

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042778.D
 Acq On : 31 Jul 2024 17:10
 Operator : JC/MD
 Sample : P3398-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L1

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042778.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	31	rBV	14212	18461	3.88%	0.477%
2	1.368	43	46	56	rVB	33653	41720	8.76%	1.078%
3	1.459	60	61	62	rBV	459	276	0.06%	0.007%
4	1.550	72	76	77	rBV3	1145	1240	0.26%	0.032%
5	1.648	88	92	101	rVB	24957	31809	6.68%	0.822%
6	1.807	117	118	121	rBV	395	286	0.06%	0.007%
7	1.837	121	123	126	rVB	563	432	0.09%	0.011%
8	1.874	126	129	130	rBV2	292	295	0.06%	0.008%
9	2.294	192	198	209	rBV	87250	136650	28.70%	3.531%
10	2.495	228	231	234	rBV2	324	348	0.07%	0.009%
11	2.550	238	240	241	rVB	324	207	0.04%	0.005%
12	2.623	249	252	254	rBB	242	232	0.05%	0.006%
13	2.654	254	257	258	rBV	178	202	0.04%	0.005%
14	2.788	273	279	284	rBV3	803	1717	0.36%	0.044%
15	2.947	298	305	311	rVV2	1624	3490	0.73%	0.090%
16	2.995	311	313	314	rVB2	471	317	0.07%	0.008%
17	3.087	326	328	331	rBV	366	365	0.08%	0.009%
18	3.233	348	352	355	rBV2	196	332	0.07%	0.009%
19	3.294	358	362	366	rVB	243	334	0.07%	0.009%
20	3.434	380	385	386	rBV	173	242	0.05%	0.006%
21	3.459	386	389	393	rVB2	200	349	0.07%	0.009%
22	3.514	394	398	399	rBV	156	215	0.05%	0.006%
23	3.587	407	410	413	rBV	164	216	0.05%	0.006%
24	3.751	433	437	440	rVB	205	326	0.07%	0.008%
25	3.946	465	469	471	rVB	250	246	0.05%	0.006%
26	3.989	474	476	477	rBV	283	196	0.04%	0.005%
27	4.026	477	482	487	rVB2	206	506	0.11%	0.013%
28	4.367	537	538	542	rVB	304	245	0.05%	0.006%
29	4.471	547	555	571	rBV2	33557	97217	20.42%	2.512%
30	5.062	640	652	667	rVV	60667	196105	41.19%	5.067%
31	5.184	670	672	675	rVB	232	244	0.05%	0.006%
32	5.263	681	685	688	rBV3	215	314	0.07%	0.008%
33	5.385	702	705	707	rBV2	416	465	0.10%	0.012%
34	5.794	769	772	774	rBV2	241	271	0.06%	0.007%
35	5.970	789	801	817	rBV2	162275	476088	100.00%	12.301%
36	6.172	833	834	838	rVB2	289	216	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042778.D
 Acq On : 31 Jul 2024 17:10
 Operator : JC/MD
 Sample : P3398-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L1

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\SFAMXML072624WMA.M
 Title : VOC Analysis

