

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051176.D
 Acq On : 06 Oct 2022 16:57
 Operator : JC/MD
 Sample : N4858-01ME
 Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGSE8ME

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\SFAMULM092922WMA.M
 Title : VOC Analysis

Signal : TIC: VU051176.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	74	80	106	rVB	117634	245772	15.49%	1.840%
2	2.523	357	368	388	rVB	322348	520518	32.81%	3.897%
3	3.176	555	571	594	rBV	47995	117917	7.43%	0.883%
4	3.469	659	662	664	rBV	471	270	0.02%	0.002%
5	3.565	690	692	696	rBV	355	250	0.02%	0.002%
6	3.662	718	722	723	rBV2	887	620	0.04%	0.005%
7	3.716	735	739	743	rVB2	566	501	0.03%	0.004%
8	3.739	743	746	748	rBV3	340	187	0.01%	0.001%
9	3.887	788	792	794	rVV2	218	168	0.01%	0.001%
10	3.944	805	810	812	rBV2	283	286	0.02%	0.002%
11	4.047	837	842	846	rBV2	297	249	0.02%	0.002%
12	4.099	853	858	861	rBV2	543	431	0.03%	0.003%
13	4.150	872	874	878	rBV	282	219	0.01%	0.002%
14	4.221	893	896	898	rBV2	223	144	0.01%	0.001%
15	4.279	912	914	920	rBV2	185	173	0.01%	0.001%
16	4.369	938	942	945	rBV2	319	257	0.02%	0.002%
17	4.424	957	959	963	rVB2	297	176	0.01%	0.001%
18	4.446	963	966	968	rBV	217	159	0.01%	0.001%
19	4.485	972	978	979	rBV2	309	305	0.02%	0.002%
20	4.514	984	987	991	rBV2	361	258	0.02%	0.002%
21	4.636	1013	1025	1046	rBV	111091	351357	22.15%	2.631%
22	5.057	1140	1156	1182	rBV	272728	631490	39.80%	4.728%
23	5.227	1207	1209	1211	rBV2	293	159	0.01%	0.001%
24	5.407	1262	1265	1266	rBV2	212	130	0.01%	0.001%
25	5.440	1272	1275	1277	rBV2	358	206	0.01%	0.002%
26	5.456	1277	1280	1285	rVB2	373	286	0.02%	0.002%
27	5.623	1329	1332	1333	rBV	154	87	0.01%	0.001%
28	5.716	1340	1361	1385	rBV2	618819	1586618	100.00%	11.879%
29	5.874	1408	1410	1414	rBV2	415	227	0.01%	0.002%
30	5.915	1418	1423	1425	rBV	294	328	0.02%	0.002%
31	5.973	1432	1441	1460	rBV3	13879	31829	2.01%	0.238%
32	6.079	1473	1474	1477	rBV2	197	101	0.01%	0.001%
33	6.102	1477	1481	1485	rVV2	561	489	0.03%	0.004%
34	6.243	1511	1525	1553	rBV	536065	1069589	67.41%	8.008%
35	6.533	1603	1615	1626	rBV	10355	21849	1.38%	0.164%
36	6.597	1628	1635	1647	rBV5	6236	12336	0.78%	0.092%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051176.D
 Acq On : 06 Oct 2022 16:57
 Operator : JC/MD
 Sample : N4858-01ME
 Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGSE8ME

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\SFAMULM092922WMA.M
 Title : VOC Analysis

