8.951	1285	1290	1304	rBV	96495	147572	10.33%	1.328%
49	9.165	1321	1325	1327	rBV3	381	579	0.04%	0.005%
50	9.275	1339	1343	1348	rVB2	1119	1503	0.11%	0.014%
51	9.311	1348	1349	1354	rBV2	179	282	0.02%	0.003%
52	9.384	1356	1361	1380	rBV	385763	566554	39.65%	5.098%
53	9.720	1414	1416	1420	rVB2	390	301	0.02%	0.003%
54	10.000	1460	1462	1465	rBV	275	227	0.02%	0.002%
55	10.055	1465	1471	1486	rBV	902513	1257092	87.98%	11.312%
56	10.244	1500	1502	1503	rVB	336	196	0.01%	0.002%
57	10.360	1519	1521	1522	rVB	455	223	0.02%	0.002%
58	10.396	1525	1527	1529	rBV2	401	299	0.02%	0.003%
59	10.567	1554	1555	1557	rBV2	360	240	0.02%	0.002%
60	10.683	1572	1574	1576	rBV	192	174	0.01%	0.002%
61	10.726	1579	1581	1584	rVV2	228	172	0.01%	0.002%
62	10.756	1584	1586	1588	rBV	361	193	0.01%	0.002%
63	10.878	1604	1606	1607	rVB	379	177	0.01%	0.002%
64	10.939	1614	1616	1617	rBV	220	178	0.01%	0.002%
65	11.079	1637	1639	1641	rBV2	249	196	0.01%	0.002%
