

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
 Data File : VU052038.D
 Acq On : 22 Nov 2022 12:33
 Operator : JC/MD
 Sample : N5658-10ME
 Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ESQT0ME

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\SFAMULM112122WMA.M
 Title : VOC Analysis

Signal : TIC: VU052038.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	112	rVB	146624	266075	15.23%	1.928%
2	2.536	360	372	395	rVB	339007	548368	31.39%	3.974%
3	2.900	482	485	487	rBV2	357	229	0.01%	0.002%
4	2.916	487	490	494	rVB4	586	474	0.03%	0.003%
5	3.035	512	527	546	rBV4	7484	18288	1.05%	0.133%
6	3.176	559	571	591	rVB	31354	70013	4.01%	0.507%
7	3.523	676	679	685	rBV3	369	389	0.02%	0.003%
8	3.594	698	701	704	rBV	321	269	0.02%	0.002%
9	3.642	714	716	718	rBV	209	124	0.01%	0.001%
10	3.671	718	725	734	rVV5	1215	2142	0.12%	0.016%
11	3.745	746	748	750	rBV	170	97	0.01%	0.001%
12	3.822	769	772	778	rVB	296	245	0.01%	0.002%
13	3.858	778	783	784	rBV	222	215	0.01%	0.002%
14	3.967	813	817	820	rBV2	152	136	0.01%	0.001%
15	3.986	820	823	828	rVV	275	255	0.01%	0.002%
16	4.099	856	858	862	rVB	501	303	0.02%	0.002%
17	4.118	862	864	868	rBV2	181	111	0.01%	0.001%
18	4.224	892	897	904	rBV	238	265	0.02%	0.002%
19	4.353	933	937	938	rBV	294	179	0.01%	0.001%
20	4.462	967	971	974	rBV	296	265	0.02%	0.002%
21	4.629	1011	1023	1063	rBV	116328	399717	22.88%	2.897%
22	5.057	1140	1156	1186	rBV	299944	680369	38.94%	4.931%
23	5.430	1268	1272	1277	rBV3	358	387	0.02%	0.003%
24	5.472	1283	1285	1290	rVB2	391	259	0.01%	0.002%
25	5.498	1290	1293	1295	rBV	249	114	0.01%	0.001%
26	5.514	1295	1298	1300	rVV	333	169	0.01%	0.001%
27	5.713	1341	1360	1395	rBV2	679914	1747225	100.00%	12.662%
28	5.977	1432	1442	1456	rBV4	3877	8346	0.48%	0.060%
29	6.099	1473	1480	1485	rBV4	644	839	0.05%	0.006%
30	6.173	1500	1503	1509	rBV2	220	298	0.02%	0.002%
31	6.243	1509	1525	1558	rBV	554010	1094775	62.66%	7.934%
32	6.469	1593	1595	1598	rBV2	313	118	0.01%	0.001%
33	6.523	1602	1612	1624	rBV10	4939	11500	0.66%	0.083%
34	6.597	1624	1635	1639	rBV3	6326	10219	0.58%	0.074%
35	6.684	1649	1662	1691	rVB	395271	789518	45.19%	5.722%
36	6.932	1736	1739	1744	rVB	369	279	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
 Data File : VU052038.D
 Acq On : 22 Nov 2022 12:33
 Operator : JC/MD
 Sample : N5658-10ME
 Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ESQTOME

Integration Parameters: LSCINT.P

Integrator: RTE

Soothing : 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\SFAMULM112122WMA.M
 Title : VOC Analysis

