

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050527.D
 Acq On : 30 Aug 2022 20:04
 Operator : SY/MD
 Sample : N4345-14ME
 Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT2ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	40	44	48	rBV2	3110	2787	0.11%	0.015%
2	1.514	49	54	63	rBV3	3454	5424	0.22%	0.029%
3	1.594	71	79	87	rBV	146574	201157	8.18%	1.075%
4	1.880	163	168	177	rBV	49768	67039	2.73%	0.358%
5	2.523	355	368	387	rBV	483026	782190	31.80%	4.180%
6	2.629	398	401	403	rBV3	686	353	0.01%	0.002%
7	2.655	403	409	415	rVV8	1422	1894	0.08%	0.010%
8	2.890	479	482	486	rBV3	326	293	0.01%	0.002%
9	3.025	514	524	539	rVB2	12567	23888	0.97%	0.128%
10	3.176	556	571	589	rBV	44882	116653	4.74%	0.623%
11	3.571	690	694	699	rVB3	356	437	0.02%	0.002%
12	3.594	699	701	705	rBV	328	226	0.01%	0.001%
13	3.658	717	721	727	rBV3	1174	1624	0.07%	0.009%
14	3.716	736	739	745	rBV3	277	271	0.01%	0.001%
15	3.877	786	789	793	rBV2	257	232	0.01%	0.001%
16	4.144	865	872	877	rBV2	229	216	0.01%	0.001%
17	4.272	908	912	915	rBV3	350	266	0.01%	0.001%
18	4.353	933	937	945	rVB	317	321	0.01%	0.002%
19	4.645	1014	1028	1098	rBV	184376	673368	27.37%	3.598%
20	4.941	1118	1120	1123	rBV4	352	236	0.01%	0.001%
21	5.060	1139	1157	1184	rBV	397797	921840	37.47%	4.926%
22	5.198	1197	1200	1206	rVB4	1027	943	0.04%	0.005%
23	5.288	1218	1228	1234	rBV4	1545	2688	0.11%	0.014%
24	5.366	1245	1252	1255	rBV3	1046	1400	0.06%	0.007%
25	5.520	1294	1300	1306	rBV2	417	572	0.02%	0.003%
26	5.562	1309	1313	1318	rBV2	300	236	0.01%	0.001%
27	5.716	1340	1361	1399	rBV2	981839	2460082	100.00%	13.145%
28	5.980	1432	1443	1470	rBV3	14379	35548	1.44%	0.190%
