

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055894.D
 Acq On : 26 Oct 2023 10:17
 Operator : MD/SY
 Sample : VU1026MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK118

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	112	rVB	305640	359251	14.68%	1.928%
2	1.882	177	184	205	rVB	205850	322801	13.19%	1.732%
3	2.557	381	394	417	rBV	512743	838948	34.29%	4.502%
4	2.779	459	463	471	rVB3	3483	4649	0.19%	0.025%
5	2.869	487	491	493	rBV	477	375	0.02%	0.002%
6	2.949	511	516	519	rBV2	373	457	0.02%	0.002%
7	3.036	534	543	554	rBV6	4488	8650	0.35%	0.046%
8	3.155	576	580	581	rBV	701	483	0.02%	0.003%
9	3.338	633	637	639	rBV3	966	904	0.04%	0.005%
10	3.454	670	673	678	rVV2	536	544	0.02%	0.003%
11	3.718	752	755	763	rBV2	488	617	0.03%	0.003%
12	3.949	824	827	831	rVV2	446	308	0.01%	0.002%
13	4.055	854	860	863	rBV2	417	413	0.02%	0.002%
14	4.168	891	895	900	rBV2	528	430	0.02%	0.002%
15	4.419	969	973	978	rVB2	628	608	0.02%	0.003%
16	4.573	1014	1021	1023	rBV2	328	419	0.02%	0.002%
17	4.615	1023	1034	1068	rBV	178372	462274	18.89%	2.481%
18	4.859	1107	1110	1114	rBV	704	547	0.02%	0.003%
19	5.055	1154	1171	1202	rBV	415461	957672	39.14%	5.139%
20	5.251	1228	1232	1236	rVB4	783	655	0.03%	0.004%
21	5.328	1245	1256	1266	rBV2	5556	10639	0.43%	0.057%
22	5.473	1299	1301	1306	rVB2	528	435	0.02%	0.002%
23	5.512	1311	1313	1318	rVV	669	518	0.02%	0.003%
24	5.718	1351	1377	1409	rBV2	896395	2446821	100.00%	13.130%
25	5.965	1451	1454	1456	rBV3	789	583	0.02%	0.003%
26	6.029	1469	1474	1477	rBV3	454	562	0.02%	0.003%
27	6.113	1496	1500	1504	rBV2	505	520	0.02%	0.003%
28	6.148	1509	1511	1519	rVB3	396	426	0.02%	0.002%
29	6.245	1526	1541	1572	rBV	638599	1257228	51.38%	6.746%
30	6.531	1620	1630	1644	rBV10	5042	9123	0.37%	0.049%
31	6.592	1644	1649	1650	rBV2	956	636	0.03%	0.003%
32	6.685	1664	1678	1699	rBV	539708	1073210	43.86%	5.759%
33	7.190	1822	1835	1848	rVV6	5782	13574	0.55%	0.073%
34	7.287	1861	1865	1869	rVB2	675	626	0.03%	0.003%
35	7.319	1872	1875	1877	rBV2	441	339	0.01%	0.002%
36	7.422	1900	1907	1908	rBV2	398	339	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055894.D
 Acq On : 26 Oct 2023 10:17
 Operator : MD/SY
 Sample : VU1026MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK118

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\SFAMULM101023WMA.M
 Title : VOC Analysis

