

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053622.D
 Acq On : 10 Apr 2023 18:48
 Operator : JC/MD
 Sample : 02251-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD7

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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	53	rBV	27155	49350	6.11%	0.756%
2	1.597	74	80	93	rBV	98076	115615	14.32%	1.770%
3	1.909	170	177	190	rVB	86518	114809	14.22%	1.758%
4	2.565	369	381	398	rBV	154248	253814	31.43%	3.886%
5	3.044	525	530	534	rBV3	674	647	0.08%	0.010%
6	3.099	542	547	549	rBV	370	280	0.03%	0.004%
7	3.263	596	598	601	rBV	165	87	0.01%	0.001%
8	3.321	614	616	617	rBV	206	78	0.01%	0.001%
9	3.928	803	805	809	rBV2	198	125	0.02%	0.002%
10	4.067	846	848	849	rBV2	149	43	0.01%	0.001%
11	4.160	872	877	883	rVB2	313	346	0.04%	0.005%
12	4.189	883	886	888	rBV	206	97	0.01%	0.001%
13	4.240	899	902	905	rBV2	267	212	0.03%	0.003%
14	4.414	954	956	958	rBV	162	80	0.01%	0.001%
15	4.453	965	968	970	rBV2	228	176	0.02%	0.003%
16	4.530	990	992	995	rBV	222	102	0.01%	0.002%
17	4.565	1000	1003	1005	rBV	218	145	0.02%	0.002%
18	4.613	1007	1018	1044	rBV2	63776	155016	19.20%	2.373%
19	4.967	1126	1128	1131	rBV	147	71	0.01%	0.001%
20	5.057	1141	1156	1177	rBV2	145500	314630	38.97%	4.817%
21	5.411	1263	1266	1269	rVB	426	281	0.03%	0.004%
22	5.436	1272	1274	1276	rVV	304	99	0.01%	0.002%
23	5.578	1316	1318	1320	rBV2	203	115	0.01%	0.002%
24	5.629	1331	1334	1339	rVB2	219	202	0.03%	0.003%
25	5.719	1340	1362	1392	rBV2	280366	807442	100.00%	12.362%
26	5.977	1437	1442	1445	rBV2	404	388	0.05%	0.006%
27	6.115	1482	1485	1487	rBV2	294	160	0.02%	0.002%
28	6.243	1512	1525	1547	rBV	278266	525382	65.07%	8.044%
29	6.475	1595	1597	1603	rBV2	227	199	0.02%	0.003%
30	6.526	1609	1613	1618	rBV4	1001	864	0.11%	0.013%
31	6.684	1648	1662	1679	rBV	175551	343758	42.57%	5.263%
32	6.784	1691	1693	1696	rBV3	392	190	0.02%	0.003%
33	6.835	1705	1709	1713	rBV3	274	199	0.02%	0.003%
34	6.970	1749	1751	1753	rBV2	160	82	0.01%	0.001%
35	7.067	1779	1781	1783	rVB	286	112	0.01%	0.002%
36	7.192	1814	1820	1830	rVB5	942	1586	0.20%	0.024%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053622.D
 Acq On : 10 Apr 2023 18:48
 Operator : JC/MD
 Sample : 02251-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD7