29	6.112	1475	1484	1499	rBV4	1068	2310	0.09%	0.012%
30	6.247	1508	1526	1550	rBV	788864	1555363	63.22%	8.311%
31	6.533	1603	1615	1625	rVV9	6403	12966	0.53%	0.069%
32	6.603	1625	1637	1649	rBV5	6019	14025	0.57%	0.075%
33	6.690	1649	1664	1692	rVB	545994	1110174	45.13%	5.932%
34	6.851	1712	1714	1717	rVB2	484	240	0.01%	0.001%
35	6.877	1717	1722	1724	rBV3	299	256	0.01%	0.001%
36	6.980	1751	1754	1759	rVV2	460	369	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050527.D
 Acq On : 30 Aug 2022 20:04
 Operator : SY/MD
 Sample : N4345-14ME
 Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT2ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

37	7.224	1813	1830	1848	rBV8	5298	15136	0.62%	0.081%
38	7.304	1852	1855	1857	rBV	719	521	0.02%	0.003%
39	7.388	1877	1881	1887	rBV3	262	289	0.01%	0.002%
40	7.436	1891	1896	1902	rVB	292	356	0.01%	0.002%
41	7.568	1922	1937	1960	rBV	231036	446549	18.15%	2.386%
42	7.777	1997	2002	2005	rBV2	486	451	0.02%	0.002%
43	7.800	2005	2009	2011	rBV2	515	366	0.01%	0.002%
44	7.896	2025	2039	2060	rBV	1074433	1926484	78.31%	10.294%
45	8.182	2116	2128	2153	rBV	151494	296697	12.06%	1.585%
46	8.552	2231	2243	2259	rBV	199916	342299	13.91%	1.829%
47	8.658	2259	2276	2313	rBV2	562977	1410740	57.35%	7.538%
48	8.893	2347	2349	2354	rVB4	555	495	0.02%	0.003%
49	8.915	2354	2356	2359	rVV2	498	287	0.01%	0.002%
50	8.941	2359	2364	2370	rVB6	754	730	0.03%	0.004%
51	8.967	2370	2372	2376	rVB3	510	357	0.01%	0.002%
52	8.992	2376	2380	2384	rBV2	516	524	0.02%	0.003%
53	9.076	2401	2406	2408	rBV3	371	232	0.01%	0.001%
54	9.118	2412	2419	2420	rBV3	503	333	0.01%	0.002%
55	9.201	2439	2445	2446	rBV2	348	303	0.01%	0.002%
