

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
 Data File : VU052888.D
 Acq On : 31 Jan 2023 18:50
 Operator : JC/MD
 Sample : 01381-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44M8

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\SFAMULM012623WMA.M
 Title : VOC Analysis

Signal : TIC: VU052888.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	97	rVB	112979	140288	13.85%	1.839%
2	1.909	170	177	192	rBV	98994	136319	13.46%	1.787%
3	2.562	367	380	395	rBV	218906	355985	35.14%	4.667%
4	2.716	424	428	431	rBV2	299	301	0.03%	0.004%
5	2.777	444	447	448	rBV2	432	240	0.02%	0.003%
6	2.858	469	472	478	rVV3	351	321	0.03%	0.004%
7	2.996	512	515	518	rBV	198	176	0.02%	0.002%
8	3.041	523	529	533	rBV3	925	1092	0.11%	0.014%
9	3.247	589	593	596	rVB	241	197	0.02%	0.003%
10	3.301	607	610	614	rVB2	294	243	0.02%	0.003%
11	3.334	615	620	625	rBV	307	337	0.03%	0.004%
12	3.398	637	640	642	rBV	391	299	0.03%	0.004%
13	3.456	655	658	663	rBV	372	304	0.03%	0.004%
14	3.498	667	671	677	rVB2	344	422	0.04%	0.006%
15	3.527	677	680	685	rBV2	621	542	0.05%	0.007%
16	3.555	685	689	695	rVB2	543	559	0.06%	0.007%
17	3.594	696	701	704	rBV2	334	303	0.03%	0.004%
18	3.633	709	713	716	rVB2	347	275	0.03%	0.004%
19	3.649	716	718	720	rBV	255	146	0.01%	0.002%
20	3.697	730	733	735	rVB	351	209	0.02%	0.003%
21	3.726	740	742	743	rBV	299	145	0.01%	0.002%
22	3.781	755	759	761	rBV	159	155	0.02%	0.002%
23	3.793	761	763	767	rBV	379	267	0.03%	0.004%
24	3.829	772	774	776	rVB	340	157	0.02%	0.002%
25	3.858	781	783	787	rBV2	209	183	0.02%	0.002%
26	4.092	853	856	859	rVB	305	204	0.02%	0.003%
27	4.208	885	892	895	rBV2	456	454	0.04%	0.006%
28	4.279	908	914	917	rBV	198	223	0.02%	0.003%
29	4.295	917	919	922	rVV2	252	152	0.02%	0.002%
30	4.334	926	931	934	rVV2	336	240	0.02%	0.003%
31	4.494	978	981	984	rBV2	327	267	0.03%	0.004%
32	4.523	987	990	993	rBV	257	204	0.02%	0.003%
33	4.623	1007	1021	1049	rBV	69800	189356	18.69%	2.482%
34	4.816	1078	1081	1083	rBV2	389	220	0.02%	0.003%
35	5.057	1140	1156	1181	rBV	188666	417489	41.22%	5.473%
36	5.295	1227	1230	1231	rBV	285	176	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
 Data File : VU052888.D
 Acq On : 31 Jan 2023 18:50
 Operator : JC/MD
 Sample : 01381-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44M8

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\SFAMULM012623WMA.M
 Title : VOC Analysis