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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.282	1846	1848	1850	rBV	158	53	0.01%	0.001%
38	7.414	1886	1889	1892	rVB2	192	140	0.02%	0.002%
39	7.436	1893	1896	1898	rBV2	274	205	0.03%	0.003%
40	7.562	1922	1935	1952	rBV	96674	172056	21.31%	2.634%
41	7.681	1969	1972	1973	rBV2	538	320	0.04%	0.005%
42	7.758	1990	1996	2000	rVB2	296	333	0.04%	0.005%
43	7.787	2001	2005	2009	rBV2	268	232	0.03%	0.004%
44	7.893	2025	2038	2061	rBV	357290	624550	77.35%	9.562%
45	8.176	2114	2126	2142	rBV2	68252	117329	14.53%	1.796%
46	8.266	2152	2154	2157	rVB2	381	233	0.03%	0.004%
47	8.292	2157	2162	2166	rBV2	381	335	0.04%	0.005%
48	8.369	2184	2186	2188	rBV	189	100	0.01%	0.002%
49	8.462	2208	2215	2217	rBV3	570	653	0.08%	0.010%
50	8.584	2252	2253	2255	rVB	255	48	0.01%	0.001%
51	8.626	2255	2266	2296	rBV	198066	359086	44.47%	5.498%
52	8.777	2312	2313	2315	rBV	252	69	0.01%	0.001%
53	8.819	2323	2326	2328	rBV	200	117	0.01%	0.002%
54	9.031	2390	2392	2396	rVB2	265	175	0.02%	0.003%
55	9.153	2428	2430	2434	rBV	160	59	0.01%	0.001%
56	9.414	2498	2511	2536	rBV2	383492	747881	92.62%	11.450%
57	9.591	2564	2566	2572	rVB2	267	180	0.02%	0.003%
58	9.629	2576	2578	2581	rVB2	383	201	0.02%	0.003%
59	9.649	2581	2584	2587	rVB	201	91	0.01%	0.001%
60	9.677	2590	2593	2595	rBV	250	152	0.02%	0.002%
61	9.980	2685	2687	2689	rVB	241	116	0.01%	0.002%
62	10.002	2689	2694	2696	rBV	173	185	0.02%	0.003%
63	10.124	2730	2732	2733	rBV	157	48	0.01%	0.001%
64	10.147	2737	2739	2741	rVB	260	96	0.01%	0.001%
65	10.266	2774	2776	2778	rBV	227	102	0.01%	0.002%
66	10.356	2801	2804	2807	rBV	173	155	0.02%	0.002%
67	10.504	2847	2850	2852	rBV	199	127	0.02%	0.002%
68	10.751	2915	2927	2947	rBV	260831	419234	51.92%	6.419%
69	10.857	2957	2960	2962	rBV	203	133	0.02%	0.002%
70	10.925	2978	2981	2984	rBV	312	229	0.03%	0.004%
71	11.099	3031	3035	3038	rBV	376	285	0.04%	0.004%
72	11.423	3133	3136	3140	rBV	306	216	0.03%	0.003%
73	11.742	3227	3235	3243	rBV2	3109	4552	0.56%	0.070%
74	11.806	3244	3255	3280	rVV	422302	726243	89.94%	11.119%
75	12.073	3334	3338	3340	rBV	844	607	0.08%	0.009%
76	12.189	3362	3374	3398	rBV	390291	654935	81.11%	10.027%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053622.D
 Acq On : 10 Apr 2023 18:48
 Operator : JC/MD
 Sample : 02251-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0MD7

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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

77	12.314	3409	3413	3419	rVB4	649	655	0.08%	0.010%
78	12.449	3452	3455	3458	rBV3	330	257	0.03%	0.004%
79	12.626	3504	3510	3514	rBV2	419	416	0.05%	0.006%
80	12.677	3525	3526	3527	rBV2	238	82	0.01%	0.001%
81	12.751	3548	3549	3552	rBV	265	102	0.01%	0.002%
82	12.780	3555	3558	3559	rBV2	382	235	0.03%	0.004%
83	13.057	3640	3644	3650	rBV3	461	539	0.07%	0.008%
84	13.799	3872	3875	3877	rBV	335	234	0.03%	0.004%
85	13.841	3882	3888	3899	rVB4	6295	9340	1.16%	0.143%
86	13.909	3908	3909	3912	rBV2	241	157	0.02%	0.002%
87	14.089	3958	3965	3967	rBV2	544	672	0.08%	0.010%
88	14.250	4012	4015	4016	rBV	384	195	0.02%	0.003%