66	11.140	1647	1649	1652	rBV2	356	321	0.02%	0.003%
67	11.189	1652	1657	1670	rBV	449600	602565	42.17%	5.422%
68	11.360	1682	1685	1688	rVB2	384	462	0.03%	0.004%
69	11.402	1690	1692	1694	rVB2	186	173	0.01%	0.002%
70	11.457	1699	1701	1704	rVV3	354	273	0.02%	0.002%
71	11.707	1740	1742	1746	rVB2	566	571	0.04%	0.005%
72	11.744	1746	1748	1749	rBV	324	268	0.02%	0.002%
73	11.811	1758	1759	1761	rBV2	244	215	0.02%	0.002%
74	11.969	1779	1785	1788	rBV3	1187	1852	0.13%	0.017%
75	12.024	1788	1794	1805	rVV	838132	1109201	77.63%	9.981%
76	12.219	1823	1826	1831	rBV2	2904	3794	0.27%	0.034%

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 Title : VOC Analysis

77	12.317	1837	1842	1862	rVB	693117	926575	64.85%	8.338%
78	12.548	1873	1880	1881	rVB2	432	496	0.03%	0.004%
79	12.835	1925	1927	1928	rBV	400	208	0.01%	0.002%
80	12.859	1928	1931	1933	rVB2	280	230	0.02%	0.002%