37	5.404	1261	1264	1266	rVB	234	148	0.01%	0.002%
38	5.478	1284	1287	1289	rBV	240	189	0.02%	0.002%
39	5.510	1294	1297	1301	rVB2	299	238	0.02%	0.003%
40	5.719	1341	1362	1383	rBV2	375176	1012919	100.00%	13.279%
41	5.957	1433	1436	1442	rVB	266	169	0.02%	0.002%
42	6.243	1510	1525	1549	rBV	299979	573999	56.67%	7.525%
43	6.385	1565	1569	1572	rVB2	213	200	0.02%	0.003%
44	6.536	1606	1616	1627	rBV6	3910	7820	0.77%	0.103%
45	6.684	1648	1662	1684	rBV	235014	451538	44.58%	5.919%
46	6.922	1732	1736	1740	rBV	193	220	0.02%	0.003%
47	7.025	1765	1768	1770	rBV	306	189	0.02%	0.002%
48	7.073	1781	1783	1787	rBV	199	172	0.02%	0.002%
49	7.182	1810	1817	1820	rBV3	1525	1880	0.19%	0.025%
50	7.456	1896	1902	1903	rBV	277	226	0.02%	0.003%
51	7.562	1920	1935	1955	rBV	118298	208883	20.62%	2.738%
52	7.649	1960	1962	1964	rBV	385	237	0.02%	0.003%
53	7.681	1969	1972	1973	rBV	620	334	0.03%	0.004%
54	7.748	1991	1993	1998	rBV2	211	203	0.02%	0.003%
55	7.800	2007	2009	2013	rVB2	277	224	0.02%	0.003%
56	7.893	2024	2038	2056	rBV	451388	778235	76.83%	10.202%
57	8.015	2074	2076	2079	rVB2	403	178	0.02%	0.002%
58	8.083	2092	2097	2101	rVB3	446	463	0.05%	0.006%
59	8.112	2101	2106	2109	rBV	380	324	0.03%	0.004%
60	8.176	2115	2126	2145	rBV	84013	142680	14.09%	1.870%
61	8.292	2159	2162	2169	rBV	604	721	0.07%	0.009%
62	8.324	2169	2172	2174	rVV	251	196	0.02%	0.003%
63	8.378	2186	2189	2191	rBV	326	185	0.02%	0.002%
64	8.555	2238	2244	2249	rBV5	1357	1663	0.16%	0.022%
65	8.636	2254	2269	2298	rBV3	205160	425589	42.02%	5.579%
66	8.957	2365	2369	2372	rBV	213	206	0.02%	0.003%
67	9.034	2388	2393	2394	rBV2	330	319	0.03%	0.004%
68	9.092	2407	2411	2416	rBV2	372	432	0.04%	0.006%
69	9.414	2496	2511	2537	rBV	417512	754592	74.50%	9.892%
70	9.578	2557	2562	2565	rVV2	604	512	0.05%	0.007%
71	9.594	2565	2567	2568	rVV2	321	158	0.02%	0.002%
72	9.616	2572	2574	2579	rVB	257	189	0.02%	0.002%
73	9.642	2579	2582	2584	rBV	179	155	0.02%	0.002%
74	9.693	2589	2598	2603	rBV3	1257	1744	0.17%	0.023%
75	9.767	2617	2621	2622	rBV	198	162	0.02%	0.002%
76	9.874	2651	2654	2660	rBV	249	340	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
 Data File : VU052888.D
 Acq On : 31 Jan 2023 18:50
 Operator : JC/MD
 Sample : 01381-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44M8

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\SFAMULM012623WMA.M
 Title : VOC Analysis

77	9.970	2681	2684	2687	rBV	222	148	0.01%	0.002%
78	10.089	2718	2721	2722	rBV	467	230	0.02%	0.003%
79	10.144	2735	2738	2742	rBV	210	159	0.02%	0.002%
80	10.269	2774	2777	2781	rVB	225	179	0.02%	0.002%
81	10.314	2788	2791	2796	rBV	182	171	0.02%	0.002%
82	10.394	2813	2816	2817	rBV	360	228	0.02%	0.003%
83	10.610	2878	2883	2884	rBV	208	192	0.02%	0.003%
84	10.751	2914	2927	2944	rBV	313819	500598	49.42%	6.562%
85	11.105	3030	3037	3042	rBV	450	637	0.06%	0.008%
86	11.275	3087	3090	3092	rBV	283	189	0.02%	0.002%
87	11.748	3228	3237	3243	rVB4	1263	1917	0.19%	0.025%
88	11.809	3243	3256	3276	rBV	389604	633123	62.50%	8.300%
89	12.060	3327	3334	3343	rBV6	2986	5033	0.50%	0.066%
90	12.189	3362	3374	3402	rBV2	435527	772583	76.27%	10.128%
91	12.410	3441	3443	3446	rBV	256	151	0.01%	0.002%
92	13.060	3642	3645	3648	rBV	430	269	0.03%	0.004%
93	13.105	3656	3659	3661	rBV2	296	179	0.02%	0.002%
94	13.150	3671	3673	3678	rVB	404	208	0.02%	0.003%
95	13.835	3876	3886	3900	rBV2	46933	74533	7.36%	0.977%
96	13.963	3922	3926	3928	rBV2	622	467	0.05%	0.006%
97	14.037	3946	3949	3951	rBV2	332	207	0.02%	0.003%
98	14.327	4031	4039	4050	rBV3	12234	18929	1.87%	0.248%
99	14.664	4141	4144	4146	rBV	402	246	0.02%	0.003%
100	14.922	4221	4224	4225	rBV	653	349	0.03%	0.005%

