

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053503.D
 Acq On : 31 Mar 2023 19:46
 Operator : JC/MD
 Sample : 02130-07ME
 Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1196ME

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: VU053503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	107	rVB	164623	238755	15.65%	1.876%
2	2.543	361	374	391	rVB	350005	570596	37.40%	4.484%
3	2.880	476	479	482	rBV2	552	383	0.03%	0.003%
4	2.941	496	498	503	rBV	311	265	0.02%	0.002%
5	2.964	503	505	507	rBV	294	190	0.01%	0.001%
6	3.034	517	527	534	rBV6	4016	7762	0.51%	0.061%
7	3.173	561	570	576	rBV5	1226	2146	0.14%	0.017%
8	3.333	616	620	622	rBV4	793	603	0.04%	0.005%
9	3.623	707	710	714	rVB2	439	242	0.02%	0.002%
10	3.671	719	725	726	rBV3	1225	1017	0.07%	0.008%
11	3.819	768	771	775	rVB	345	198	0.01%	0.002%
12	3.896	790	795	799	rBV2	272	324	0.02%	0.003%
13	4.044	837	841	843	rBV2	233	209	0.01%	0.002%
14	4.160	872	877	880	rBV	184	195	0.01%	0.002%
15	4.462	961	971	975	rBV2	273	335	0.02%	0.003%
16	4.514	982	987	991	rVV	306	278	0.02%	0.002%
17	4.620	1007	1020	1065	rVV	94947	295292	19.35%	2.320%
18	5.054	1138	1155	1178	rVV	269502	626237	41.05%	4.921%
19	5.221	1203	1207	1210	rBV	393	327	0.02%	0.003%
20	5.266	1215	1221	1222	rBV	247	191	0.01%	0.002%
21	5.327	1236	1240	1243	rBV2	718	627	0.04%	0.005%
22	5.346	1243	1246	1247	rBV	435	227	0.01%	0.002%
23	5.440	1269	1275	1277	rBV2	243	245	0.02%	0.002%
24	5.555	1307	1311	1314	rBV	212	209	0.01%	0.002%
25	5.584	1317	1320	1324	rVB3	567	369	0.02%	0.003%
26	5.713	1337	1360	1388	rBV2	582669	1525724	100.00%	11.989%
27	5.967	1432	1439	1440	rBV2	1146	1142	0.07%	0.009%
28	6.031	1454	1459	1461	rBV2	362	345	0.02%	0.003%
29	6.115	1477	1485	1489	rBV6	1223	1504	0.10%	0.012%
30	6.185	1503	1507	1510	rVB	417	231	0.02%	0.002%
31	6.240	1510	1524	1552	rBV	456713	892583	58.50%	7.014%
32	6.420	1577	1580	1582	rBV2	395	250	0.02%	0.002%
33	6.526	1602	1613	1626	rBV7	12770	25596	1.68%	0.201%
34	6.684	1648	1662	1681	rBV	335615	663698	43.50%	5.215%
35	6.845	1709	1712	1717	rVB2	469	366	0.02%	0.003%
36	6.893	1723	1727	1729	rBV2	248	224	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053503.D
 Acq On : 31 Mar 2023 19:46
 Operator : JC/MD
 Sample : 02130-07ME
 Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1196ME

