

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035180.D
 Acq On : 19 Apr 2023 19:20
 Operator : JC/MD
 Sample : 02378-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ6

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: VX035180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	25	33	43	rBV	37991	140535	10.46%	1.323%
2	1.367	43	46	61	rVB	159529	187464	13.95%	1.765%
3	1.672	92	96	108	rBV	114049	149155	11.10%	1.404%
4	2.306	194	200	212	rBV	310649	475789	35.40%	4.480%
5	2.556	240	241	243	rBV	400	249	0.02%	0.002%
6	2.745	270	272	273	rBV	370	226	0.02%	0.002%
7	2.940	297	304	315	rBV2	12352	29659	2.21%	0.279%
8	3.044	318	321	324	rBV	324	423	0.03%	0.004%
9	3.196	344	346	347	rBV	228	196	0.01%	0.002%
10	3.251	353	355	357	rVB	290	234	0.02%	0.002%
11	3.300	360	363	365	rBV3	327	353	0.03%	0.003%
12	3.391	376	378	381	rVV	393	324	0.02%	0.003%
13	3.568	404	407	408	rBV2	159	214	0.02%	0.002%
14	3.617	413	415	417	rVV	301	208	0.02%	0.002%
15	3.654	419	421	424	rVV2	249	295	0.02%	0.003%
16	3.678	424	425	429	rVV	318	288	0.02%	0.003%
17	3.721	431	432	437	rVV2	252	261	0.02%	0.002%
18	3.904	461	462	465	rVB	312	228	0.02%	0.002%
19	3.928	465	466	468	rBV2	287	217	0.02%	0.002%
20	3.952	468	470	472	rBV2	225	226	0.02%	0.002%
21	3.989	472	476	478	rVV	401	390	0.03%	0.004%
22	4.019	478	481	483	rVV	291	322	0.02%	0.003%
23	4.086	487	492	494	rVB2	229	371	0.03%	0.003%
24	4.184	506	508	511	rBV	335	376	0.03%	0.004%
25	4.288	524	525	528	rBV2	172	201	0.01%	0.002%
26	4.470	546	555	571	rBV	72914	240667	17.91%	2.266%
27	4.763	601	603	605	rBV	489	349	0.03%	0.003%
28	4.781	605	606	610	rVB3	289	193	0.01%	0.002%
29	4.861	617	619	622	rVB2	290	292	0.02%	0.003%
30	4.891	622	624	627	rVB2	341	364	0.03%	0.003%
31	4.983	637	639	640	rBV	337	298	0.02%	0.003%
32	5.056	640	651	670	rVV	173525	515988	38.39%	4.859%
33	5.385	701	705	707	rBV3	560	816	0.06%	0.008%
34	5.452	715	716	720	rBV2	354	403	0.03%	0.004%
35	5.489	720	722	725	rVB	319	203	0.02%	0.002%
36	5.562	725	734	738	rBV5	2093	4849	0.36%	0.046%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035180.D
 Acq On : 19 Apr 2023 19:20
 Operator : JC/MD
 Sample : 02378-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ6

