

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035152.D
 Acq On : 19 Apr 2023 02:52
 Operator : JC/MD
 Sample : 02397-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM8

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: VX035152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	42	rBV	154938	330045	1.44%	0.657%
2	1.368	43	46	60	rVB	233404	265391	1.16%	0.528%
3	1.672	92	96	107	rVB	171895	226368	0.99%	0.451%
4	2.306	194	200	211	rBV	416431	660964	2.89%	1.316%
5	2.508	230	233	239	rVB4	652	1326	0.01%	0.003%
6	2.556	239	241	243	rBV2	308	285	0.00%	0.001%
7	2.660	255	258	260	rVB2	450	432	0.00%	0.001%
8	2.727	267	269	271	rVB	405	277	0.00%	0.001%
9	2.788	276	279	283	rVV2	1203	1689	0.01%	0.003%
10	2.831	283	286	287	rVB2	305	203	0.00%	0.000%
11	2.898	295	297	299	rBV	276	245	0.00%	0.000%
12	2.934	301	303	304	rBV2	418	356	0.00%	0.001%
13	3.105	329	331	332	rBV	254	170	0.00%	0.000%
14	3.166	338	341	343	rVB3	222	200	0.00%	0.000%
15	3.264	356	357	360	rVB2	235	195	0.00%	0.000%
16	3.373	373	375	378	rBV	375	259	0.00%	0.001%
17	3.507	393	397	398	rBV3	231	280	0.00%	0.001%
18	3.544	401	403	404	rBV2	243	169	0.00%	0.000%
19	3.562	404	406	408	rVB3	184	159	0.00%	0.000%
20	3.715	429	431	433	rVB2	316	255	0.00%	0.001%
21	3.831	446	450	452	rVV	279	235	0.00%	0.000%
22	3.916	460	464	466	rBV2	218	208	0.00%	0.000%
23	3.946	466	469	471	rBV	410	497	0.00%	0.001%
24	4.074	488	490	492	rBV	231	187	0.00%	0.000%
25	4.148	499	502	504	rVB2	211	197	0.00%	0.000%
26	4.391	540	542	544	rBV2	188	202	0.00%	0.000%
27	4.459	544	553	575	rBV2	120001	370480	1.62%	0.737%
28	4.745	598	600	601	rVB	387	194	0.00%	0.000%
29	4.946	630	633	636	rVB3	221	228	0.00%	0.000%
30	5.056	638	651	671	rBV	239815	746925	3.27%	1.487%
31	5.379	701	704	705	rBV2	601	556	0.00%	0.001%
32	5.477	718	720	724	rBV3	340	513	0.00%	0.001%
33	5.556	726	733	735	rBV3	1283	2059	0.01%	0.004%
34	5.641	745	747	752	rVB2	304	361	0.00%	0.001%
35	5.678	752	753	755	rBV	369	222	0.00%	0.000%
36	5.769	766	768	770	rBV	305	390	0.00%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035152.D
 Acq On : 19 Apr 2023 02:52
 Operator : JC/MD
 Sample : 02397-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM8