37	6.318	854	858	859	rBV	267	318	0.07%	0.008%
38	6.403	870	872	875	rVB	267	257	0.05%	0.007%
39	6.629	906	909	912	rBV2	187	249	0.05%	0.006%
40	6.696	917	920	921	rBV	246	244	0.05%	0.006%
41	6.763	921	931	948	rBV	121655	298438	62.69%	7.711%
42	6.934	958	959	964	rVB2	405	395	0.08%	0.010%
43	7.043	975	977	980	rVB	414	251	0.05%	0.006%
44	7.220	1003	1006	1009	rBV2	262	333	0.07%	0.009%
45	7.312	1012	1021	1032	rBV	100009	215216	45.21%	5.561%
46	7.495	1049	1051	1052	rVB	383	212	0.04%	0.005%
47	7.531	1054	1057	1059	rBV	201	244	0.05%	0.006%
48	7.604	1067	1069	1071	rBV	178	239	0.05%	0.006%
49	7.769	1093	1096	1100	rBV2	180	275	0.06%	0.007%
50	7.824	1100	1105	1106	rBV2	350	349	0.07%	0.009%
51	7.909	1116	1119	1121	rVV2	255	295	0.06%	0.008%
52	8.330	1182	1188	1200	rBV	61954	112434	23.62%	2.905%
53	8.647	1234	1240	1249	rBV	269566	439612	92.34%	11.358%
54	8.872	1275	1277	1280	rVB2	258	219	0.05%	0.006%
55	8.952	1285	1290	1301	rBV	48387	74718	15.69%	1.930%
56	9.067	1307	1309	1310	rBV	327	235	0.05%	0.006%
57	9.281	1338	1344	1350	rBV2	3761	5893	1.24%	0.152%
58	9.391	1357	1362	1382	rBV	181728	286880	60.26%	7.412%
59	10.055	1465	1471	1484	rBV	284462	401283	84.29%	10.368%
60	10.305	1509	1512	1516	rBV4	848	1432	0.30%	0.037%
61	10.378	1523	1524	1526	rBV	319	269	0.06%	0.007%
62	10.646	1564	1568	1572	rBV3	703	1144	0.24%	0.030%
63	11.018	1627	1629	1630	rBV	313	228	0.05%	0.006%
64	11.037	1630	1632	1635	rVB2	428	457	0.10%	0.012%
65	11.195	1652	1658	1667	rBV	216878	294431	61.84%	7.607%
66	11.317	1673	1678	1683	rVB3	3162	4469	0.94%	0.115%
67	11.396	1689	1691	1692	rBV	314	219	0.05%	0.006%
68	11.457	1698	1701	1704	rBV3	233	263	0.06%	0.007%
69	11.573	1718	1720	1725	rVB2	267	274	0.06%	0.007%
70	11.750	1747	1749	1753	rBV3	454	697	0.15%	0.018%
71	11.951	1780	1782	1783	rBV	365	202	0.04%	0.005%
72	12.024	1789	1794	1803	rBV	258349	331189	69.56%	8.557%
73	12.219	1824	1826	1829	rBV3	403	538	0.11%	0.014%
74	12.323	1837	1843	1850	rBV	267260	354621	74.49%	9.162%
75	12.488	1868	1870	1872	rVV	343	244	0.05%	0.006%
76	12.707	1901	1906	1908	rBV2	212	332	0.07%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042778.D
 Acq On : 31 Jul 2024 17:10
 Operator : JC/MD
 Sample : P3398-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L1

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\SFAMXML072624WMA.M
 Title : VOC Analysis

77	12.762	1912	1915	1920	rVB2	1184	1653	0.35%	0.043%
78	12.872	1930	1933	1936	rVV2	407	405	0.09%	0.010%
79	12.914	1938	1940	1942	rBV2	240	200	0.04%	0.005%
80	13.122	1971	1974	1975	rBV2	448	320	0.07%	0.008%
81	13.780	2077	2082	2088	rBV2	8939	12741	2.68%	0.329%
82	13.865	2094	2096	2097	rVB	507	220	0.05%	0.006%
83	14.127	2134	2139	2144	rVV2	2044	2850	0.60%	0.074%
84	14.231	2151	2156	2159	rBV2	286	451	0.09%	0.012%
85	14.353	2174	2176	2177	rVB2	286	202	0.04%	0.005%
86	14.597	2215	2216	2218	rBV2	366	316	0.07%	0.008%
87	14.640	2221	2223	2228	rVB4	678	1088	0.23%	0.028%
88	14.786	2243	2247	2250	rBV2	752	856	0.18%	0.022%
89	14.847	2256	2257	2263	rVB2	316	388	0.08%	0.010%
90	15.011	2283	2284	2287	rBV2	228	205	0.04%	0.005%
91	15.316	2333	2334	2338	rVB2	345	357	0.07%	0.009%
92	15.389	2340	2346	2350	rBV3	2195	3505	0.74%	0.091%
93	15.566	2373	2375	2377	rBV2	330	298	0.06%	0.008%
94	15.639	2385	2387	2388	rBV	350	263	0.06%	0.007%
95	15.944	2435	2437	2439	rVB2	609	461	0.10%	0.012%
96	16.097	2459	2462	2463	rBV2	371	420	0.09%	0.011%
97	16.328	2497	2500	2503	rBV3	403	527	0.11%	0.014%
98	16.408	2511	2513	2515	rBV2	332	213	0.04%	0.006%
99	16.578	2539	2541	2542	rVB	502	310	0.07%	0.008%
100	16.688	2556	2559	2560	rBV	540	404	0.08%	0.010%