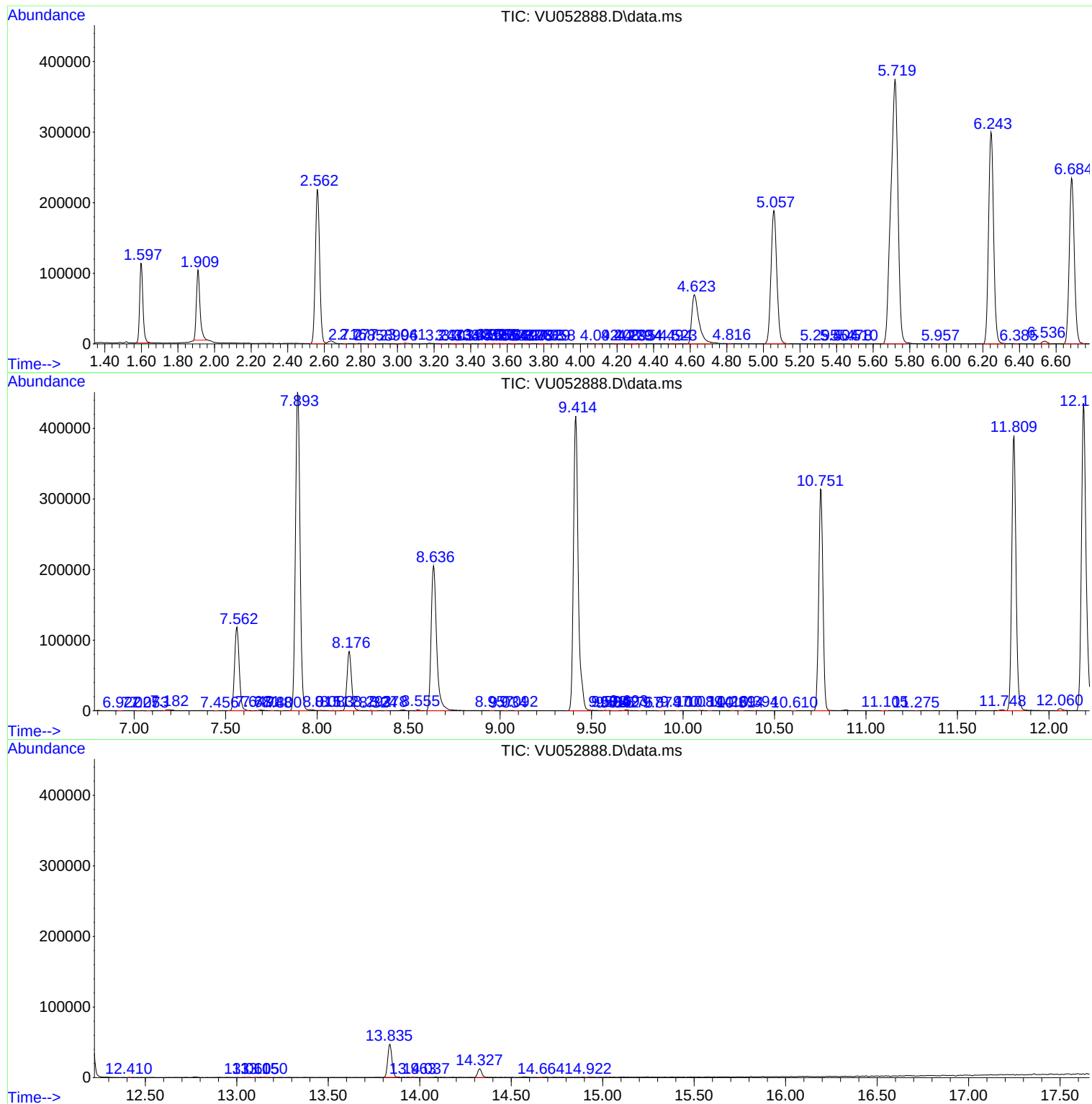
Sum of corrected areas: 7628206

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
Data File : VU052888.D
Acq On : 31 Jan 2023 18:50
Operator : JC/MD
Sample : 01381-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44M8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
Data File : VU052888.D
Acq On : 31 Jan 2023 18:50
Operator : JC/MD
Sample : 01381-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44M8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013123\
Data File : VU052888.D
Acq On : 31 Jan 2023 18:50
Operator : JC/MD
Sample : 01381-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44M8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------