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

37	5.970	788	801	823	rBV2	651417	1977746	8.65%	3.937%
38	6.342	860	862	864	rVB2	333	251	0.00%	0.000%
39	6.513	888	890	893	rBV2	227	211	0.00%	0.000%
40	6.544	893	895	896	rBV2	356	227	0.00%	0.000%
41	6.617	905	907	909	rBV2	182	177	0.00%	0.000%
42	6.659	912	914	916	rBV	197	158	0.00%	0.000%
43	6.763	920	931	947	rBV	450673	1098972	4.81%	2.188%
44	7.110	983	988	996	rVB5	1326	3090	0.01%	0.006%
45	7.202	1001	1003	1005	rBV2	164	196	0.00%	0.000%
46	7.306	1010	1020	1040	rBV	406590	887506	3.88%	1.767%
47	7.488	1044	1050	1054	rBV7	1089	2101	0.01%	0.004%
48	7.665	1075	1079	1081	rBV2	244	248	0.00%	0.000%
49	7.763	1093	1095	1098	rVB2	306	235	0.00%	0.000%
50	7.793	1098	1100	1103	rVB2	248	291	0.00%	0.001%
51	7.824	1103	1105	1106	rBV	245	251	0.00%	0.000%
52	7.897	1115	1117	1119	rBV2	163	168	0.00%	0.000%
53	7.952	1121	1126	1130	rVV5	1080	2257	0.01%	0.004%
54	8.062	1143	1144	1146	rBV	294	184	0.00%	0.000%
55	8.098	1148	1150	1155	rVB3	258	288	0.00%	0.001%
56	8.171	1159	1162	1164	rVB	331	324	0.00%	0.001%
57	8.196	1164	1166	1168	rBV2	311	367	0.00%	0.001%
58	8.257	1174	1176	1179	rVB2	183	170	0.00%	0.000%
59	8.324	1181	1187	1199	rBV	246671	405148	1.77%	0.806%
60	8.568	1225	1227	1230	rVB2	369	230	0.00%	0.000%
61	8.647	1233	1240	1258	rBV	1023558	1577405	6.90%	3.140%
62	8.952	1284	1290	1306	rBV	166214	259132	1.13%	0.516%
63	9.202	1329	1331	1332	rBV	412	229	0.00%	0.000%
64	9.275	1340	1343	1346	rVB4	1141	1209	0.01%	0.002%
65	9.317	1348	1350	1353	rVB2	226	198	0.00%	0.000%
66	9.384	1355	1361	1376	rBV	584826	821414	3.59%	1.635%
67	9.860	1437	1439	1443	rBV2	352	507	0.00%	0.001%
68	9.945	1448	1453	1454	rBV2	362	437	0.00%	0.001%
69	10.079	1465	1475	1500	rBV2	5060557	8011161	35.05%	15.947%
70	10.695	1575	1576	1581	rVB3	607	766	0.00%	0.002%
71	10.750	1581	1585	1586	rBV	322	421	0.00%	0.001%
72	10.963	1619	1620	1623	rBV2	174	174	0.00%	0.000%
73	11.189	1652	1657	1667	rBV	654919	848788	3.71%	1.690%
74	11.707	1740	1742	1744	rVB3	573	374	0.00%	0.001%
75	11.908	1772	1775	1777	rVB2	309	317	0.00%	0.001%
76	11.969	1779	1785	1789	rBV	508471	621780	2.72%	1.238%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035152.D
 Acq On : 19 Apr 2023 02:52
 Operator : JC/MD
 Sample : 02397-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM8

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

77	12.036	1789	1796	1809	rVB2	1956694	3593216	15.72%	7.153%
78	12.219	1822	1826	1831	rBV6	2585	4573	0.02%	0.009%
79	12.335	1837	1845	1851	rBV	17088320	22853623	100.00%	45.492%
80	12.701	1903	1905	1909	rVB4	983	777	0.00%	0.002%
81	12.829	1924	1926	1927	rVB	340	163	0.00%	0.000%
82	12.920	1936	1941	1949	rVB2	24587	32465	0.14%	0.065%
83	12.981	1949	1951	1952	rBV	406	242	0.00%	0.000%
84	13.061	1959	1964	1969	rVB3	4819	7971	0.03%	0.016%
85	13.116	1969	1973	1979	rVB4	3908	4676	0.02%	0.009%
86	13.195	1982	1986	1991	rBV	8959	11961	0.05%	0.024%
87	13.378	2014	2016	2020	rVB3	515	525	0.00%	0.001%
88	13.426	2022	2024	2025	rBV	374	318	0.00%	0.001%
89	13.585	2045	2050	2068	rVB	3025595	3834225	16.78%	7.632%
90	13.829	2088	2090	2094	rBV2	393	329	0.00%	0.001%
91	13.902	2101	2102	2106	rBV3	396	443	0.00%	0.001%
92	13.957	2106	2111	2121	rVV	485876	642338	2.81%	1.279%
93	14.249	2157	2159	2160	rBV	464	402	0.00%	0.001%
94	14.353	2175	2176	2177	rBV	305	175	0.00%	0.000%
95	14.432	2187	2189	2192	rBV2	363	403	0.00%	0.001%
96	14.591	2214	2215	2216	rVB	435	159	0.00%	0.000%
97	14.670	2227	2228	2229	rBV	382	192	0.00%	0.000%
98	14.780	2240	2246	2251	rVB	32415	47687	0.21%	0.095%
99	14.944	2271	2273	2275	rBV2	617	450	0.00%	0.001%
100	15.249	2317	2323	2333	rVB	42004	60952	0.27%	0.121%