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	6.931	1737	1739	1750	rVB	269	238	0.02%	0.002%
38	7.034	1766	1771	1774	rBV2	219	204	0.01%	0.002%
39	7.095	1786	1790	1793	rVB2	322	213	0.01%	0.002%
40	7.182	1810	1817	1819	rBV	1056	981	0.06%	0.008%
41	7.282	1844	1848	1851	rVB2	327	241	0.02%	0.002%
42	7.317	1854	1859	1862	rBV3	469	455	0.03%	0.004%
43	7.365	1871	1874	1878	rBV	266	231	0.02%	0.002%
44	7.558	1920	1934	1957	rBV	192555	359616	23.57%	2.826%
45	7.677	1969	1971	1974	rBV2	397	261	0.02%	0.002%
46	7.828	2013	2018	2021	rBV	228	205	0.01%	0.002%
47	7.893	2025	2038	2057	rBV	757882	1334749	87.48%	10.488%
48	8.124	2106	2110	2114	rBV3	1043	951	0.06%	0.007%
49	8.176	2114	2126	2147	rVV	129969	252017	16.52%	1.980%
50	8.349	2179	2180	2184	rVB	423	191	0.01%	0.002%
51	8.430	2203	2205	2209	rBV2	287	219	0.01%	0.002%
52	8.549	2229	2242	2258	rBV	234035	404013	26.48%	3.175%
53	8.642	2258	2271	2307	rVB	371500	711570	46.64%	5.591%
54	8.864	2337	2340	2344	rBV	311	214	0.01%	0.002%
55	9.163	2429	2433	2440	rBV2	440	398	0.03%	0.003%
56	9.324	2479	2483	2484	rBV2	409	300	0.02%	0.002%
57	9.414	2498	2511	2537	rBV	614028	1118609	73.32%	8.790%
58	9.693	2591	2598	2600	rBV3	979	1119	0.07%	0.009%
59	9.735	2608	2611	2612	rBV	518	262	0.02%	0.002%
60	9.980	2685	2687	2691	rVB2	302	239	0.02%	0.002%
61	10.095	2720	2723	2725	rBV3	516	379	0.02%	0.003%
62	10.121	2727	2731	2740	rVB6	1196	1669	0.11%	0.013%
63	10.391	2811	2815	2818	rBV	305	302	0.02%	0.002%
64	10.478	2839	2842	2844	rBV	466	337	0.02%	0.003%
65	10.545	2857	2863	2867	rBV2	516	536	0.04%	0.004%
66	10.584	2872	2875	2879	rBV2	365	286	0.02%	0.002%
67	10.603	2879	2881	2883	rVV2	375	191	0.01%	0.002%
68	10.619	2883	2886	2892	rVV3	517	431	0.03%	0.003%
69	10.648	2892	2895	2899	rVV2	351	250	0.02%	0.002%
70	10.758	2916	2929	2946	rBV	562226	883839	57.93%	6.945%
71	10.857	2958	2960	2964	rBV3	286	195	0.01%	0.002%
72	11.092	3025	3033	3035	rBV3	750	820	0.05%	0.006%
73	11.188	3059	3063	3067	rBV2	216	220	0.01%	0.002%
74	11.317	3096	3103	3113	rVB6	2530	3706	0.24%	0.029%
75	11.378	3114	3122	3124	rBV5	582	654	0.04%	0.005%
76	11.410	3127	3132	3139	rBV4	952	1126	0.07%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053503.D
 Acq On : 31 Mar 2023 19:46
 Operator : JC/MD
 Sample : 02130-07ME
 Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1196ME

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	11.465	3143	3149	3154	rBV3	1152	1673	0.11%	0.013%
78	11.578	3181	3184	3187	rBV2	466	270	0.02%	0.002%
79	11.661	3207	3210	3213	rBV3	469	253	0.02%	0.002%
80	11.716	3224	3227	3230	rBV2	504	309	0.02%	0.002%
81	11.745	3230	3236	3243	rBV4	1270	1680	0.11%	0.013%
82	11.809	3243	3256	3273	rBV	843749	1313513	86.09%	10.321%
83	12.050	3328	3331	3334	rBV2	261	224	0.01%	0.002%
84	12.192	3362	3375	3394	rBV	906456	1451546	95.14%	11.406%
85	12.420	3443	3446	3448	rBV2	526	308	0.02%	0.002%
86	12.462	3456	3459	3462	rBV	714	434	0.03%	0.003%
87	12.481	3462	3465	3467	rBV2	466	322	0.02%	0.003%
88	12.658	3517	3520	3522	rBV2	721	432	0.03%	0.003%
89	12.767	3551	3554	3556	rBV2	362	212	0.01%	0.002%
90	12.777	3556	3557	3561	rVV3	363	242	0.02%	0.002%
91	12.854	3580	3581	3585	rBV3	441	254	0.02%	0.002%
92	13.127	3662	3666	3668	rBV2	693	546	0.04%	0.004%
93	13.172	3678	3680	3682	rBV2	381	209	0.01%	0.002%
94	13.198	3685	3688	3691	rBV2	437	353	0.02%	0.003%
95	13.227	3691	3697	3699	rBV3	1104	1021	0.07%	0.008%
96	13.426	3754	3759	3769	rVB6	3016	3766	0.25%	0.030%
97	13.793	3869	3873	3876	rBV3	713	607	0.04%	0.005%
98	13.918	3908	3912	3915	rBV4	405	427	0.03%	0.003%
99	14.089	3961	3965	3977	rVB4	3254	5089	0.33%	0.040%
100	15.011	4249	4252	4254	rBV4	1591	1111	0.07%	0.009%