37	7.563	1937	1951	1974	rBV	296411	537470	21.97%	2.884%
38	7.695	1988	1992	2001	rVB6	2032	2961	0.12%	0.016%
39	7.756	2009	2011	2014	rVB4	745	402	0.02%	0.002%
40	7.795	2016	2023	2025	rBV4	1672	1568	0.06%	0.008%
41	7.894	2041	2054	2095	rBV	1120258	1960318	80.12%	10.519%
42	8.177	2130	2142	2172	rVV	207514	366176	14.97%	1.965%
43	8.280	2172	2174	2178	rVB2	754	458	0.02%	0.002%
44	8.367	2198	2201	2208	rVB3	630	734	0.03%	0.004%
45	8.402	2208	2212	2216	rBV4	873	795	0.03%	0.004%
46	8.463	2224	2231	2238	rBV5	2625	4280	0.17%	0.023%
47	8.553	2252	2259	2271	rVB8	4885	9352	0.38%	0.050%
48	8.634	2271	2284	2316	rBV	679953	1324807	54.14%	7.109%
49	8.962	2382	2386	2391	rBV3	868	916	0.04%	0.005%
50	8.997	2395	2397	2400	rVV2	1036	584	0.02%	0.003%
51	9.013	2400	2402	2404	rVV2	597	328	0.01%	0.002%
52	9.026	2404	2406	2410	rVV2	654	439	0.02%	0.002%
53	9.049	2410	2413	2417	rVB5	718	536	0.02%	0.003%
54	9.164	2446	2449	2451	rBV2	615	399	0.02%	0.002%
55	9.335	2497	2502	2506	rBV3	820	775	0.03%	0.004%
56	9.415	2514	2527	2553	rBV	953366	1614150	65.97%	8.662%
57	9.560	2568	2572	2573	rBV3	604	470	0.02%	0.003%
58	9.569	2573	2575	2583	rVB5	1627	1579	0.06%	0.008%
59	9.679	2603	2609	2611	rBV4	1057	1097	0.04%	0.006%
60	9.766	2630	2636	2639	rBV	545	512	0.02%	0.003%
61	9.987	2700	2705	2709	rVV3	436	380	0.02%	0.002%
62	10.106	2734	2742	2745	rBV4	1679	1867	0.08%	0.010%
63	10.193	2765	2769	2771	rVB4	596	441	0.02%	0.002%
64	10.270	2789	2793	2796	rBV2	524	429	0.02%	0.002%
65	10.286	2796	2798	2803	rVB2	542	408	0.02%	0.002%
66	10.457	2846	2851	2854	rBV3	609	647	0.03%	0.003%
67	10.489	2856	2861	2870	rVB4	1172	1453	0.06%	0.008%
68	10.595	2890	2894	2901	rVB2	519	574	0.02%	0.003%
69	10.753	2928	2943	2970	rBV	840016	1385106	56.61%	7.433%
70	10.894	2983	2987	2996	rVB3	1848	2239	0.09%	0.012%
71	11.084	3043	3046	3048	rBV2	700	426	0.02%	0.002%
72	11.161	3065	3070	3073	rVB	489	420	0.02%	0.002%
73	11.200	3078	3082	3085	rVB2	483	343	0.01%	0.002%
74	11.229	3089	3091	3098	rVB	623	446	0.02%	0.002%
75	11.296	3108	3112	3115	rVB2	606	516	0.02%	0.003%
76	11.319	3115	3119	3122	rBV2	640	440	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055894.D
 Acq On : 26 Oct 2023 10:17
 Operator : MD/SY
 Sample : VU1026MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK118

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\SFAMULM101023WMA.M
 Title : VOC Analysis

77	11.393	3137	3142	3143	rBV2	539	432	0.02%	0.002%
78	11.405	3143	3146	3147	rVV2	874	519	0.02%	0.003%
79	11.415	3147	3149	3152	rVV2	958	600	0.02%	0.003%
80	11.476	3161	3168	3173	rBV5	1445	1869	0.08%	0.010%
81	11.656	3219	3224	3228	rVB3	473	495	0.02%	0.003%
82	11.753	3244	3254	3259	rBV9	2775	4118	0.17%	0.022%
83	11.811	3259	3272	3297	rBV	1017794	1672278	68.34%	8.974%
84	12.097	3358	3361	3365	rVB	762	498	0.02%	0.003%
85	12.190	3377	3390	3418	rBV	1152722	1902770	77.76%	10.210%
86	12.428	3460	3464	3467	rBV4	914	794	0.03%	0.004%
87	12.579	3509	3511	3515	rBV3	575	442	0.02%	0.002%
88	12.601	3515	3518	3521	rVB3	807	429	0.02%	0.002%
89	12.630	3524	3527	3532	rVB4	559	390	0.02%	0.002%
90	12.823	3584	3587	3590	rBV2	458	325	0.01%	0.002%
91	12.904	3608	3612	3616	rVB2	440	429	0.02%	0.002%
92	12.926	3616	3619	3622	rBV2	610	446	0.02%	0.002%
93	13.007	3640	3644	3646	rBV4	454	450	0.02%	0.002%
94	13.232	3709	3714	3727	rVB7	2876	5056	0.21%	0.027%
95	13.714	3861	3864	3866	rBV	600	405	0.02%	0.002%
96	13.849	3899	3906	3917	rBV4	5368	9006	0.37%	0.048%
97	14.103	3976	3985	3998	rBV	8009	16051	0.66%	0.086%
98	14.335	4049	4057	4066	rBV6	7270	12527	0.51%	0.067%
99	14.698	4168	4170	4173	rBV2	660	423	0.02%	0.002%
100	14.884	4226	4228	4235	rVB6	830	865	0.04%	0.005%

