

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020223\
 Data File : VU052928.D
 Acq On : 02 Feb 2023 16:12
 Operator : JC/MD
 Sample : 01412-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44K2

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: VU052928.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	72	80	99	rBV	95049	116361	12.59%	1.726%
2	1.909	169	177	197	rVB	87604	123048	13.31%	1.826%
3	2.562	368	380	398	rVV	192379	310812	33.63%	4.611%
4	2.636	398	403	415	rVB3	1345	2386	0.26%	0.035%
5	2.758	437	441	444	rBV2	227	204	0.02%	0.003%
6	2.842	462	467	476	rBB	318	421	0.05%	0.006%
7	2.884	476	480	482	rBV	221	202	0.02%	0.003%
8	3.041	522	529	539	rVB2	2811	4759	0.51%	0.071%
9	3.176	563	571	575	rBV3	792	1260	0.14%	0.019%
10	3.311	611	613	617	rVV	220	207	0.02%	0.003%
11	3.449	654	656	659	rBV	241	151	0.02%	0.002%
12	3.556	685	689	691	rBV2	346	290	0.03%	0.004%
13	3.658	718	721	726	rBV	174	221	0.02%	0.003%
14	3.790	760	762	767	rBV	172	183	0.02%	0.003%
15	3.861	780	784	786	rBB	257	186	0.02%	0.003%
16	3.887	787	792	795	rBB	180	194	0.02%	0.003%
17	3.970	816	818	822	rBV	187	176	0.02%	0.003%
18	4.118	860	864	866	rBB2	280	150	0.02%	0.002%
19	4.215	891	894	896	rBV2	243	158	0.02%	0.002%
20	4.375	938	944	947	rBV	192	260	0.03%	0.004%
21	4.488	975	979	982	rBB	314	223	0.02%	0.003%
22	4.623	1010	1021	1049	rBV	55114	144654	15.65%	2.146%
23	4.838	1086	1088	1092	rBV	296	238	0.03%	0.004%
24	4.893	1100	1105	1109	rBV	307	303	0.03%	0.004%
25	4.919	1110	1113	1115	rVB2	337	152	0.02%	0.002%
26	4.938	1115	1119	1122	rBV2	364	275	0.03%	0.004%
27	4.986	1129	1134	1137	rBB2	256	203	0.02%	0.003%
28	5.057	1138	1156	1176	rBV	178669	391073	42.31%	5.802%
29	5.510	1295	1297	1301	rVB2	278	211	0.02%	0.003%
30	5.719	1340	1362	1385	rBV2	339475	924288	100.00%	13.713%
31	5.874	1407	1410	1413	rBB3	430	312	0.03%	0.005%
32	5.899	1414	1418	1420	rBV	300	223	0.02%	0.003%
33	5.941	1427	1431	1434	rBV	175	208	0.02%	0.003%
34	6.092	1475	1478	1482	rBV	280	234	0.03%	0.003%
35	6.160	1495	1499	1502	rBB2	287	213	0.02%	0.003%
36	6.244	1511	1525	1550	rBV	281621	531185	57.47%	7.881%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020223\
 Data File : VU052928.D
 Acq On : 02 Feb 2023 16:12
 Operator : JC/MD
 Sample : 01412-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44K2