81	12.878	1933	1934	1936	rBV	413	241	0.02%	0.002%
82	13.000	1951	1954	1955	rBV	287	270	0.02%	0.002%
83	13.182	1982	1984	1988	rVB	334	304	0.02%	0.003%
84	13.371	2014	2015	2018	rVB	381	203	0.01%	0.002%
85	13.499	2034	2036	2039	rVB	388	256	0.02%	0.002%
86	13.524	2039	2040	2042	rBV	216	192	0.01%	0.002%
87	13.591	2047	2051	2058	rBV5	3973	5437	0.38%	0.049%
88	13.713	2069	2071	2073	rVB	455	305	0.02%	0.003%
89	13.737	2073	2075	2080	rBV2	388	456	0.03%	0.004%
90	13.969	2106	2113	2117	rBV4	623	1106	0.08%	0.010%
91	14.115	2133	2137	2141	rVB2	320	561	0.04%	0.005%
92	14.194	2149	2150	2154	rVB2	337	367	0.03%	0.003%
93	14.231	2154	2156	2160	rBV3	294	442	0.03%	0.004%
94	14.463	2192	2194	2195	rBV	353	259	0.02%	0.002%
95	14.627	2219	2221	2222	rBV2	363	225	0.02%	0.002%
96	14.737	2238	2239	2241	rBV2	551	455	0.03%	0.004%
97	14.761	2241	2243	2244	rVV	434	322	0.02%	0.003%
98	15.188	2311	2313	2316	rBV	444	533	0.04%	0.005%