37	6.960	1744	1748	1750	rBV	290	206	0.01%	0.001%
38	7.012	1762	1764	1769	rBV2	315	241	0.01%	0.002%
39	7.038	1769	1772	1774	rBV2	259	177	0.01%	0.001%
40	7.067	1777	1781	1782	rBV	174	125	0.01%	0.001%
41	7.102	1789	1792	1797	rBV	340	286	0.02%	0.002%
42	7.128	1797	1800	1803	rBV2	172	119	0.01%	0.001%
43	7.198	1809	1822	1842	rBV10	5104	15224	0.87%	0.110%
44	7.314	1853	1858	1862	rBV2	348	337	0.02%	0.002%
45	7.350	1865	1869	1873	rBV	452	384	0.02%	0.003%
46	7.420	1887	1891	1893	rBV2	330	247	0.01%	0.002%
47	7.491	1910	1913	1916	rBV2	208	177	0.01%	0.001%
48	7.562	1920	1935	1960	rBV	190859	368096	21.07%	2.668%
49	7.745	1989	1992	1996	rVB3	610	465	0.03%	0.003%
50	7.787	1996	2005	2010	rBV5	2398	4141	0.24%	0.030%
51	7.893	2025	2038	2057	rBV	741064	1360410	77.86%	9.859%
52	8.179	2114	2127	2154	rBV2	122526	255115	14.60%	1.849%
53	8.353	2179	2181	2183	rBV	528	310	0.02%	0.002%
54	8.423	2201	2203	2206	rBV	263	147	0.01%	0.001%
55	8.446	2206	2210	2212	rBV2	309	216	0.01%	0.002%
56	8.542	2236	2240	2241	rBV3	552	366	0.02%	0.003%
57	8.597	2253	2257	2259	rBV	329	269	0.02%	0.002%
58	8.649	2259	2273	2307	rBV	462272	959827	54.93%	6.956%
59	8.919	2354	2357	2359	rBV2	827	596	0.03%	0.004%
60	8.957	2367	2369	2371	rBV2	347	147	0.01%	0.001%
61	9.230	2451	2454	2456	rVV2	257	177	0.01%	0.001%
62	9.259	2460	2463	2466	rVB	219	106	0.01%	0.001%
63	9.298	2470	2475	2478	rVB2	265	229	0.01%	0.002%
64	9.321	2478	2482	2486	rBV	187	162	0.01%	0.001%
65	9.343	2486	2489	2491	rBV2	161	109	0.01%	0.001%
66	9.420	2497	2513	2533	rBV	756710	1396322	79.92%	10.119%
67	9.671	2582	2591	2593	rBV10	2455	3422	0.20%	0.025%
68	9.790	2625	2628	2631	rBV	207	182	0.01%	0.001%
69	9.832	2637	2641	2644	rBV2	290	274	0.02%	0.002%
70	9.883	2652	2657	2660	rBV2	317	309	0.02%	0.002%
71	9.902	2660	2663	2665	rBV2	229	174	0.01%	0.001%
72	10.005	2689	2695	2697	rBV2	240	231	0.01%	0.002%
73	10.034	2701	2704	2707	rBV2	279	189	0.01%	0.001%
74	10.066	2711	2714	2717	rBV	306	146	0.01%	0.001%
75	10.095	2718	2723	2724	rBV2	691	492	0.03%	0.004%
76	10.266	2773	2776	2778	rBV2	176	96	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
 Data File : VU052038.D
 Acq On : 22 Nov 2022 12:33
 Operator : JC/MD
 Sample : N5658-10ME
 Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ESQTOME

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\SFAMULM112122WMA.M
 Title : VOC Analysis

77	10.317	2781	2792	2806	rVB3	16883	29513	1.69%	0.214%
78	10.372	2806	2809	2811	rBV2	195	139	0.01%	0.001%
79	10.462	2829	2837	2850	rBV5	8335	13943	0.80%	0.101%
80	10.555	2863	2866	2869	rBV2	264	180	0.01%	0.001%
81	10.626	2881	2888	2892	rBV4	787	966	0.06%	0.007%
82	10.758	2912	2929	2950	rBV	696776	1183286	67.72%	8.575%
83	10.996	3000	3003	3006	rBV	276	168	0.01%	0.001%
84	11.410	3130	3132	3138	rVB2	852	681	0.04%	0.005%
85	11.645	3202	3205	3213	rVB5	956	965	0.06%	0.007%
86	11.719	3226	3228	3231	rVB	373	186	0.01%	0.001%
87	11.738	3231	3234	3243	rBV6	1384	1652	0.09%	0.012%
88	11.812	3244	3257	3281	rBV	773513	1223470	70.02%	8.866%
89	12.192	3362	3375	3395	rBV	773579	1253305	71.73%	9.083%
90	12.410	3441	3443	3446	rBV2	427	228	0.01%	0.002%
91	12.452	3453	3456	3458	rBV2	717	421	0.02%	0.003%
92	12.533	3479	3481	3483	rBV2	336	136	0.01%	0.001%
93	12.652	3515	3518	3519	rBV2	485	287	0.02%	0.002%
94	12.684	3527	3528	3532	rVB3	278	144	0.01%	0.001%
95	12.951	3607	3611	3614	rBV3	483	482	0.03%	0.003%
96	13.221	3688	3695	3706	rBV3	5664	9354	0.54%	0.068%
97	13.735	3850	3855	3860	rBV5	884	1057	0.06%	0.008%
98	13.812	3877	3879	3881	rBV	638	364	0.02%	0.003%
99	14.330	4031	4040	4056	rBV2	12743	21432	1.23%	0.155%
100	14.905	4211	4219	4229	rBV4	23003	33650	1.93%	0.244%