56	9.282	2467	2470	2473	rBV2	275	225	0.01%	0.001%
57	9.420	2497	2513	2536	rBV	1021323	1871765	76.09%	10.001%
58	9.574	2556	2561	2569	rVB5	1181	1597	0.06%	0.009%
59	9.610	2570	2572	2578	rVB3	327	257	0.01%	0.001%
60	9.693	2594	2598	2599	rBV2	562	422	0.02%	0.002%
61	9.799	2628	2631	2638	rVB2	310	279	0.01%	0.001%
62	9.996	2688	2692	2697	rVB2	338	302	0.01%	0.002%
63	10.099	2722	2724	2728	rBV3	512	417	0.02%	0.002%
64	10.201	2747	2756	2758	rBV2	246	352	0.01%	0.002%
65	10.291	2782	2784	2791	rVB2	331	306	0.01%	0.002%
66	10.359	2802	2805	2808	rBV3	367	220	0.01%	0.001%
67	10.500	2844	2849	2852	rVB3	524	512	0.02%	0.003%
68	10.555	2864	2866	2870	rVB3	378	288	0.01%	0.002%
69	10.626	2881	2888	2890	rBV4	803	885	0.04%	0.005%
70	10.642	2891	2893	2896	rBV2	338	236	0.01%	0.001%
71	10.764	2916	2931	2949	rBV	812088	1344719	54.66%	7.185%
72	10.963	2990	2993	2997	rBV	252	235	0.01%	0.001%
73	11.028	3008	3013	3015	rBV2	322	295	0.01%	0.002%
74	11.115	3033	3040	3050	rVB9	2968	4895	0.20%	0.026%
75	11.156	3050	3053	3057	rBV2	336	321	0.01%	0.002%
76	11.320	3097	3104	3105	rBV3	471	409	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050527.D
 Acq On : 30 Aug 2022 20:04
 Operator : SY/MD
 Sample : N4345-14ME
 Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT2ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

77	11.362	3116	3117	3120	rBV	370	233	0.01%	0.001%
78	11.471	3148	3151	3154	rBV2	496	419	0.02%	0.002%
79	11.584	3183	3186	3188	rBV2	649	441	0.02%	0.002%
80	11.751	3232	3238	3245	rVB6	1224	1962	0.08%	0.010%
81	11.815	3245	3258	3280	rBV	952224	1500093	60.98%	8.016%
82	12.198	3364	3377	3397	rBV	943519	1526744	62.06%	8.158%