37	6.687	1650	1663	1682	rVB	360793	732720	46.18%	5.486%
38	6.858	1711	1716	1717	rBV3	599	497	0.03%	0.004%
39	6.906	1728	1731	1732	rBV	210	120	0.01%	0.001%
40	7.018	1764	1766	1768	rBV2	253	138	0.01%	0.001%
41	7.031	1768	1770	1771	rBV	209	95	0.01%	0.001%
42	7.124	1796	1799	1802	rBV2	328	223	0.01%	0.002%
43	7.224	1810	1830	1845	rBV10	5500	19452	1.23%	0.146%
44	7.301	1851	1854	1857	rBV4	1102	828	0.05%	0.006%
45	7.346	1865	1868	1871	rVB3	463	274	0.02%	0.002%
46	7.411	1886	1888	1890	rVB	314	138	0.01%	0.001%
47	7.433	1891	1895	1897	rBV3	330	224	0.01%	0.002%
48	7.497	1912	1915	1920	rBV2	404	377	0.02%	0.003%
49	7.565	1923	1936	1954	rBV	165850	319046	20.11%	2.389%
50	7.767	1994	1999	2001	rBV2	693	578	0.04%	0.004%
51	7.896	2024	2039	2054	rBV	645712	1154285	72.75%	8.642%
52	8.182	2115	2128	2146	rBV	112653	221785	13.98%	1.660%
53	8.353	2173	2181	2185	rBV6	2141	2988	0.19%	0.022%
54	8.398	2192	2195	2197	rVB2	477	261	0.02%	0.002%
55	8.462	2213	2215	2218	rBV3	507	319	0.02%	0.002%
56	8.549	2226	2242	2259	rBV	561082	962527	60.67%	7.206%
57	8.648	2260	2273	2307	rVV2	374671	838275	52.83%	6.276%
58	9.015	2385	2387	2391	rVB	418	200	0.01%	0.001%
59	9.054	2396	2399	2402	rBV2	342	170	0.01%	0.001%
60	9.076	2402	2406	2407	rBV2	523	336	0.02%	0.003%
61	9.118	2417	2419	2421	rBV2	297	132	0.01%	0.001%
62	9.156	2428	2431	2432	rBV2	561	354	0.02%	0.003%
63	9.202	2443	2445	2446	rBV2	217	97	0.01%	0.001%
64	9.224	2450	2452	2454	rBV	216	91	0.01%	0.001%
65	9.266	2460	2465	2467	rBV2	440	338	0.02%	0.003%
66	9.330	2481	2485	2491	rVB3	385	403	0.03%	0.003%
67	9.369	2491	2497	2499	rBV2	574	537	0.03%	0.004%
68	9.420	2499	2513	2534	rBV	768929	1378367	86.87%	10.320%
69	9.648	2581	2584	2586	rBV2	370	231	0.01%	0.002%
70	9.697	2588	2599	2610	rVV4	4165	7839	0.49%	0.059%
71	9.777	2619	2624	2626	rBV3	308	301	0.02%	0.002%
72	9.845	2639	2645	2646	rBV	404	359	0.02%	0.003%
73	9.873	2651	2654	2659	rVB3	451	343	0.02%	0.003%
74	9.912	2660	2666	2670	rBV3	477	552	0.03%	0.004%
75	10.015	2691	2698	2705	rBV3	561	677	0.04%	0.005%
76	10.047	2705	2708	2710	rBV	353	188	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051176.D
 Acq On : 06 Oct 2022 16:57
 Operator : JC/MD
 Sample : N4858-01ME
 Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGSE8ME

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\SFAMULM092922WMA.M
 Title : VOC Analysis

77	10.102	2718	2725	2730	rBV4	728	972	0.06%	0.007%
78	10.227	2761	2764	2768	rBV	235	176	0.01%	0.001%
79	10.279	2777	2780	2784	rBV2	441	352	0.02%	0.003%
80	10.301	2784	2787	2790	rBV2	282	195	0.01%	0.001%
81	10.488	2842	2845	2846	rBV2	313	171	0.01%	0.001%
82	10.555	2859	2866	2870	rBV	470	491	0.03%	0.004%
83	10.591	2875	2877	2878	rBV	495	170	0.01%	0.001%
84	10.626	2885	2888	2891	rBV	442	360	0.02%	0.003%
85	10.652	2891	2896	2901	rVB5	1117	1026	0.06%	0.008%
86	10.761	2916	2930	2946	rBV	580488	934653	58.91%	6.998%
87	10.890	2965	2970	2977	rVB4	875	1149	0.07%	0.009%
88	10.970	2992	2995	2997	rBV2	316	218	0.01%	0.002%
89	11.115	3029	3040	3051	rVB7	6129	10285	0.65%	0.077%
90	11.192	3062	3064	3066	rBV	184	101	0.01%	0.001%
91	11.311	3099	3101	3107	rVB2	552	397	0.03%	0.003%
92	11.404	3128	3130	3133	rBV	607	387	0.02%	0.003%
93	11.449	3141	3144	3146	rBV3	525	354	0.02%	0.003%
94	11.574	3181	3183	3186	rVB2	400	199	0.01%	0.001%
95	11.664	3209	3211	3213	rVB	352	139	0.01%	0.001%
96	11.812	3245	3257	3278	rBV	717661	1137962	71.72%	8.520%
97	12.195	3362	3376	3393	rBV	630959	1022064	64.42%	7.652%
98	12.494	3466	3469	3472	rBV4	882	652	0.04%	0.005%
99	12.668	3519	3523	3526	rBV2	795	615	0.04%	0.005%
100	13.989	3931	3934	3940	rBV4	1079	1174	0.07%	0.009%