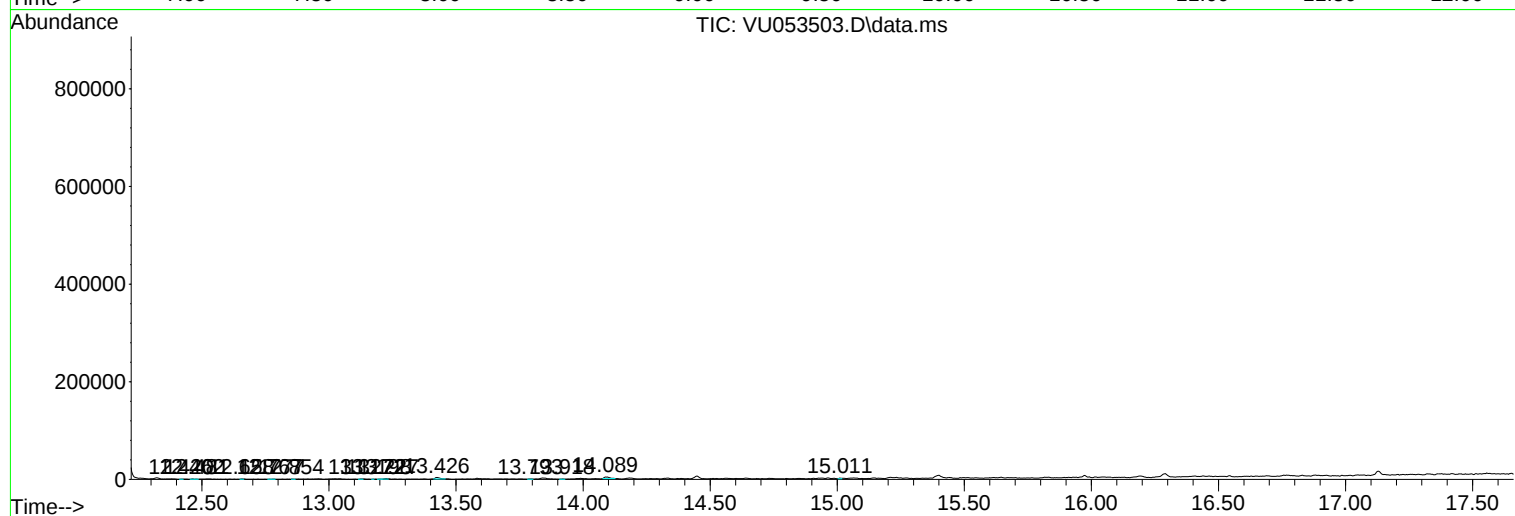
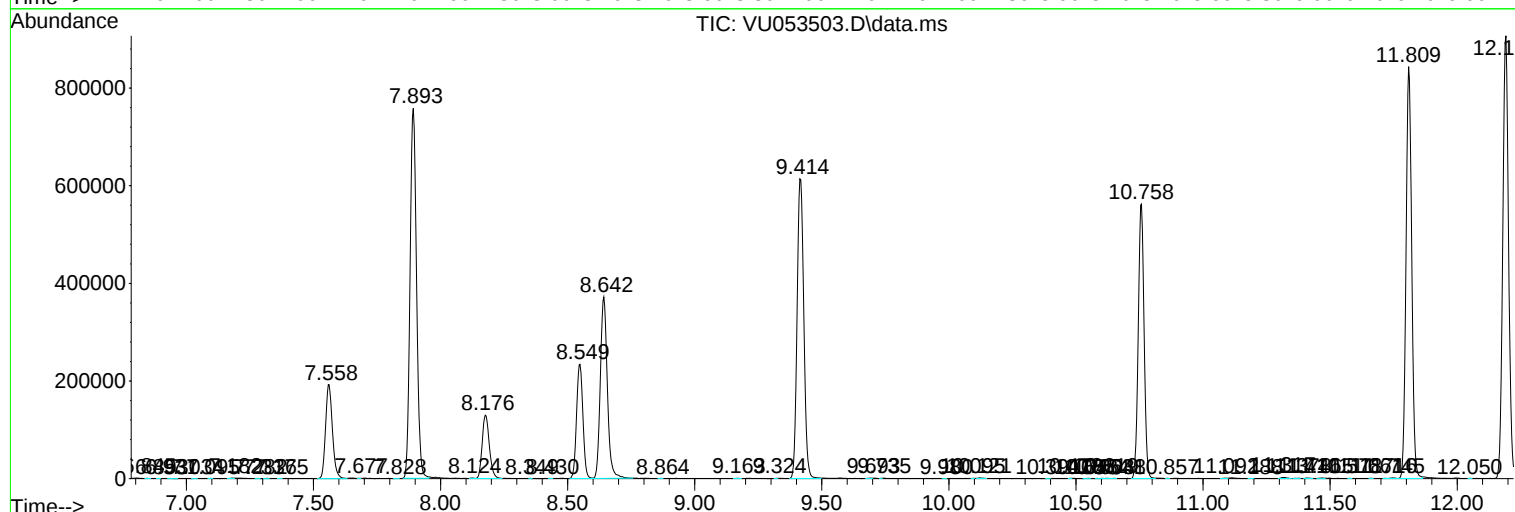
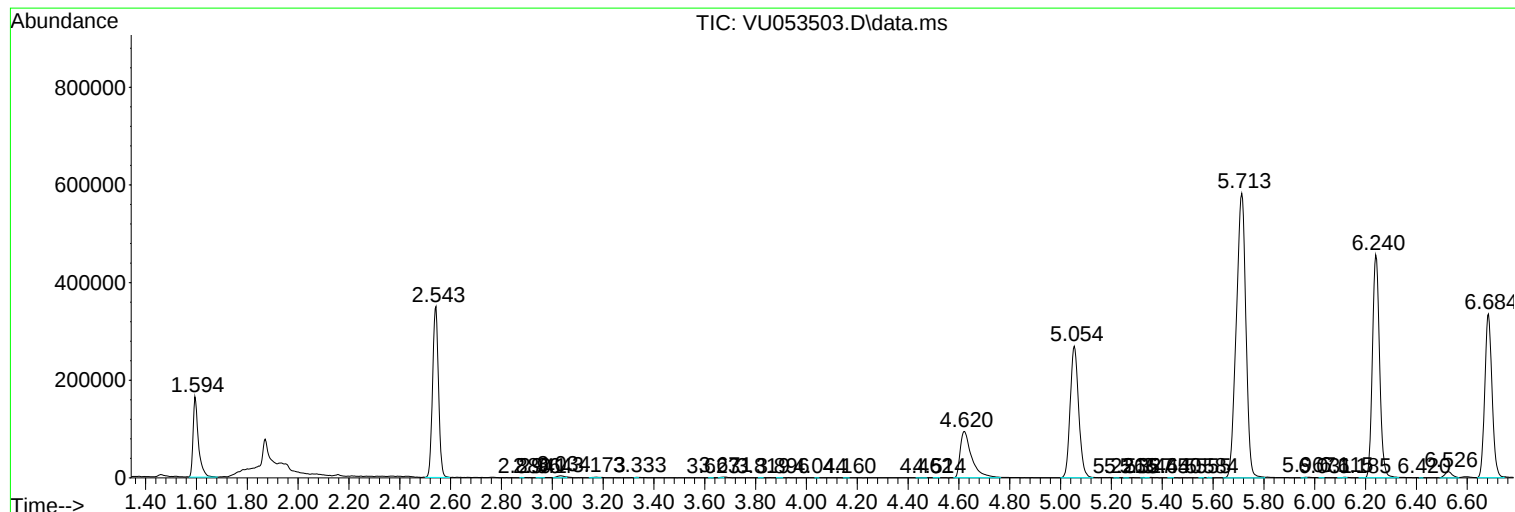
Sum of corrected areas: 12726123

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053503.D
Acq On : 31 Mar 2023 19:46
Operator : JC/MD
Sample : 02130-07ME
Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1196ME

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\VU033123\
Data File : VU053503.D
Acq On : 31 Mar 2023 19:46
Operator : JC/MD
Sample : 02130-07ME
Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1196ME

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053503.D
Acq On : 31 Mar 2023 19:46
Operator : JC/MD
Sample : 02130-07ME
Misc : 5.62g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1196ME

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	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------