

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046338.D
 Acq On : 13 Dec 2021 23:49
 Operator : SY/MD
 Sample : M5062-04 20X
 Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL03

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\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	103	rVB	76473	88060	16.02%	1.972%
2	1.919	172	180	192	rVB	53938	69056	12.56%	1.547%
3	2.205	267	269	276	rVB2	345	328	0.06%	0.007%
4	2.243	277	281	284	rBV	368	251	0.05%	0.006%
5	2.356	313	316	319	rBV2	470	314	0.06%	0.007%
6	2.407	329	332	336	rVB	431	341	0.06%	0.008%
7	2.436	336	341	344	rBV3	401	409	0.07%	0.009%
8	2.456	344	347	350	rVV2	453	302	0.05%	0.007%
9	2.523	362	368	371	rBV2	323	367	0.07%	0.008%
10	2.571	371	383	414	rVV	115963	194414	35.37%	4.354%
11	2.739	431	435	438	rBV	301	278	0.05%	0.006%
12	2.796	447	453	455	rBV	558	644	0.12%	0.014%
13	2.915	484	490	496	rVB	252	346	0.06%	0.008%
14	2.954	497	502	505	rVB2	321	316	0.06%	0.007%
15	3.054	525	533	541	rVB4	2006	3271	0.60%	0.073%
16	3.134	555	558	563	rVB2	412	330	0.06%	0.007%
17	3.189	563	575	585	rBV2	3457	7744	1.41%	0.173%
18	3.388	634	637	642	rBV2	368	244	0.04%	0.005%
19	3.436	646	652	654	rBV2	359	371	0.07%	0.008%
20	3.510	670	675	676	rBV	374	308	0.06%	0.007%
21	3.829	768	774	777	rBV2	354	426	0.08%	0.010%
22	3.870	783	787	789	rBV	424	278	0.05%	0.006%
23	4.147	869	873	876	rBV	348	321	0.06%	0.007%
24	4.272	905	912	915	rBV	419	415	0.08%	0.009%
25	4.401	949	952	957	rVB	293	274	0.05%	0.006%
26	4.642	1013	1027	1059	rBV	45131	138122	25.13%	3.093%
27	4.845	1088	1090	1095	rVB2	386	313	0.06%	0.007%
28	4.877	1095	1100	1102	rBV2	322	294	0.05%	0.007%
29	4.938	1116	1119	1127	rBV	462	518	0.09%	0.012%
30	5.066	1143	1159	1182	rBV	96147	223444	40.65%	5.004%
31	5.430	1267	1272	1276	rBV	337	350	0.06%	0.008%
32	5.529	1300	1303	1306	rVB2	365	247	0.04%	0.006%
33	5.549	1306	1309	1312	rBV	520	419	0.08%	0.009%
34	5.642	1335	1338	1343	rVB	627	485	0.09%	0.011%
35	5.729	1343	1365	1390	rBV2	203935	549720	100.00%	12.311%
36	5.938	1424	1430	1435	rBV	539	592	0.11%	0.013%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046338.D
 Acq On : 13 Dec 2021 23:49
 Operator : SY/MD
 Sample : M5062-04 20X
 Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL03

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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.144	1490	1494	1496	rBV	380	269	0.05%	0.006%
38	6.160	1496	1499	1504	rVV2	306	269	0.05%	0.006%
39	6.201	1509	1512	1514	rBV	361	251	0.05%	0.006%
40	6.253	1514	1528	1549	rVV	181532	343260	62.44%	7.687%
41	6.417	1576	1579	1585	rBV2	339	366	0.07%	0.008%
42	6.533	1607	1615	1625	rVV5	1719	3208	0.58%	0.072%
43	6.693	1652	1665	1688	rBV	126125	246119	44.77%	5.512%
44	6.812	1697	1702	1705	rBV	426	312	0.06%	0.007%
45	6.841	1708	1711	1717	rVB2	336	306	0.06%	0.007%
46	7.192	1814	1820	1823	rBV2	365	328	0.06%	0.007%
47	7.340	1863	1866	1869	rBV2	495	349	0.06%	0.008%
48	7.568	1925	1937	1957	rVB	65522	116008	21.10%	2.598%
49	7.899	2028	2040	2058	rBV	245799	420608	76.51%	9.420%
50	8.070	2088	2093	2099	rVB2	310	328	0.06%	0.007%
51	8.108	2100	2105	2110	rVB2	264	278	0.05%	0.006%
52	8.182	2116	2128	2144	rVV	46843	78080	14.20%	1.749%
53	8.246	2144	2148	2151	rVV2	381	342	0.06%	0.008%
54	8.279	2155	2158	2161	rBV2	338	253	0.05%	0.006%
55	8.555	2235	2244	2255	rVB4	3919	6967	1.27%	0.156%
56	8.639	2255	2270	2296	rBV	153812	282214	51.34%	6.320%
57	8.838	2327	2332	2337	rBV2	319	382	0.07%	0.009%
58	8.864	2338	2340	2345	rVB	429	295	0.05%	0.007%
59	8.915	2345	2356	2363	rBV3	1026	2243	0.41%	0.050%
60	8.983	2372	2377	2380	rBV2	301	355	0.06%	0.008%
61	9.050	2395	2398	2404	rVB2	524	536	0.10%	0.012%
62	9.092	2404	2411	2413	rBV	458	557	0.10%	0.012%
63	9.108	2413	2416	2419	rVV	522	388	0.07%	0.009%
64	9.127	2419	2422	2427	rVV	431	456	0.08%	0.010%
65	9.153	2427	2430	2438	rVB2	384	397	0.07%	0.009%
66	9.192	2438	2442	2447	rBV2	438	511	0.09%	0.011%
67	9.234	2451	2455	2462	rBV2	379	540	0.10%	0.012%
68	9.285	2468	2471	2476	rVB	353	310	0.06%	0.007%
69	9.320	2476	2482	2484	rBV2	305	283	0.05%	0.006%
70	9.333	2484	2486	2492	rVB2	418	369	0.07%	0.008%
71	9.365	2492	2496	2498	rBV	397	283	0.05%	0.006%
72	9.420	2499	2513	2538	rBV	283416	466959	84.94%	10.458%
73	9.729	2605	2609	2612	rBV	468	364	0.07%	0.008%
74	9.951	2674	2678	2679	rBV	334	245	0.04%	0.005%
75	10.671	2900	2902	2912	rVB5	877	967	0.18%	0.022%
76	10.758	2917	2929	2944	rBV	196648	311254	56.62%	6.971%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046338.D
 Acq On : 13 Dec 2021 23:49
 Operator : SY/MD
 Sample : M5062-04 20X
 Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL03