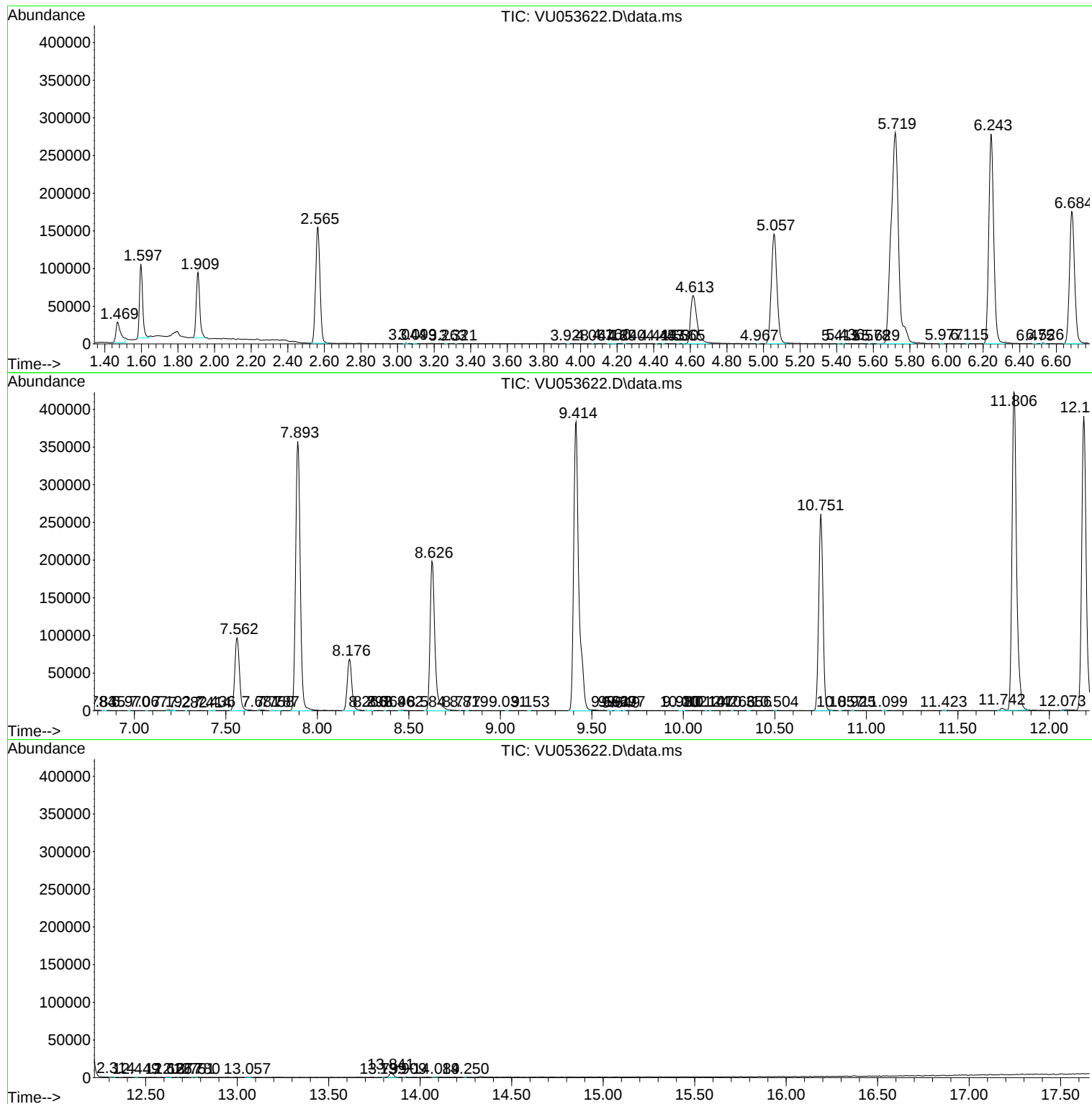
Sum of corrected areas: 6531527

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
Data File : VU053622.D
Acq On : 10 Apr 2023 18:48
Operator : JC/MD
Sample : 02251-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COMD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
Data File : VU053622.D
Acq On : 10 Apr 2023 18:48
Operator : JC/MD
Sample : 02251-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COMD7

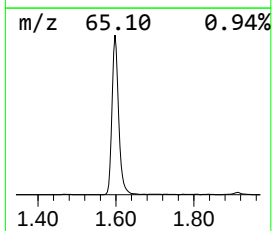
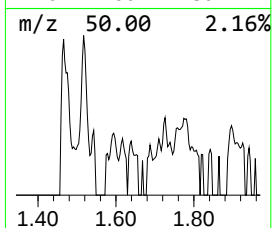
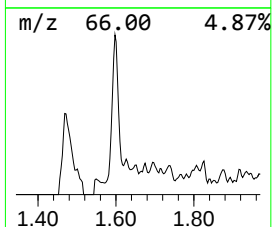
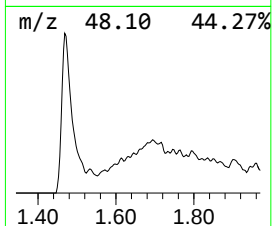
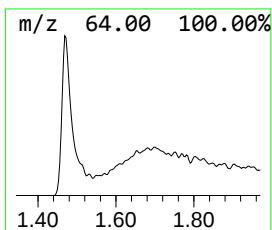
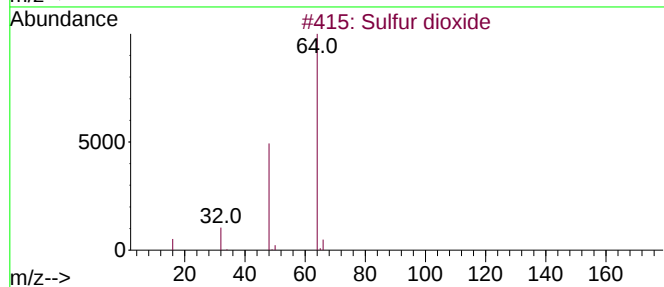
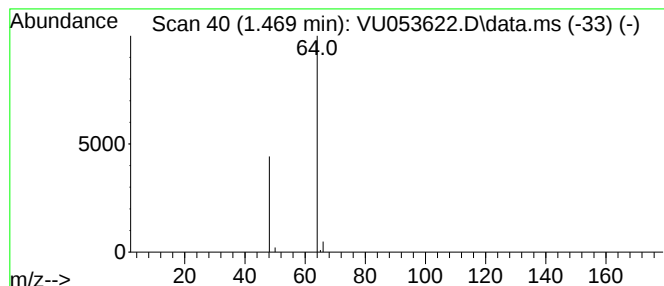
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
1.469	4.70 ug/L	49350	1,4-Difluorobenzene	6.243

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
Data File : VU053622.D
Acq On : 10 Apr 2023 18:48
Operator : JC/MD
Sample : 02251-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0MD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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	1.469	4.7	ug/L	49350	1	6.243	525382	50.0