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	6.449	1585	1589	1591	rBB2	286	197	0.02%	0.003%
38	6.530	1610	1614	1615	rBV2	1138	768	0.08%	0.011%
39	6.684	1649	1662	1685	rBV	215761	416153	45.02%	6.174%
40	6.764	1685	1687	1692	rVV2	437	264	0.03%	0.004%
41	6.809	1695	1701	1707	rVB2	552	615	0.07%	0.009%
42	7.012	1759	1764	1767	rBB	206	199	0.02%	0.003%
43	7.115	1792	1796	1799	rBV	172	179	0.02%	0.003%
44	7.186	1811	1818	1828	rVB5	1665	2586	0.28%	0.038%
45	7.362	1868	1873	1876	rBB	197	189	0.02%	0.003%
46	7.427	1885	1893	1899	rBV	204	450	0.05%	0.007%
47	7.562	1923	1935	1956	rBV	110433	196306	21.24%	2.913%
48	7.694	1968	1976	1984	rVB3	1104	1336	0.14%	0.020%
49	7.777	1997	2002	2005	rBV	330	293	0.03%	0.004%
50	7.845	2020	2023	2025	rBV2	284	165	0.02%	0.002%
51	7.893	2025	2038	2056	rBV	420813	715241	77.38%	10.612%
52	8.173	2114	2125	2145	rVV	76937	132459	14.33%	1.965%
53	8.259	2149	2152	2155	rVV2	376	282	0.03%	0.004%
54	8.452	2209	2212	2213	rBV	513	271	0.03%	0.004%
55	8.636	2257	2269	2297	rBV3	164587	332920	36.02%	4.939%
56	8.816	2321	2325	2329	rBV	269	236	0.03%	0.004%
57	9.063	2399	2402	2406	rBV	269	254	0.03%	0.004%
58	9.157	2428	2431	2434	rBV2	346	283	0.03%	0.004%
59	9.327	2481	2484	2487	rBV	183	179	0.02%	0.003%
60	9.414	2498	2511	2530	rBV	386637	635905	68.80%	9.435%
61	9.542	2548	2551	2555	rBV2	433	283	0.03%	0.004%
62	9.623	2571	2576	2581	rBV2	274	389	0.04%	0.006%
63	9.938	2670	2674	2677	rBV	395	329	0.04%	0.005%
64	10.079	2716	2718	2720	rBV	367	161	0.02%	0.002%
65	10.112	2726	2728	2733	rVB	314	252	0.03%	0.004%
66	10.230	2763	2765	2770	rVB	237	179	0.02%	0.003%
67	10.256	2770	2773	2778	rVB	409	319	0.03%	0.005%
68	10.398	2814	2817	2820	rBV	282	184	0.02%	0.003%
69	10.417	2820	2823	2829	rVV	132	153	0.02%	0.002%
70	10.549	2860	2864	2866	rBV	209	203	0.02%	0.003%
71	10.677	2901	2904	2909	rBB	177	191	0.02%	0.003%
72	10.751	2910	2927	2945	rBV	279155	447715	48.44%	6.643%
73	10.890	2967	2970	2976	rVB3	513	400	0.04%	0.006%
74	11.070	3023	3026	3029	rBV2	273	189	0.02%	0.003%
75	11.092	3030	3033	3038	rVV	225	174	0.02%	0.003%
76	11.192	3060	3064	3066	rBV	326	260	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020223\
 Data File : VU052928.D
 Acq On : 02 Feb 2023 16:12
 Operator : JC/MD
 Sample : 01412-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44K2

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	11.330	3104	3107	3109	rBV	208	167	0.02%	0.002%
78	11.375	3118	3121	3125	rBV2	270	187	0.02%	0.003%
79	11.584	3184	3186	3188	rBV	266	157	0.02%	0.002%
80	11.632	3198	3201	3204	rVB	290	158	0.02%	0.002%
81	11.809	3240	3256	3273	rBV	384630	611339	66.14%	9.070%
82	12.057	3325	3333	3346	rBV5	7235	12640	1.37%	0.188%
83	12.144	3357	3360	3362	rBV	287	161	0.02%	0.002%
84	12.189	3362	3374	3394	rVV	403794	660115	71.42%	9.794%
85	12.327	3415	3417	3421	rVB2	280	154	0.02%	0.002%
86	12.436	3447	3451	3457	rBV2	343	346	0.04%	0.005%
87	12.546	3481	3485	3488	rVB2	291	211	0.02%	0.003%
88	12.838	3572	3576	3578	rBV2	376	254	0.03%	0.004%
89	12.864	3581	3584	3587	rBV2	246	163	0.02%	0.002%
90	12.890	3589	3592	3596	rBV2	694	653	0.07%	0.010%
91	13.217	3689	3694	3707	rVB5	1338	2047	0.22%	0.030%
92	13.488	3775	3778	3784	rBV2	299	307	0.03%	0.005%
93	13.838	3882	3887	3895	rBV4	1844	2552	0.28%	0.038%
94	13.967	3925	3927	3930	rVB2	349	158	0.02%	0.002%
95	14.092	3962	3966	3969	rVV2	486	460	0.05%	0.007%
96	14.333	4034	4041	4047	rBV4	1329	1791	0.19%	0.027%
97	14.417	4065	4067	4072	rVB2	677	485	0.05%	0.007%
98	14.446	4072	4076	4077	rBV	398	198	0.02%	0.003%
99	14.639	4133	4136	4138	rBV	263	200	0.02%	0.003%
100	15.221	4314	4317	4322	rBV3	520	393	0.04%	0.006%