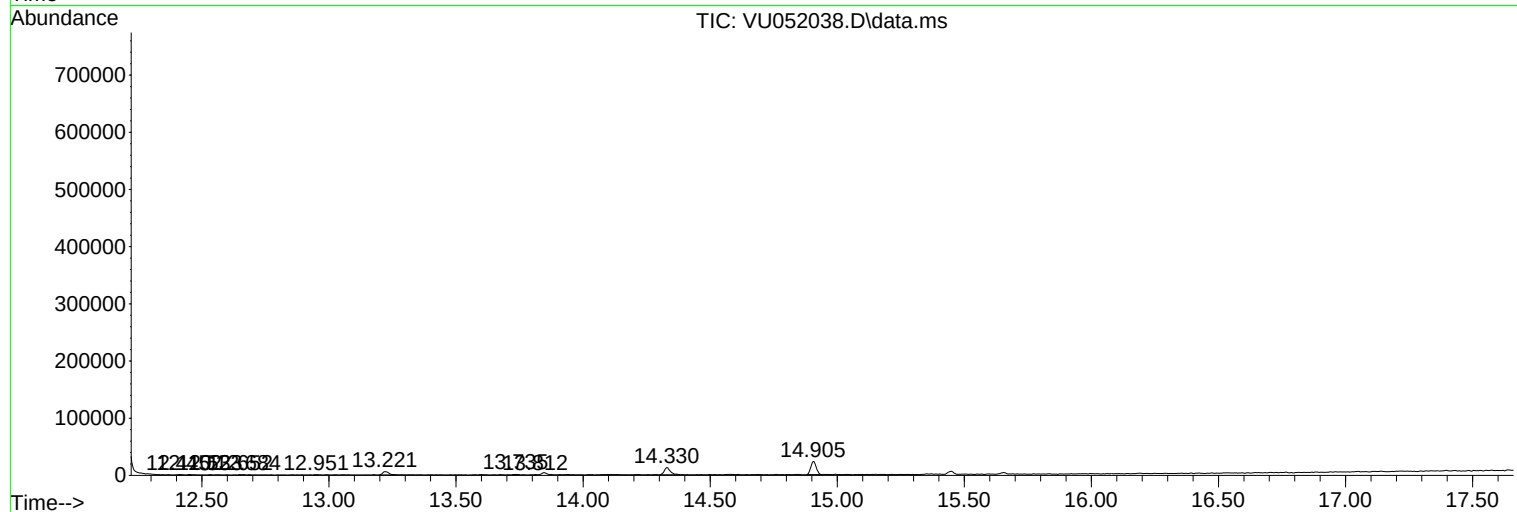
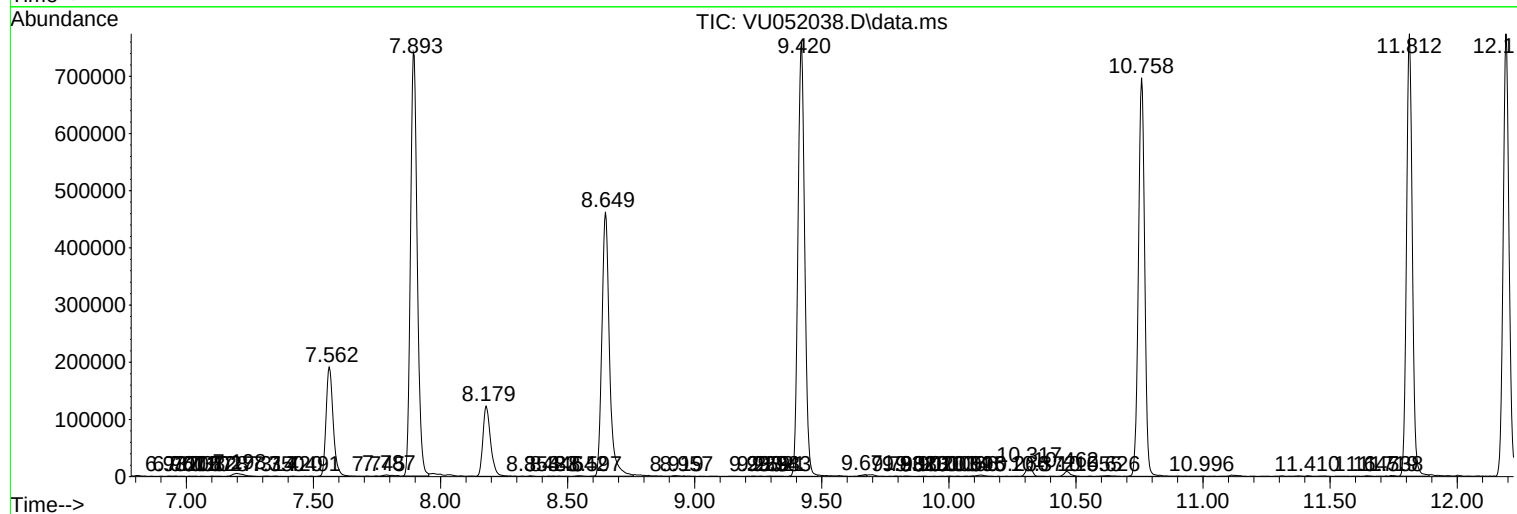
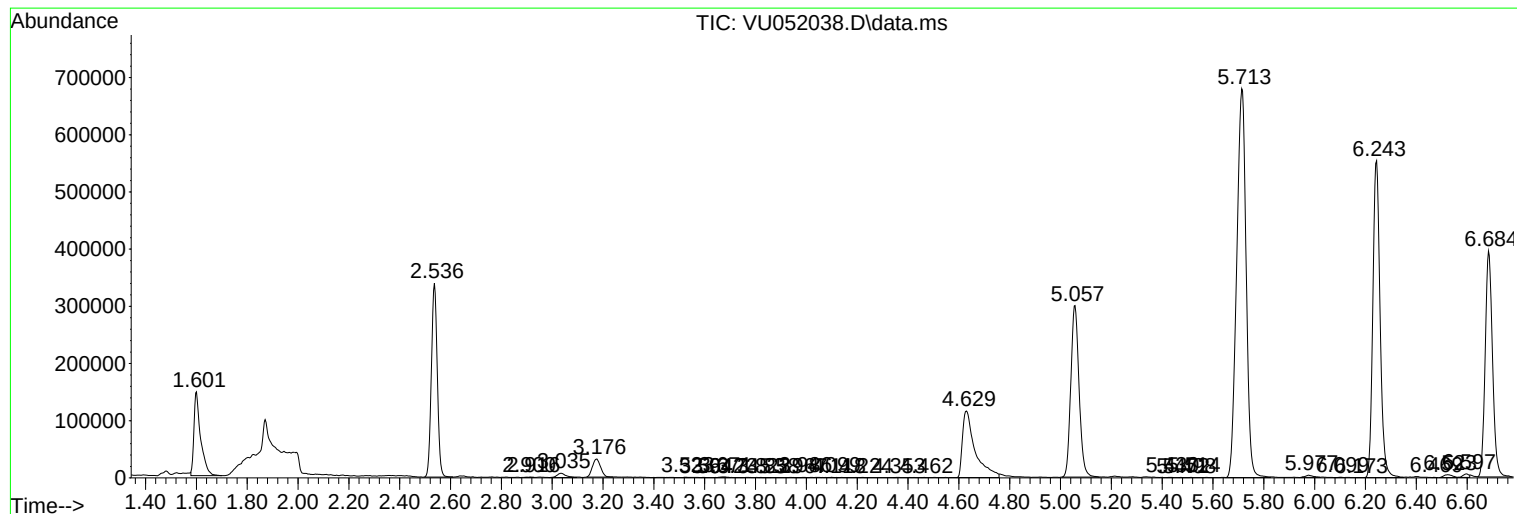
Sum of corrected areas: 13798831

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
Data File : VU052038.D
Acq On : 22 Nov 2022 12:33
Operator : JC/MD
Sample : N5658-10ME
Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ESQT0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
Data File : VU052038.D
Acq On : 22 Nov 2022 12:33
Operator : JC/MD
Sample : N5658-10ME
Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ESQT0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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\VU112122\
Data File : VU052038.D
Acq On : 22 Nov 2022 12:33
Operator : JC/MD
Sample : N5658-10ME
Misc : 2.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ESQT0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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
------------------	----	---------	-------	----------	---	----	------	------