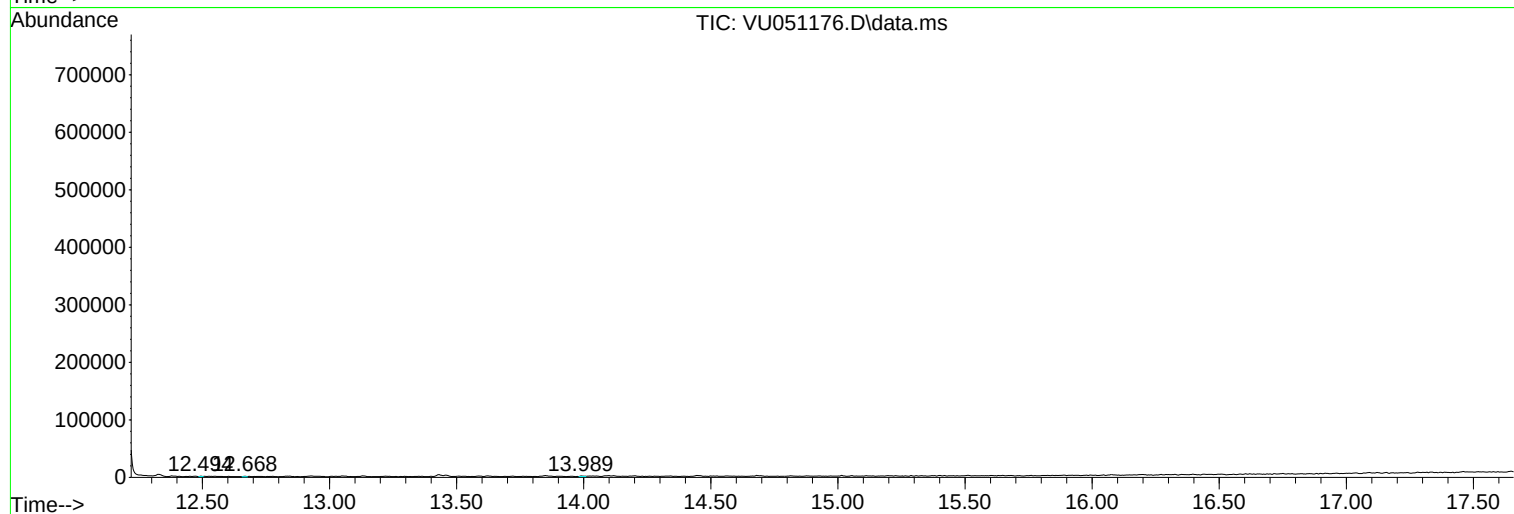
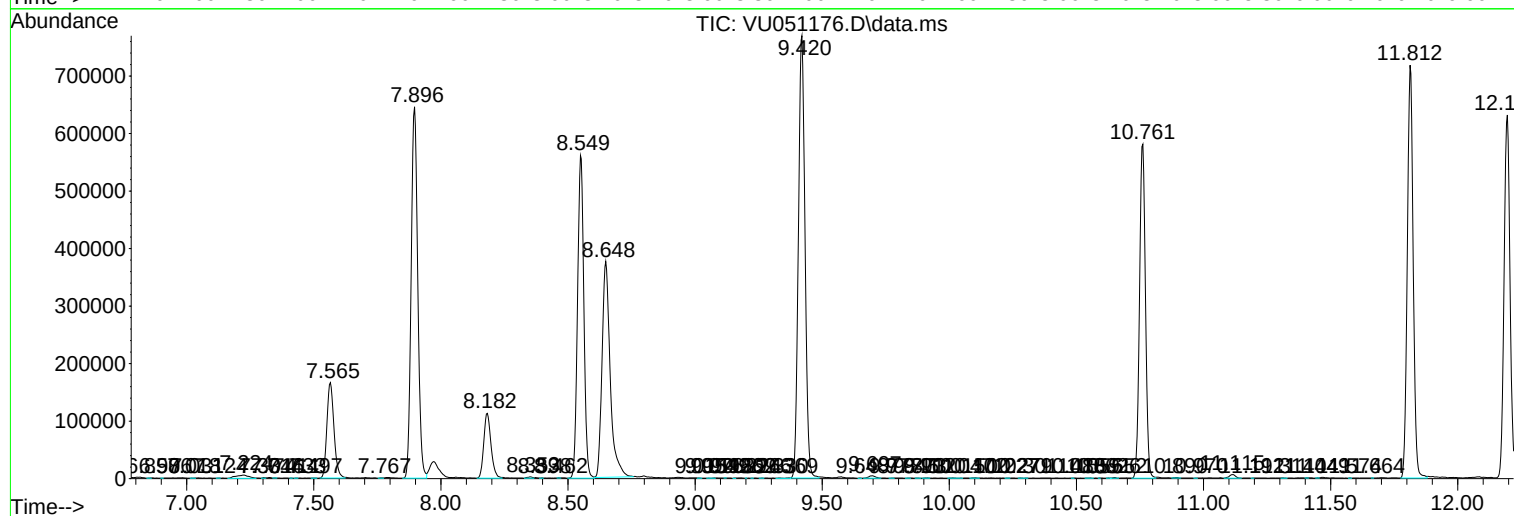
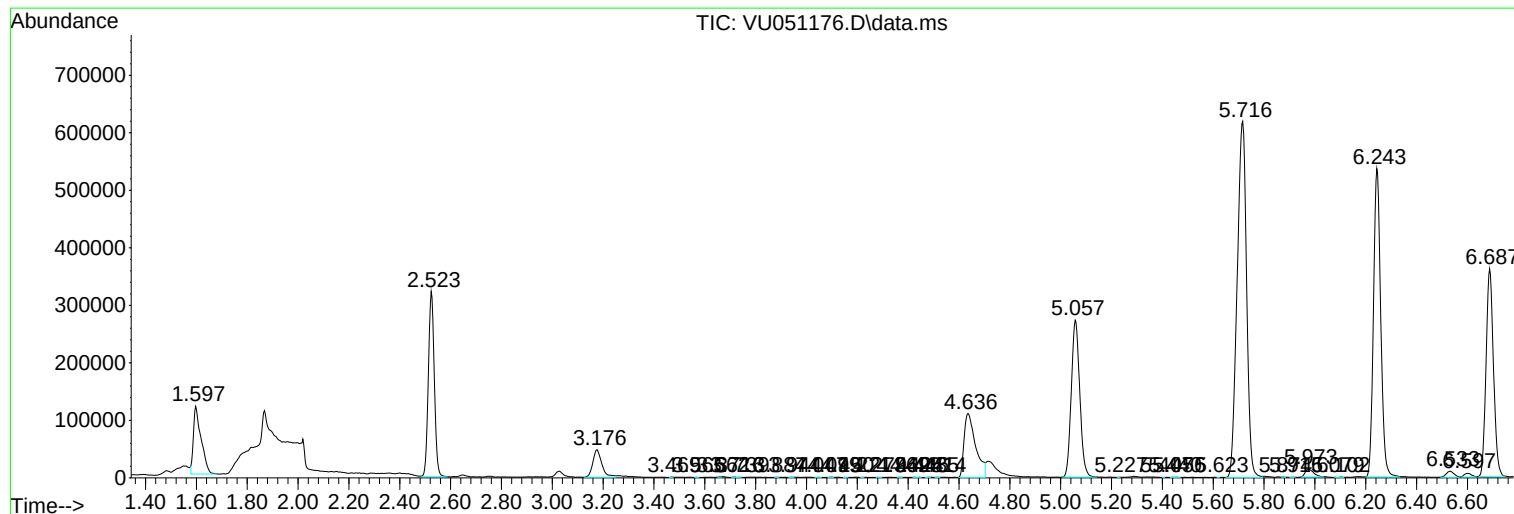
Sum of corrected areas: 13356868

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
Data File : VU051176.D
Acq On : 06 Oct 2022 16:57
Operator : JC/MD
Sample : N4858-01ME
Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGSE8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
Data File : VU051176.D
Acq On : 06 Oct 2022 16:57
Operator : JC/MD
Sample : N4858-01ME
Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGSE8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.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\VU100622\
Data File : VU051176.D
Acq On : 06 Oct 2022 16:57
Operator : JC/MD
Sample : N4858-01ME
Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGSE8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.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
------------------	----	---------	-------	----------	---	----	------	------