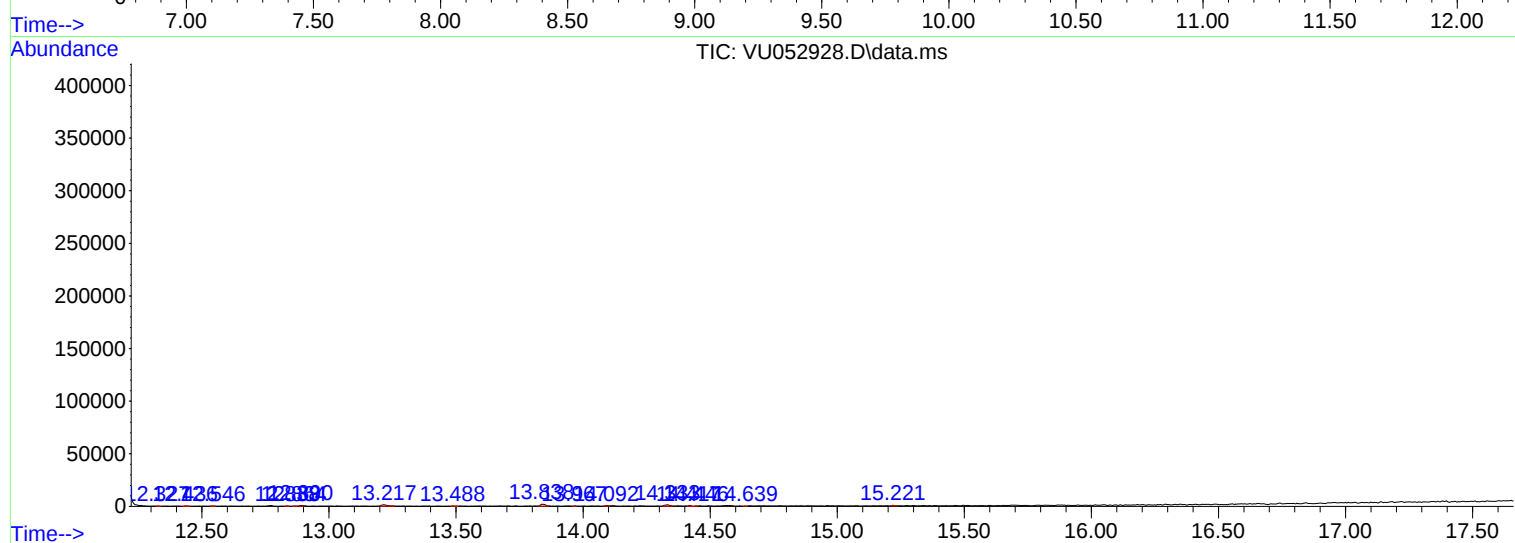
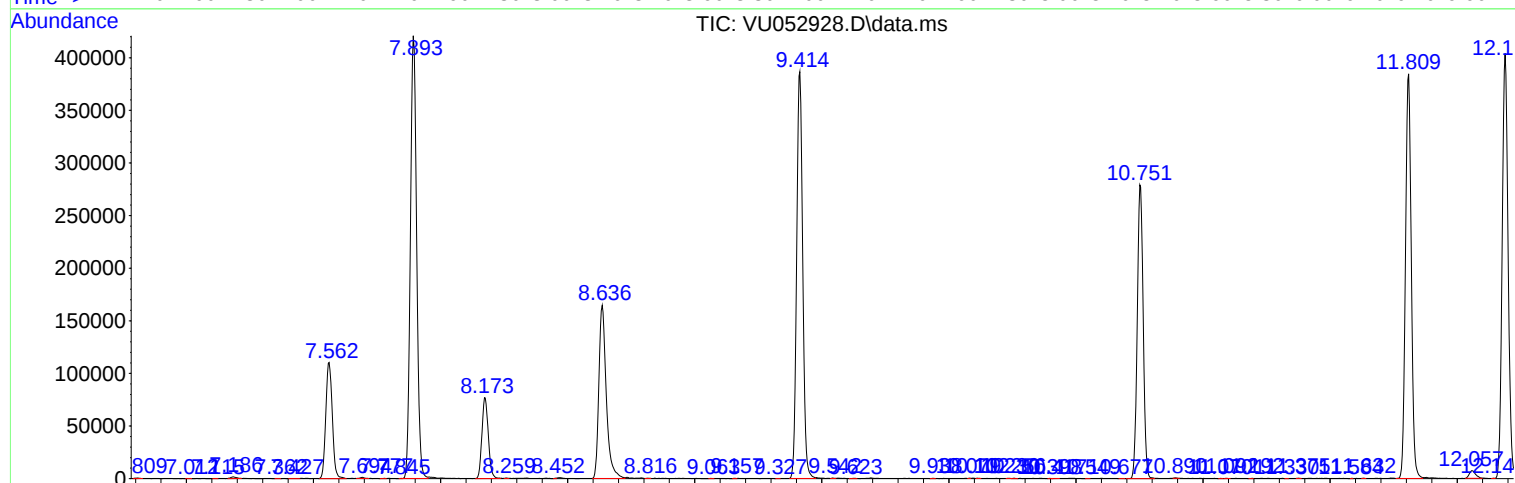
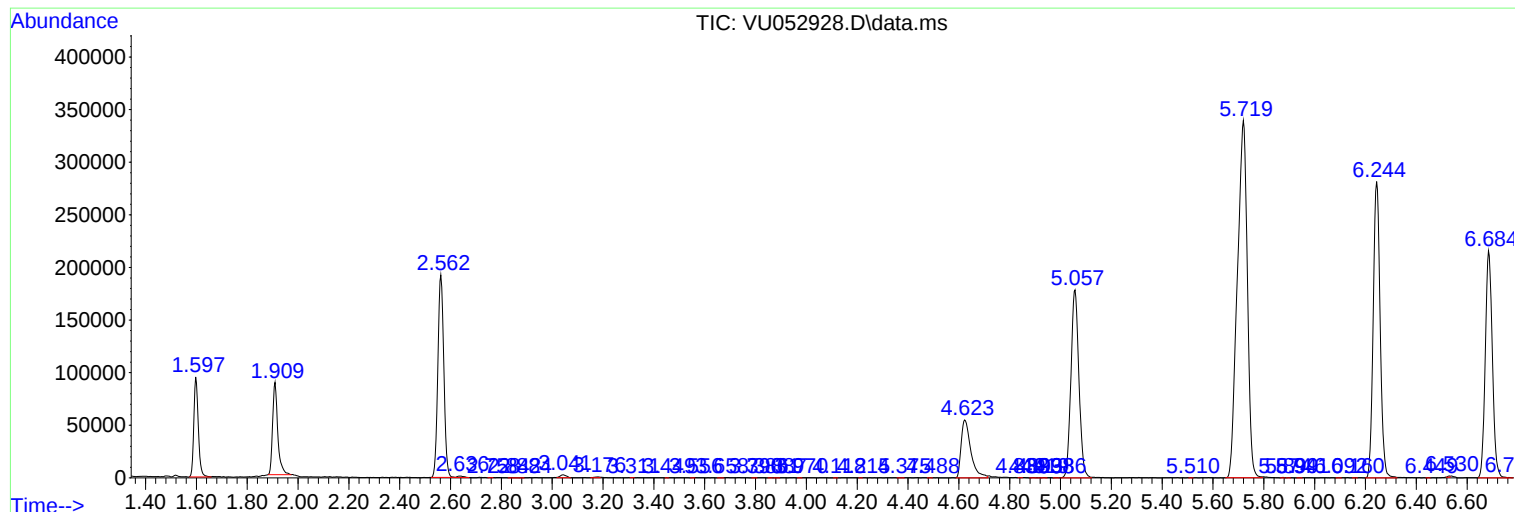
Sum of corrected areas: 6740031

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020223\
Data File : VU052928.D
Acq On : 02 Feb 2023 16:12
Operator : JC/MD
Sample : 01412-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44K2

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\VU020223\
Data File : VU052928.D
Acq On : 02 Feb 2023 16:12
Operator : JC/MD
Sample : 01412-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44K2

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\VU020223\
Data File : VU052928.D
Acq On : 02 Feb 2023 16:12
Operator : JC/MD
Sample : 01412-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44K2

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	--Internal Standard--			
					#	RT	Resp	Conc