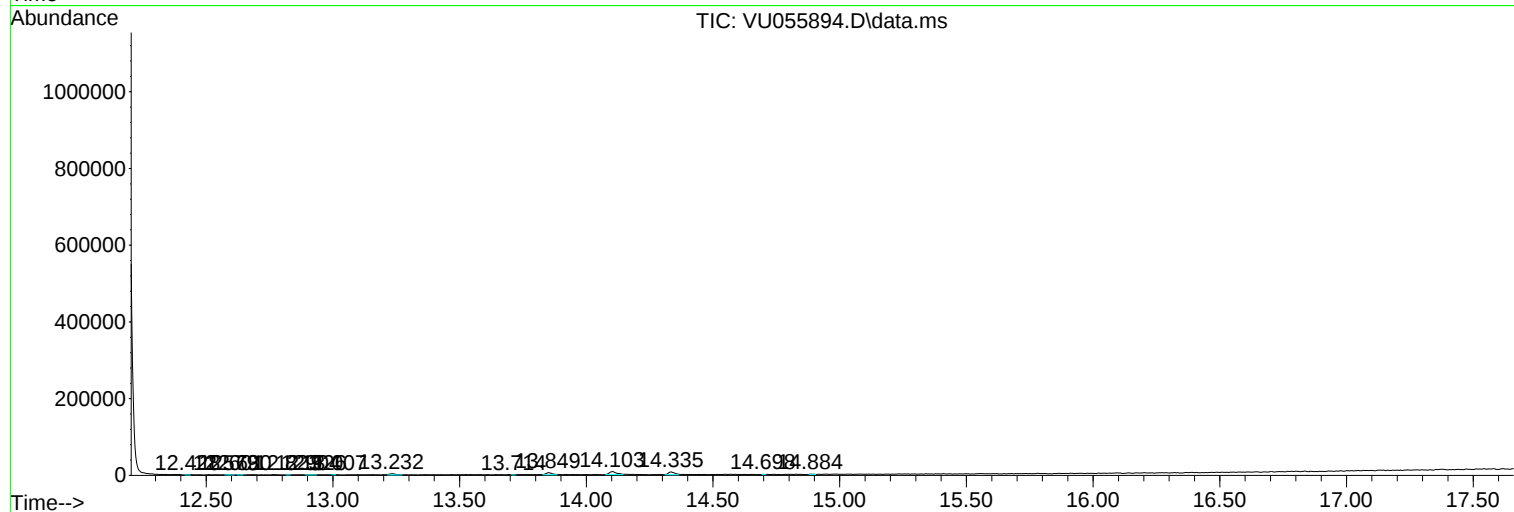
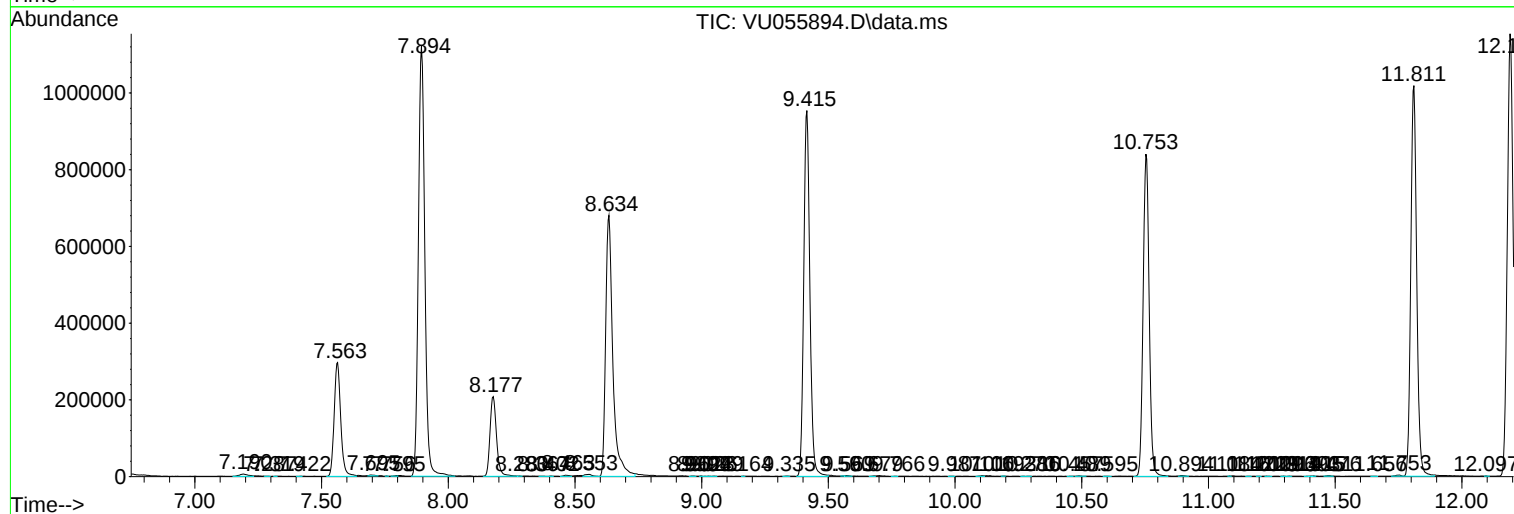
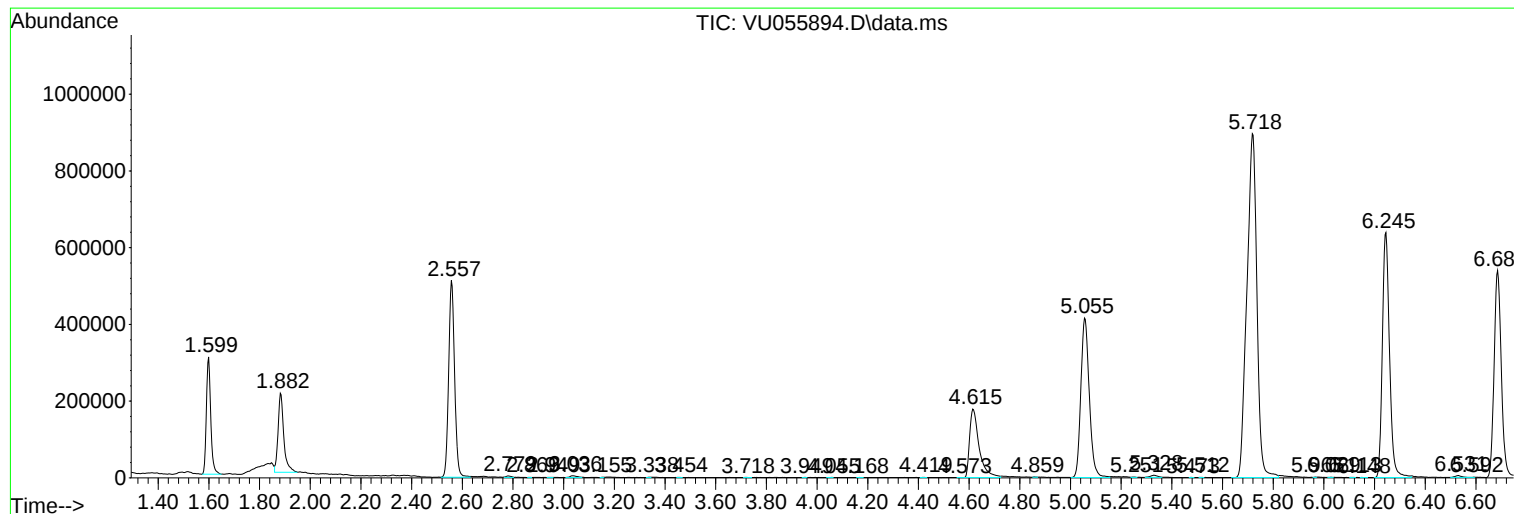
Sum of corrected areas: 18635442

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055894.D
Acq On : 26 Oct 2023 10:17
Operator : MD/SY
Sample : VU1026MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK118

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
Data File : VU055894.D
Acq On : 26 Oct 2023 10:17
Operator : MD/SY
Sample : VU1026MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK118

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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\VU102623\
Data File : VU055894.D
Acq On : 26 Oct 2023 10:17
Operator : MD/SY
Sample : VU1026MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK118

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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