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	789	801	818	rBV2	455584	1344013	100.00%	12.655%
38	6.324	857	859	861	rBV	289	218	0.02%	0.002%
39	6.543	891	895	897	rBV2	483	558	0.04%	0.005%
40	6.763	921	931	948	rBV	466451	1112311	82.76%	10.474%
41	7.001	968	970	972	rBV3	241	229	0.02%	0.002%
42	7.122	984	990	995	rBV7	1953	4994	0.37%	0.047%
43	7.305	1012	1020	1040	rBV	274405	603039	44.87%	5.678%
44	7.482	1044	1049	1052	rBV3	729	1219	0.09%	0.011%
45	7.665	1077	1079	1081	rVB	286	204	0.02%	0.002%
46	7.945	1123	1125	1126	rBV	563	372	0.03%	0.004%
47	8.208	1165	1168	1171	rBV2	208	322	0.02%	0.003%
48	8.323	1180	1187	1201	rBV	131530	222170	16.53%	2.092%
49	8.458	1207	1209	1211	rBV3	378	312	0.02%	0.003%
50	8.531	1219	1221	1222	rVB2	496	280	0.02%	0.003%
51	8.549	1222	1224	1226	rBV2	270	287	0.02%	0.003%
52	8.647	1234	1240	1254	rBV	710958	1097407	81.65%	10.333%
53	8.951	1284	1290	1304	rVV	92950	138499	10.30%	1.304%
54	9.110	1314	1316	1318	rBV2	302	210	0.02%	0.002%
55	9.274	1340	1343	1351	rVB3	2277	3091	0.23%	0.029%
56	9.384	1356	1361	1383	rBV	357695	525402	39.09%	4.947%
57	9.732	1417	1418	1422	rBV2	438	560	0.04%	0.005%
58	9.768	1422	1424	1427	rVB	352	413	0.03%	0.004%
59	9.811	1429	1431	1434	rBV	252	275	0.02%	0.003%
60	9.921	1448	1449	1453	rBV2	256	266	0.02%	0.003%
61	10.055	1465	1471	1483	rBV	902804	1244735	92.61%	11.720%
62	10.171	1488	1490	1491	rVV	550	251	0.02%	0.002%
63	10.354	1518	1520	1524	rBV2	416	389	0.03%	0.004%
64	10.823	1596	1597	1600	rBV2	278	294	0.02%	0.003%
65	10.890	1607	1608	1612	rBV2	219	237	0.02%	0.002%
66	10.963	1617	1620	1622	rBV2	361	315	0.02%	0.003%
67	11.195	1652	1658	1667	rBV	423733	562478	41.85%	5.296%
68	11.311	1674	1677	1682	rVB2	1150	1511	0.11%	0.014%
69	11.555	1716	1717	1719	rBV	228	221	0.02%	0.002%
70	11.713	1741	1743	1747	rBV2	449	580	0.04%	0.005%
71	11.817	1758	1760	1763	rVB2	295	278	0.02%	0.003%
72	11.975	1781	1786	1788	rBV3	2580	3216	0.24%	0.030%
73	12.024	1788	1794	1803	rVV	847674	1106964	82.36%	10.423%
74	12.219	1823	1826	1829	rBV2	1669	1885	0.14%	0.018%
75	12.317	1837	1842	1853	rBV	667615	873091	64.96%	8.221%
76	12.457	1863	1865	1867	rVB	394	238	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035180.D
 Acq On : 19 Apr 2023 19:20
 Operator : JC/MD
 Sample : 02378-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMJ6

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	12.512	1872	1874	1877	rBV2	301	229	0.02%	0.002%
78	12.561	1881	1882	1884	rBV	322	250	0.02%	0.002%
79	12.762	1911	1915	1919	rVB4	330	579	0.04%	0.005%
80	12.896	1935	1937	1940	rBV	330	307	0.02%	0.003%
81	12.975	1948	1950	1954	rBV2	256	300	0.02%	0.003%
82	13.091	1965	1969	1971	rBV2	265	434	0.03%	0.004%
83	13.121	1971	1974	1977	rVV2	417	405	0.03%	0.004%
84	13.158	1978	1980	1982	rVV	405	244	0.02%	0.002%
85	13.195	1984	1986	1989	rBV2	316	290	0.02%	0.003%
86	13.231	1989	1992	1993	rBV	184	204	0.02%	0.002%
87	13.341	2008	2010	2011	rBV	307	220	0.02%	0.002%
88	13.402	2018	2020	2022	rBV	350	280	0.02%	0.003%
89	13.512	2036	2038	2041	rBV	254	207	0.02%	0.002%
90	13.591	2047	2051	2056	rBV3	3817	5545	0.41%	0.052%
91	13.688	2066	2067	2069	rBV2	286	252	0.02%	0.002%
92	13.786	2081	2083	2086	rBV2	360	465	0.03%	0.004%
93	13.963	2110	2112	2116	rVB2	1516	1734	0.13%	0.016%
94	14.005	2116	2119	2120	rBV	398	277	0.02%	0.003%
95	14.072	2128	2130	2131	rBV2	219	217	0.02%	0.002%
96	14.127	2137	2139	2142	rVB	351	242	0.02%	0.002%
97	14.164	2142	2145	2147	rBV3	337	392	0.03%	0.004%
98	14.780	2244	2246	2248	rBV2	459	399	0.03%	0.004%
99	15.042	2287	2289	2291	rVB	615	456	0.03%	0.004%
100	15.158	2307	2308	2309	rBV	633	280	0.02%	0.003%