83	12.497	3466	3470	3477	rVV4	323	354	0.01%	0.002%
84	12.574	3490	3494	3495	rBV2	346	224	0.01%	0.001%
85	12.619	3504	3508	3514	rBV2	405	609	0.02%	0.003%
86	12.677	3523	3526	3530	rBV3	403	318	0.01%	0.002%
87	12.738	3543	3545	3548	rBV	436	352	0.01%	0.002%
88	13.031	3633	3636	3639	rBV2	447	336	0.01%	0.002%
89	13.102	3652	3658	3661	rVV3	433	481	0.02%	0.003%
90	13.118	3661	3663	3667	rVB3	331	273	0.01%	0.001%
91	13.446	3760	3765	3770	rVB3	643	666	0.03%	0.004%
92	13.471	3771	3773	3778	rBV2	289	275	0.01%	0.001%
93	13.622	3817	3820	3822	rBV2	350	230	0.01%	0.001%
94	13.854	3888	3892	3901	rVB5	1551	1915	0.08%	0.010%
95	14.057	3952	3955	3957	rBV2	366	267	0.01%	0.001%
96	14.105	3962	3970	3981	rVB5	2715	4840	0.20%	0.026%
97	14.307	4030	4033	4036	rVB3	502	352	0.01%	0.002%
98	14.343	4038	4044	4051	rVB6	1967	2731	0.11%	0.015%
99	14.600	4122	4124	4131	rBV3	372	302	0.01%	0.002%
100	15.057	4263	4266	4270	rBV2	731	497	0.02%	0.003%

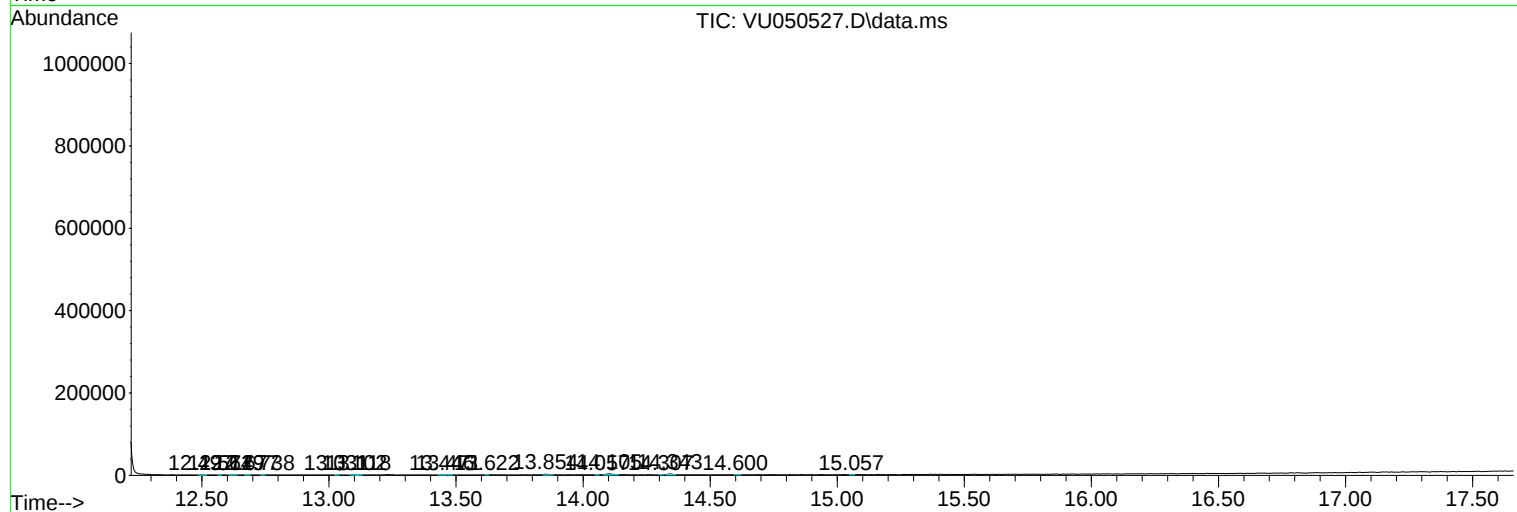
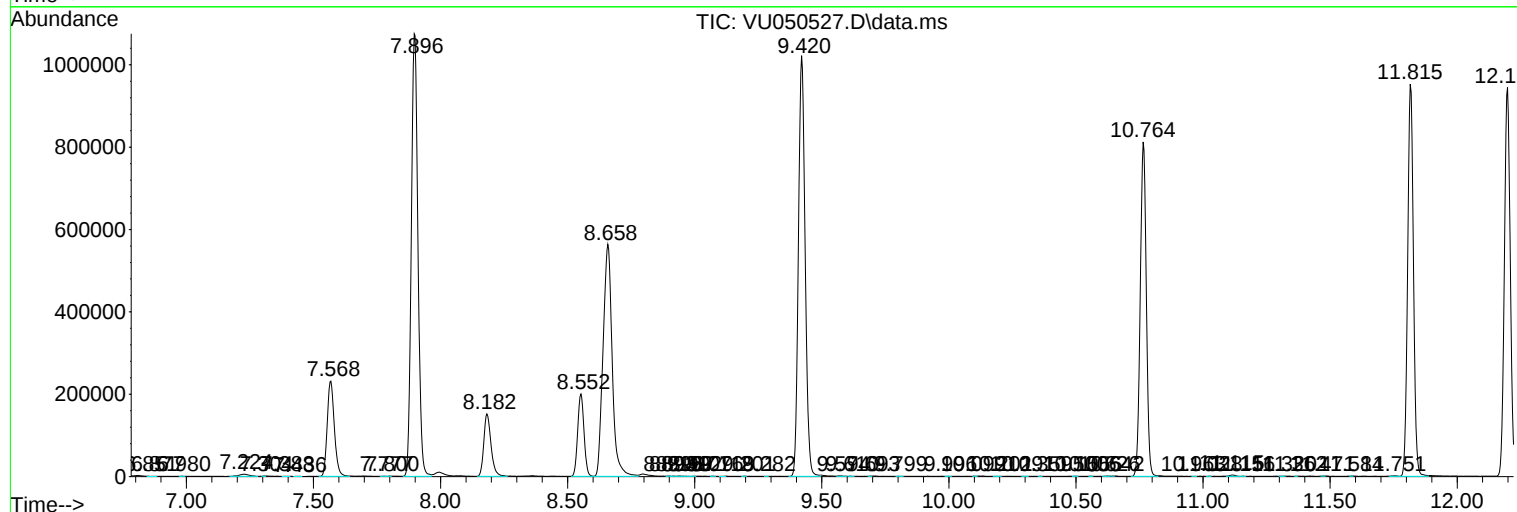
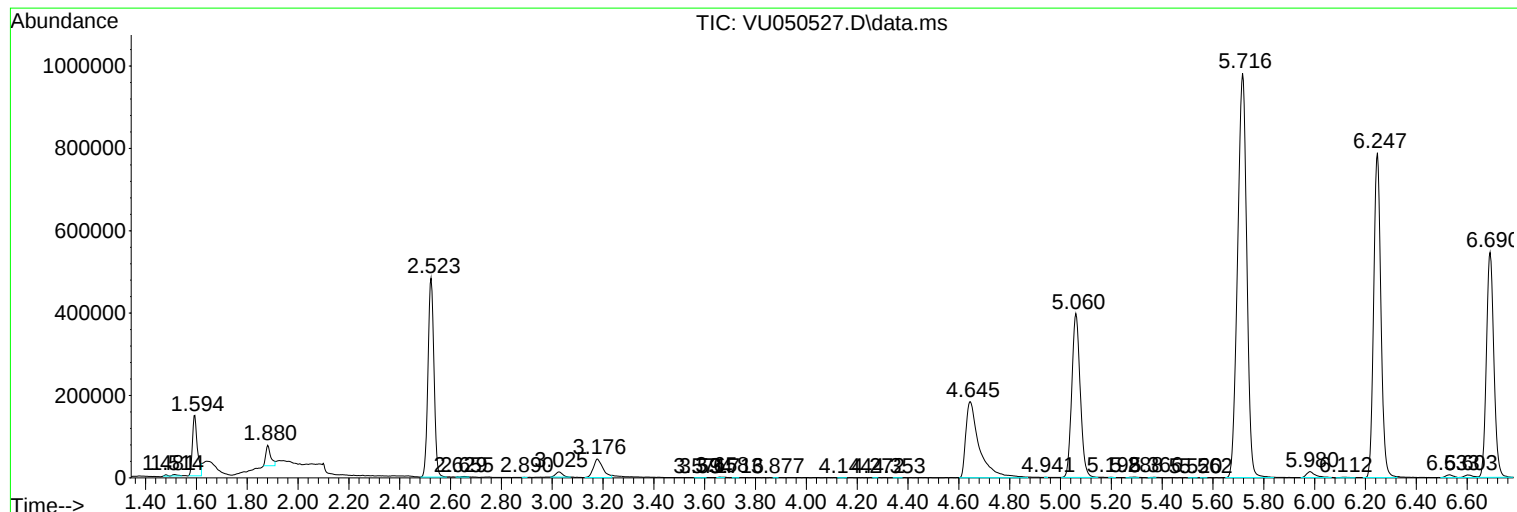
Sum of corrected areas: 18714887

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050527.D
Acq On : 30 Aug 2022 20:04
Operator : SY/MD
Sample : N4345-14ME
Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050527.D
Acq On : 30 Aug 2022 20:04
Operator : SY/MD
Sample : N4345-14ME
Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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\VU083022\
Data File : VU050527.D
Acq On : 30 Aug 2022 20:04
Operator : SY/MD
Sample : N4345-14ME
Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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