99	15.975	2441	2442	2444	rBV2	725	450	0.03%	0.004%
100	16.633	2548	2550	2552	rBV2	597	583	0.04%	0.005%

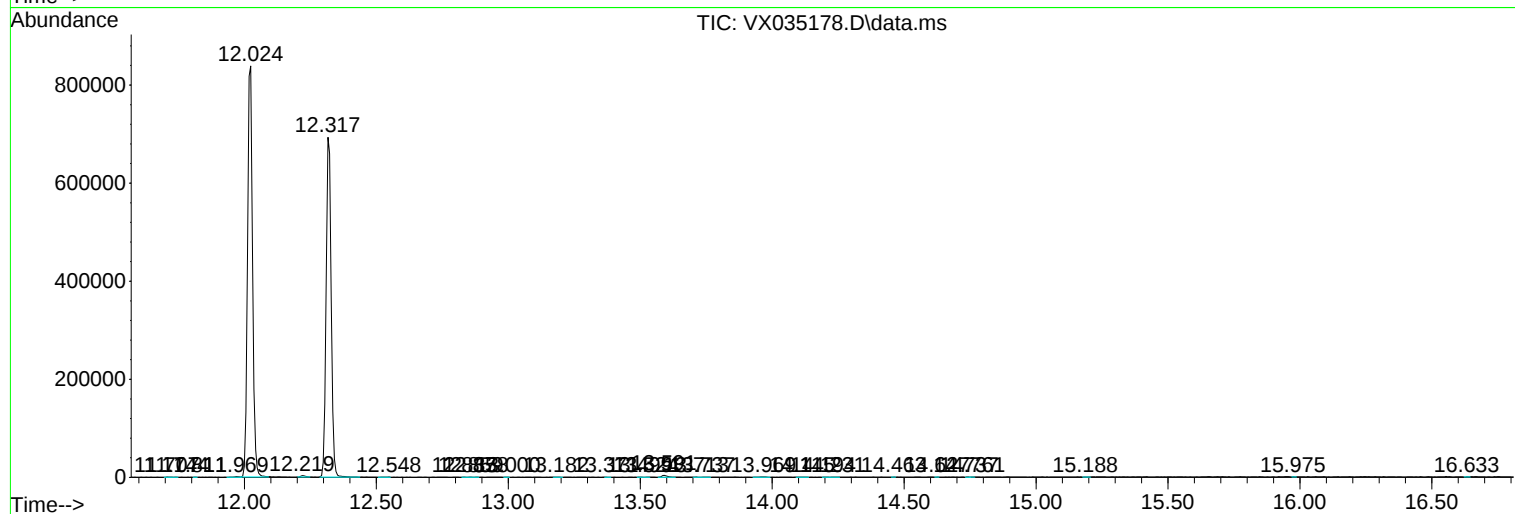
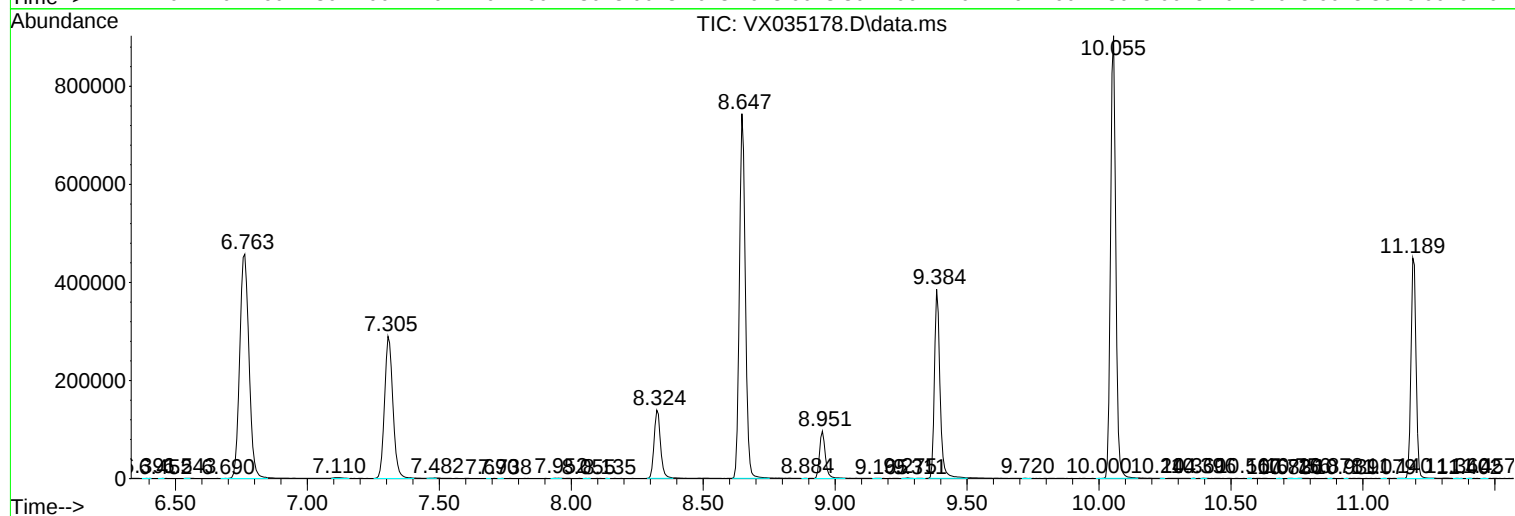
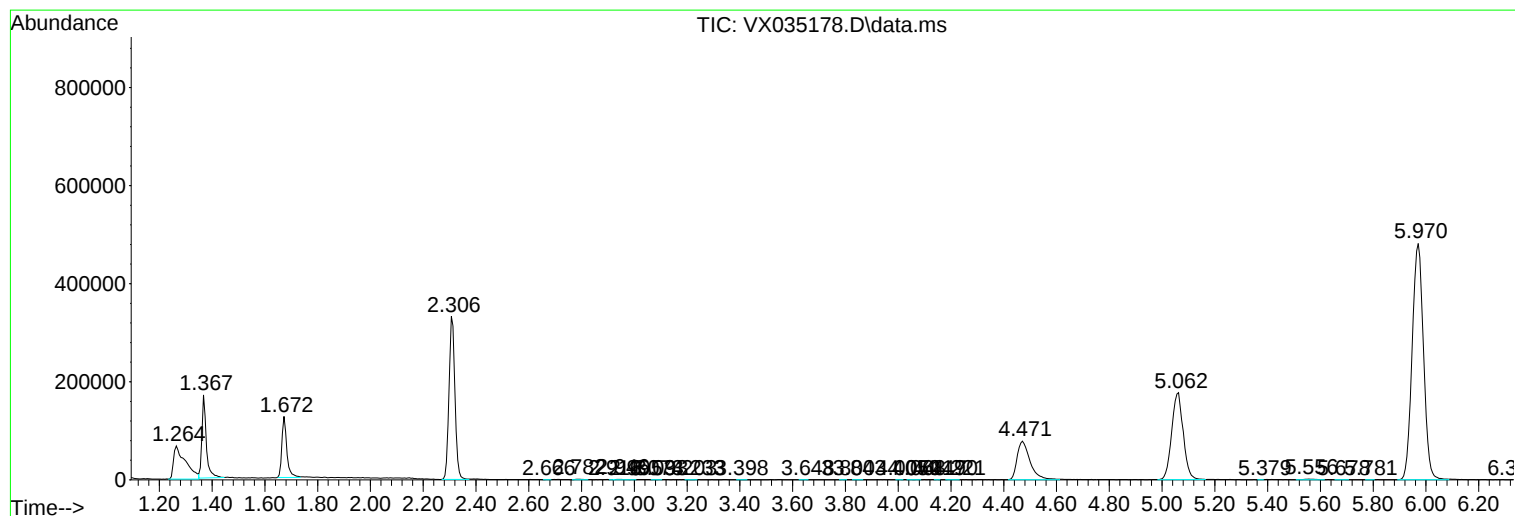
Sum of corrected areas: 11113145

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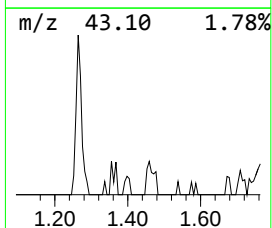
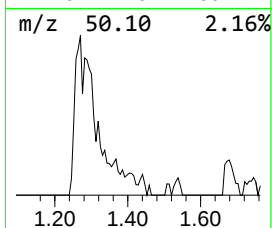
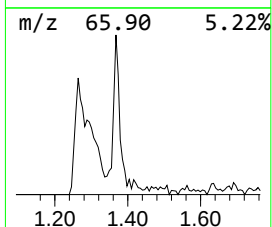
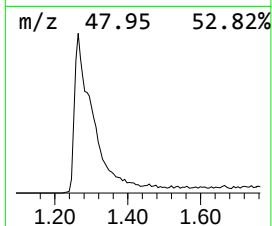
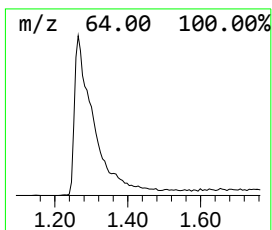
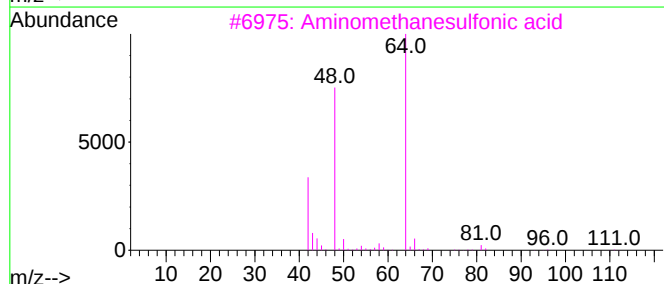
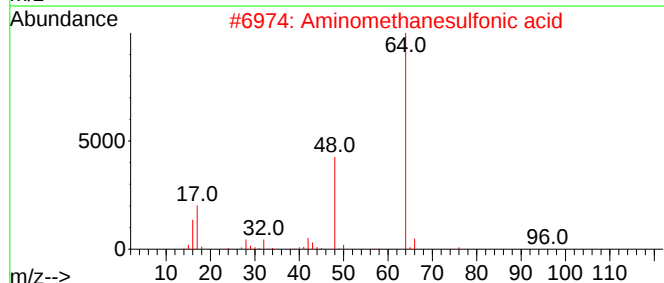
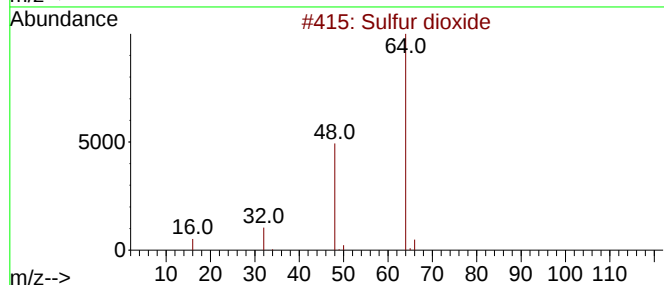
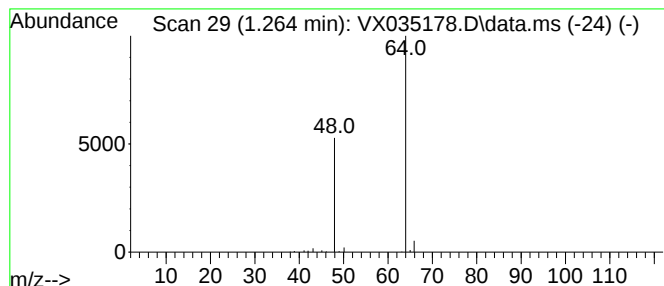
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	9.59 ug/L	212849	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
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
Sulfur dioxide	1.264	9.6	ug/L	212849	1	6.763	1110030	50.0