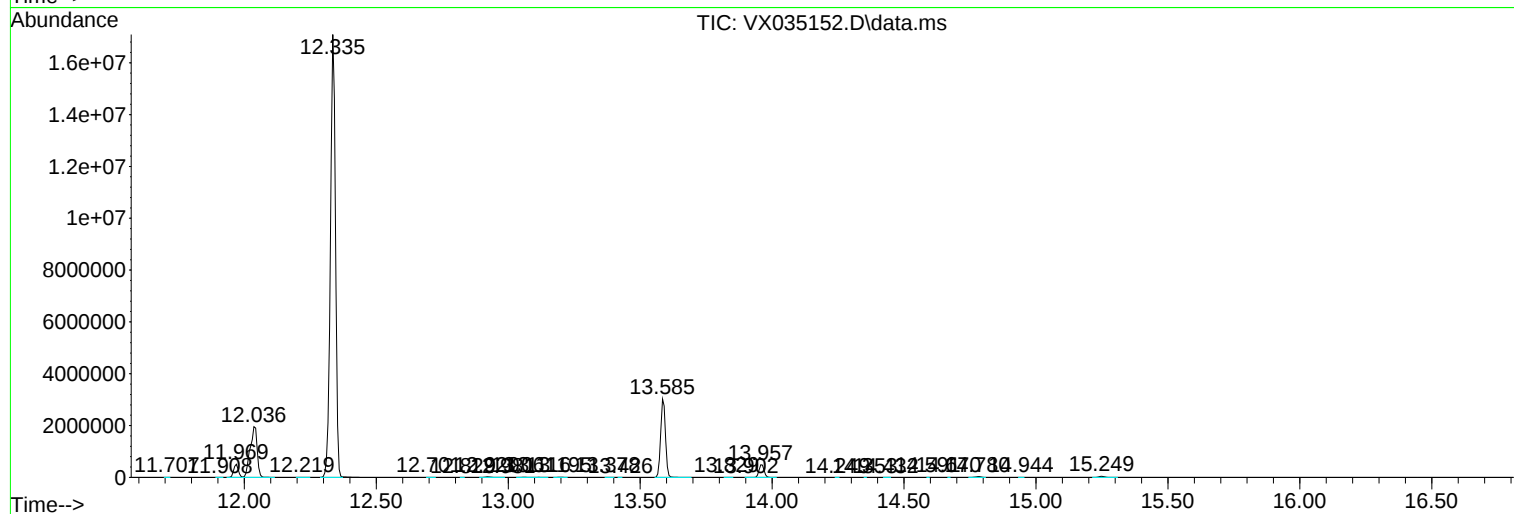
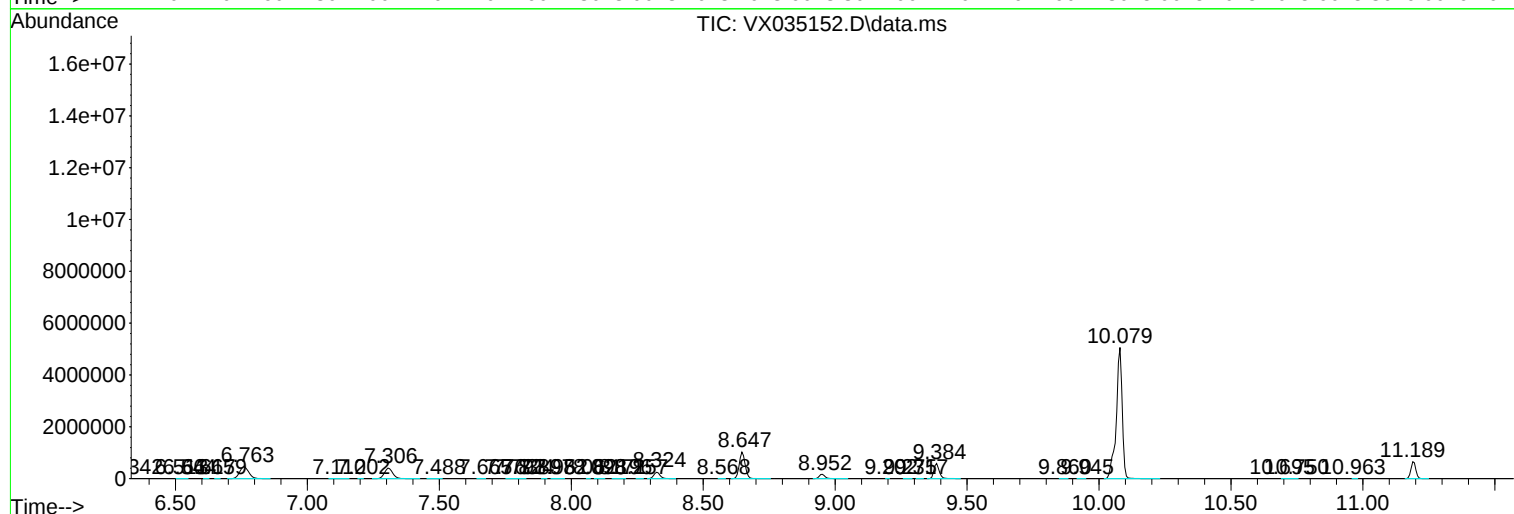