Sum of corrected areas: 3870425

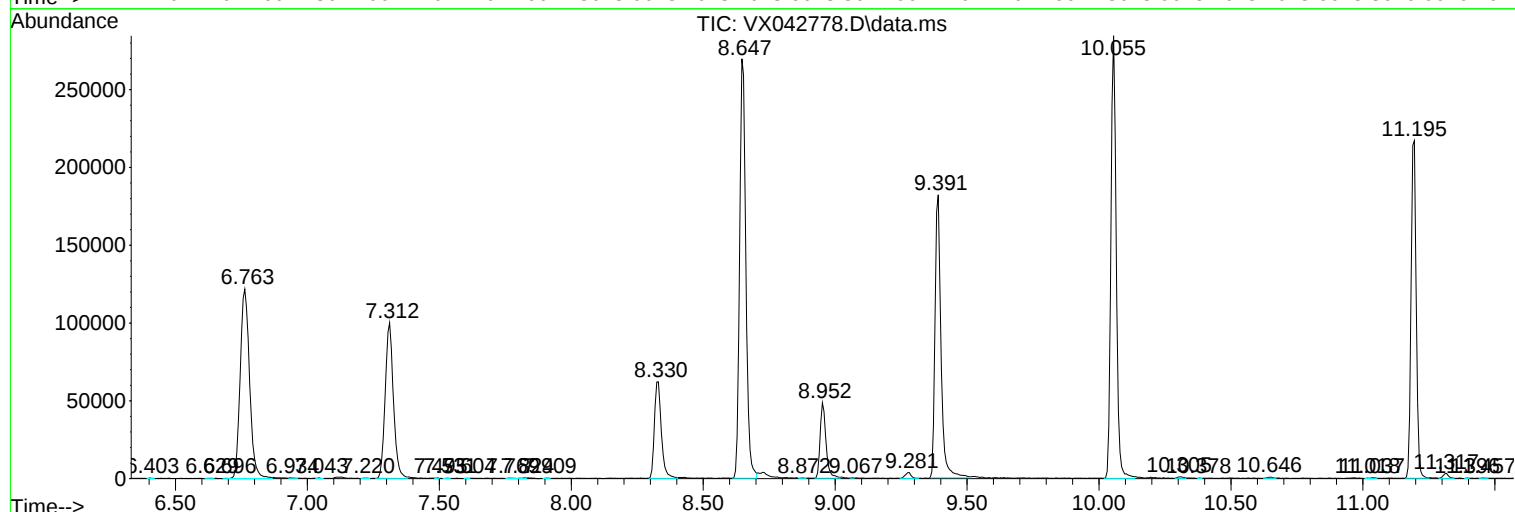
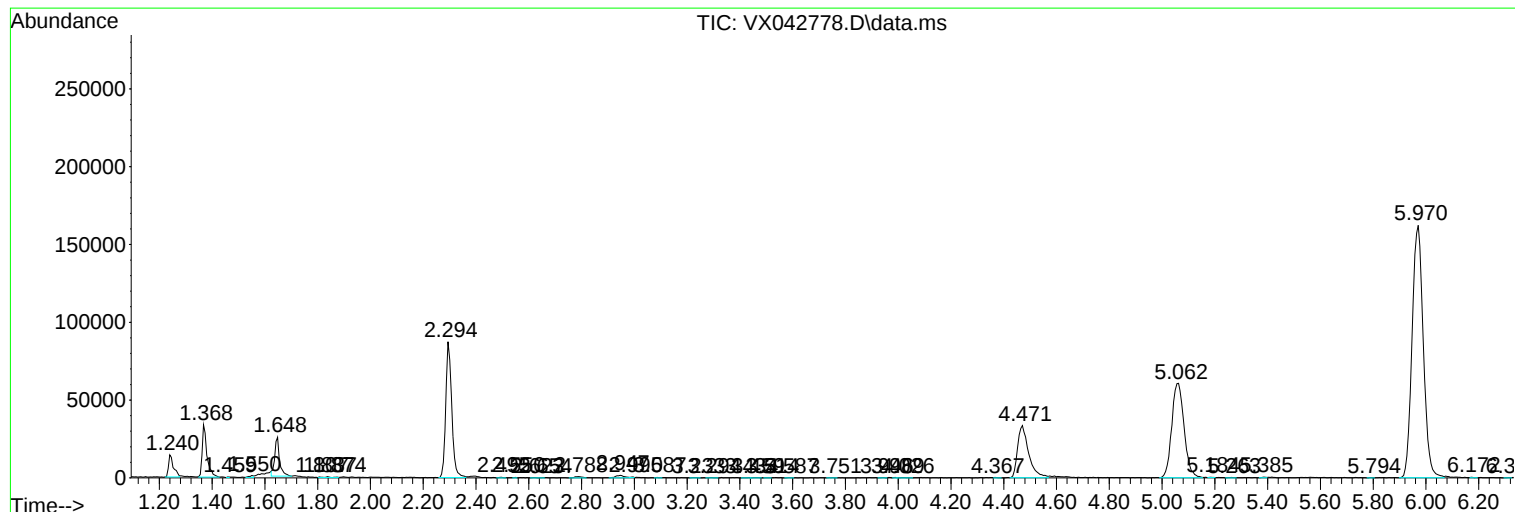
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042778.D
Acq On : 31 Jul 2024 17:10
Operator : JC/MD
Sample : P3398-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042778.D
Acq On : 31 Jul 2024 17:10
Operator : JC/MD
Sample : P3398-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L1