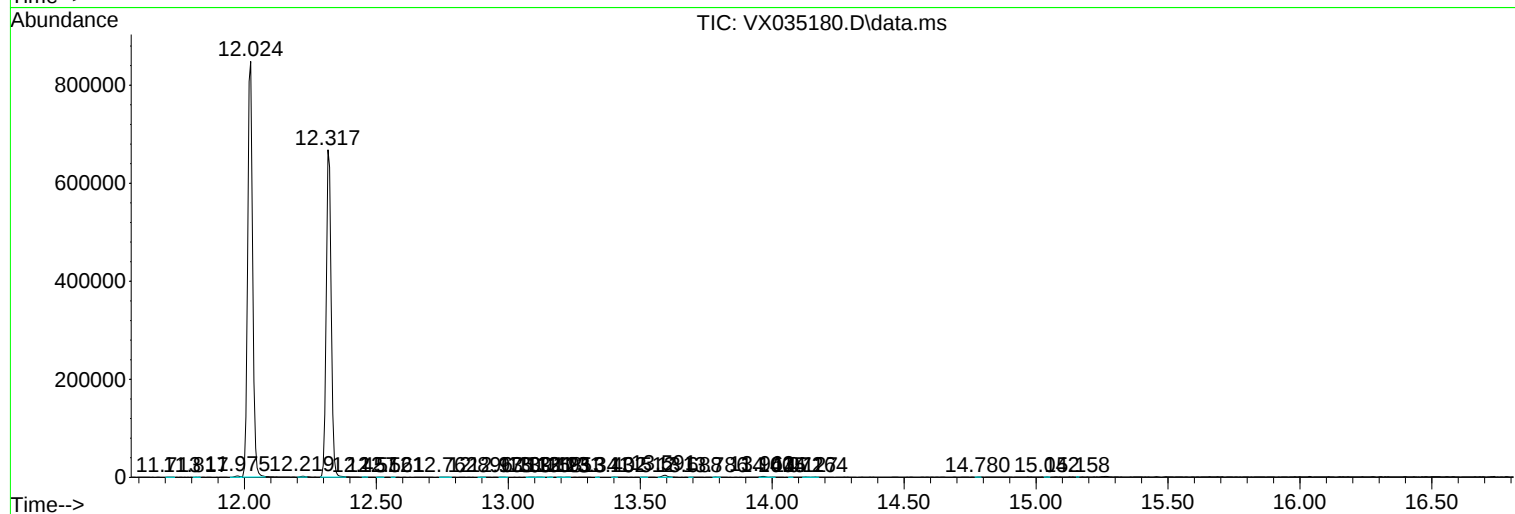
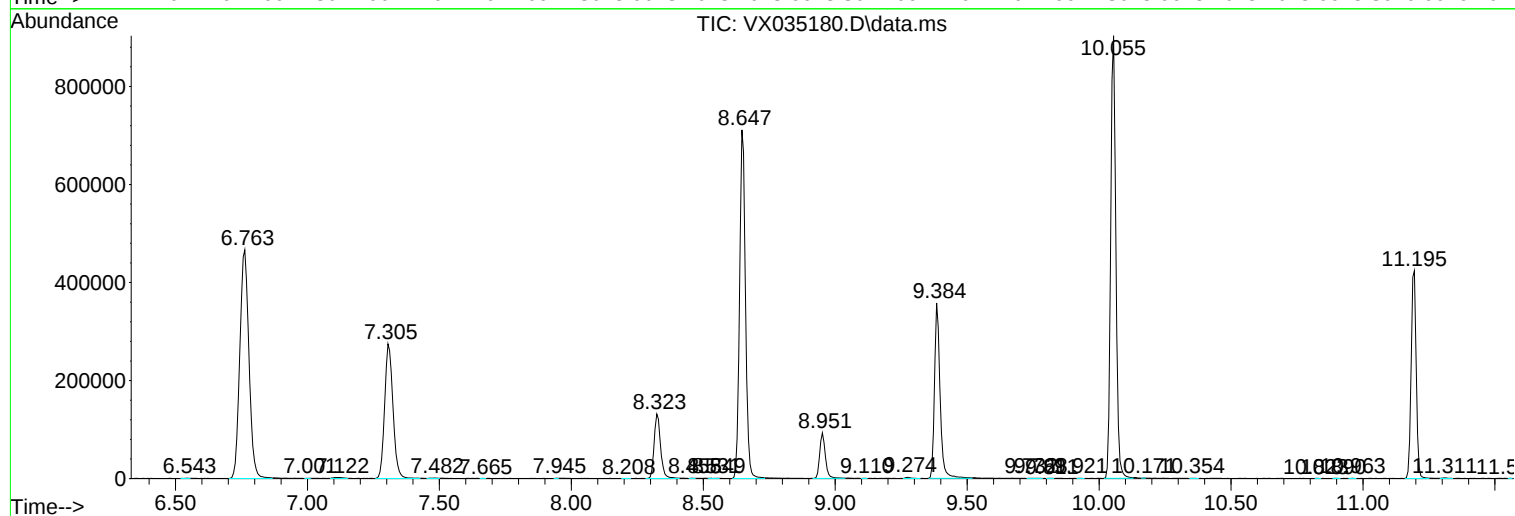
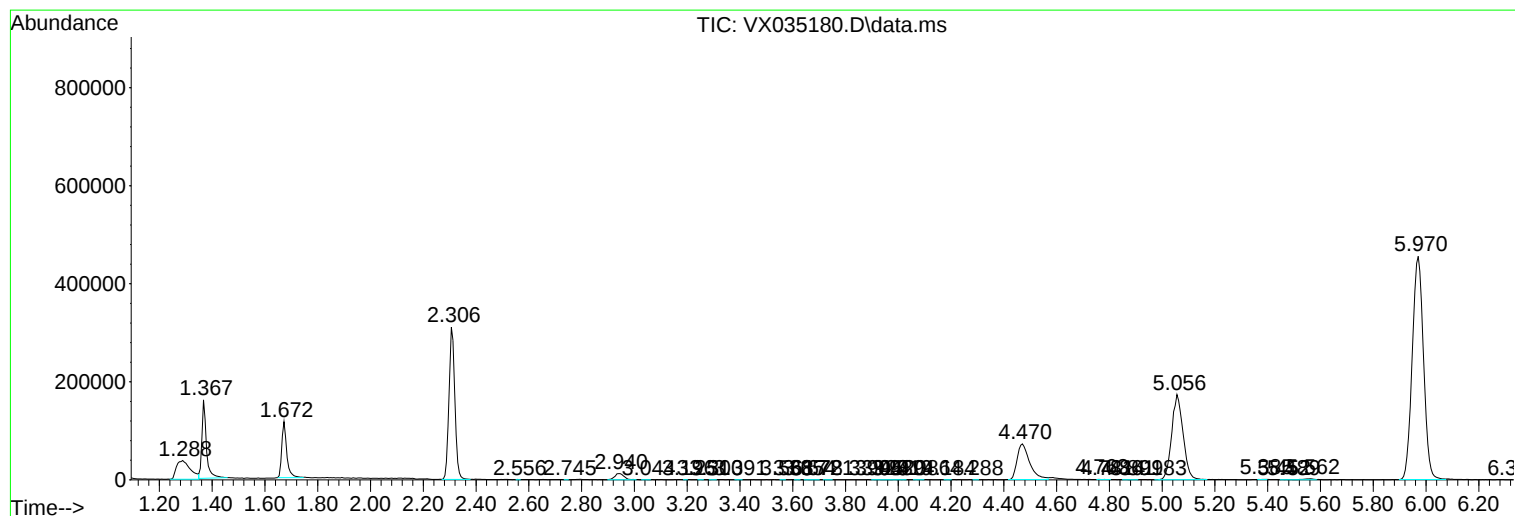
Sum of corrected areas: 10620168