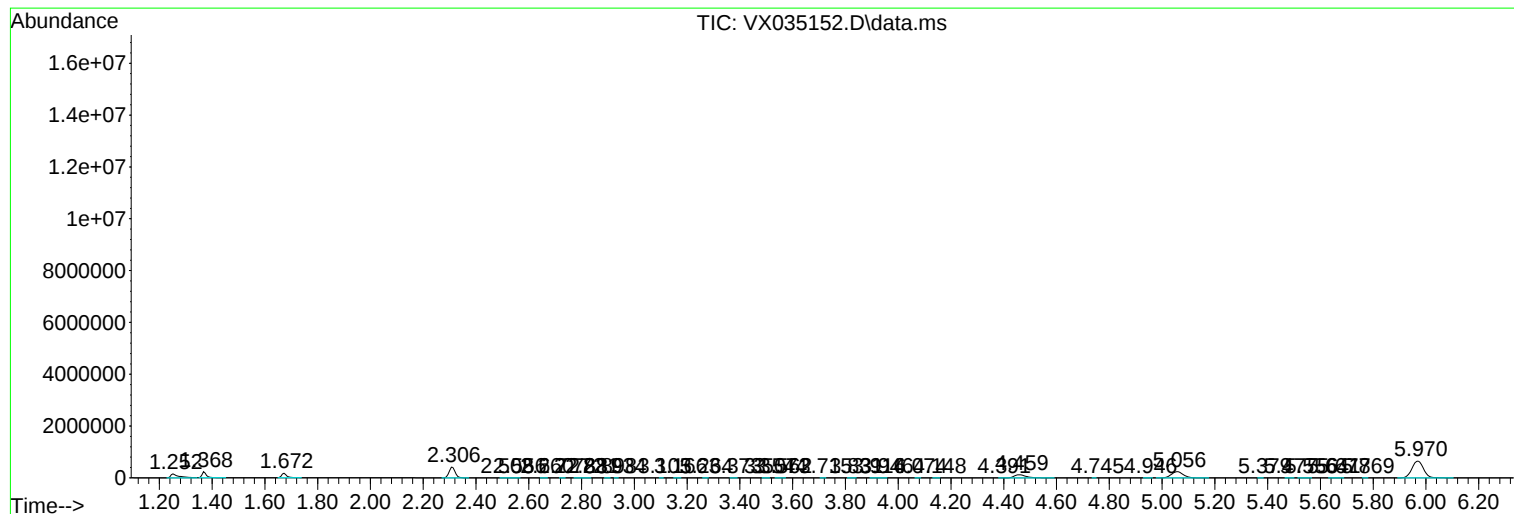
Sum of corrected areas: 50236095