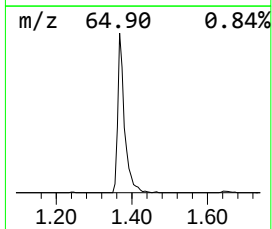
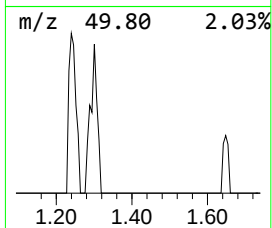
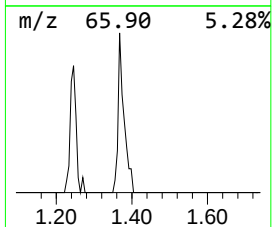
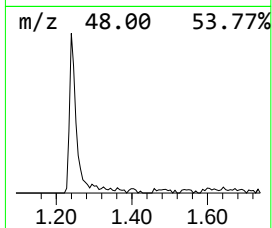
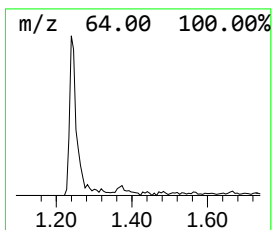
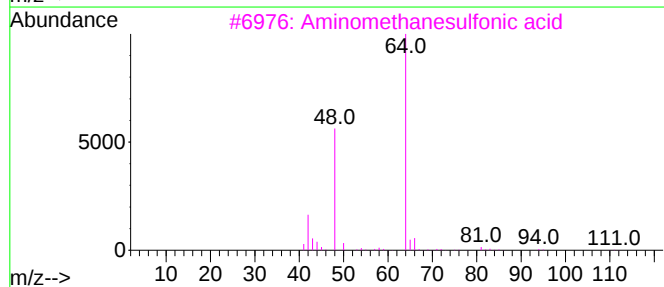
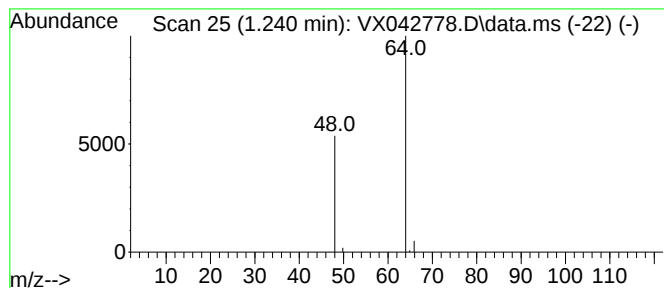
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.240	3.09 ug/L	18461	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042778.D
Acq On : 31 Jul 2024 17:10
Operator : JC/MD
Sample : P3398-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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	1.240	3.1	ug/L	18461	1	6.763	298438	50.0