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
Data File : VX035180.D
Acq On : 19 Apr 2023 19:20
Operator : JC/MD
Sample : 02378-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMJ6

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\VX041923\
Data File : VX035180.D
Acq On : 19 Apr 2023 19:20
Operator : JC/MD
Sample : 02378-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMJ6

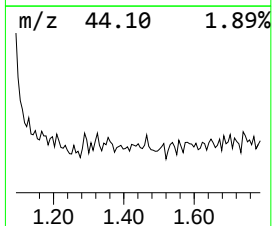
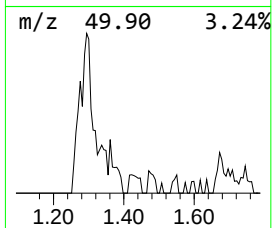
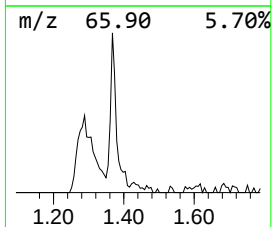
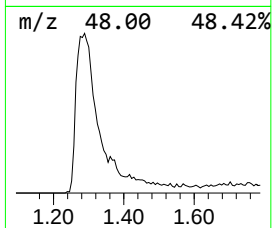
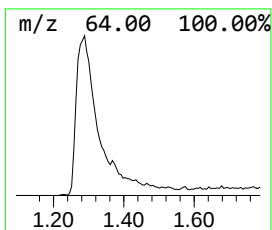
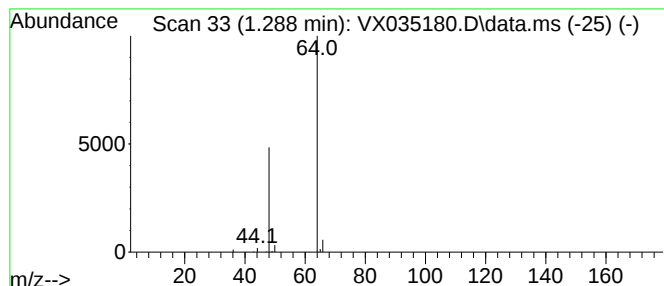
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.288	6.32 ug/L	140535	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			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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
Data File : VX035180.D
Acq On : 19 Apr 2023 19:20
Operator : JC/MD
Sample : 02378-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMJ6

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	1.288	6.3	ug/L	140535	1	6.763	1112310	50.0