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035152.D
Acq On : 19 Apr 2023 02:52
Operator : JC/MD
Sample : 02397-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMM8

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035152.D
Acq On : 19 Apr 2023 02:52
Operator : JC/MD
Sample : 02397-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMM8

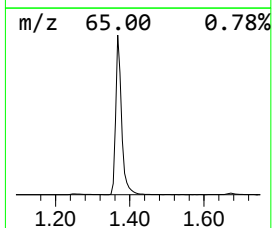
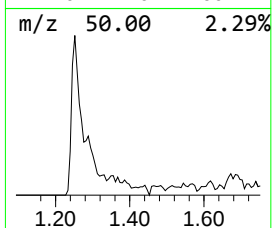
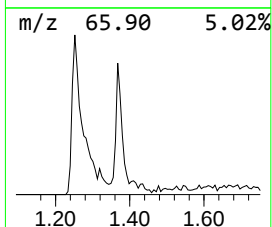
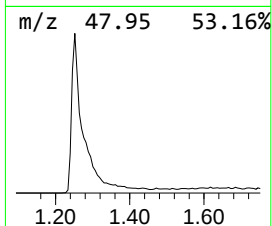
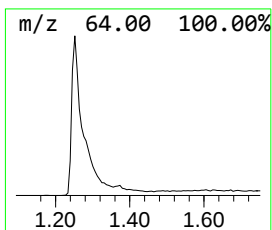
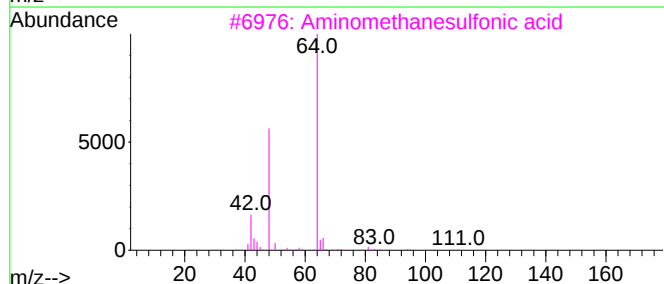
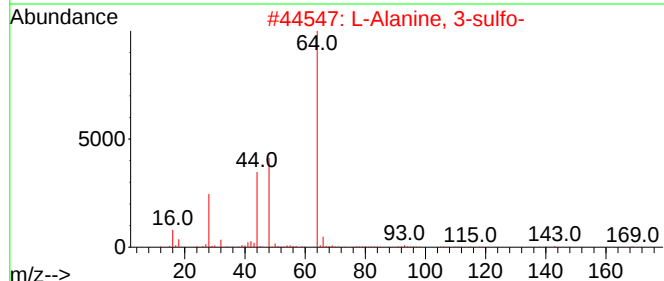
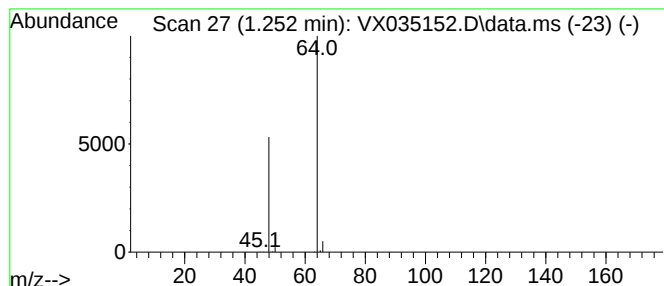
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	15.02 ug/L	330045	1,4-Difluorobenzene	6.763

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035152.D
Acq On : 19 Apr 2023 02:52
Operator : JC/MD
Sample : 02397-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMM8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	15.0	ug/L	330045	1	6.763	1098970	50.0