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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	10.838	2949	2954	2958	rBV	395	402	0.07%	0.009%
78	10.896	2967	2972	2975	rBV2	436	498	0.09%	0.011%
79	10.944	2985	2987	2990	rVB	456	251	0.05%	0.006%
80	10.963	2990	2993	2995	rBV	416	278	0.05%	0.006%
81	11.124	3040	3043	3048	rVB2	337	338	0.06%	0.008%
82	11.156	3048	3053	3060	rBV	533	669	0.12%	0.015%
83	11.237	3073	3078	3082	rBV	455	455	0.08%	0.010%
84	11.423	3133	3136	3139	rBV	520	376	0.07%	0.008%
85	11.571	3178	3182	3185	rBV2	401	316	0.06%	0.007%
86	11.629	3197	3200	3202	rBV	386	293	0.05%	0.007%
87	11.812	3245	3257	3275	rBV	304409	470041	85.51%	10.527%
88	12.150	3358	3362	3364	rBV	469	355	0.06%	0.008%
89	12.195	3364	3376	3391	rVV	259086	412876	75.11%	9.246%
90	12.375	3428	3432	3436	rBV2	366	346	0.06%	0.008%
91	12.397	3437	3439	3442	rBV	327	246	0.04%	0.006%
92	12.510	3471	3474	3479	rBV	323	301	0.05%	0.007%
93	12.774	3551	3556	3562	rVB3	1170	1564	0.28%	0.035%
94	13.005	3624	3628	3631	rBV	415	377	0.07%	0.008%
95	13.471	3767	3773	3776	rBV2	359	395	0.07%	0.009%
96	14.574	4109	4116	4124	rBV2	1257	1944	0.35%	0.044%
97	15.169	4296	4301	4305	rBV2	385	425	0.08%	0.010%
98	15.491	4398	4401	4404	rVB2	349	259	0.05%	0.006%
99	16.005	4559	4561	4564	rBV2	396	245	0.04%	0.005%
100	16.593	4742	4744	4748	rBV2	383	290	0.05%	0.006%

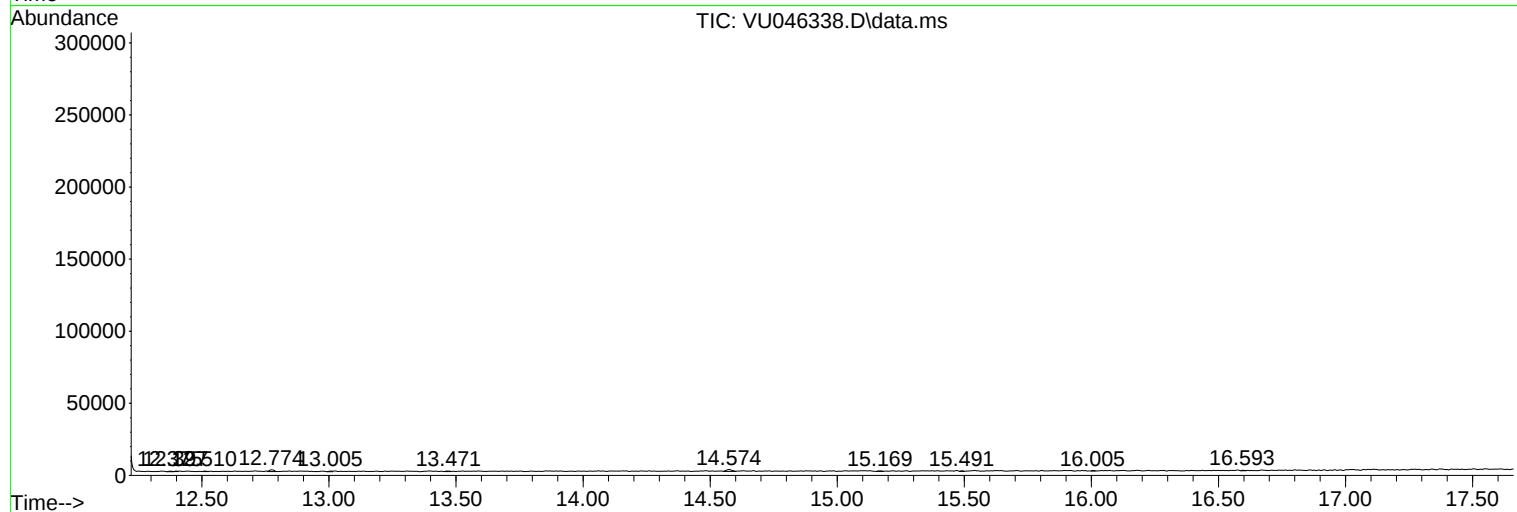
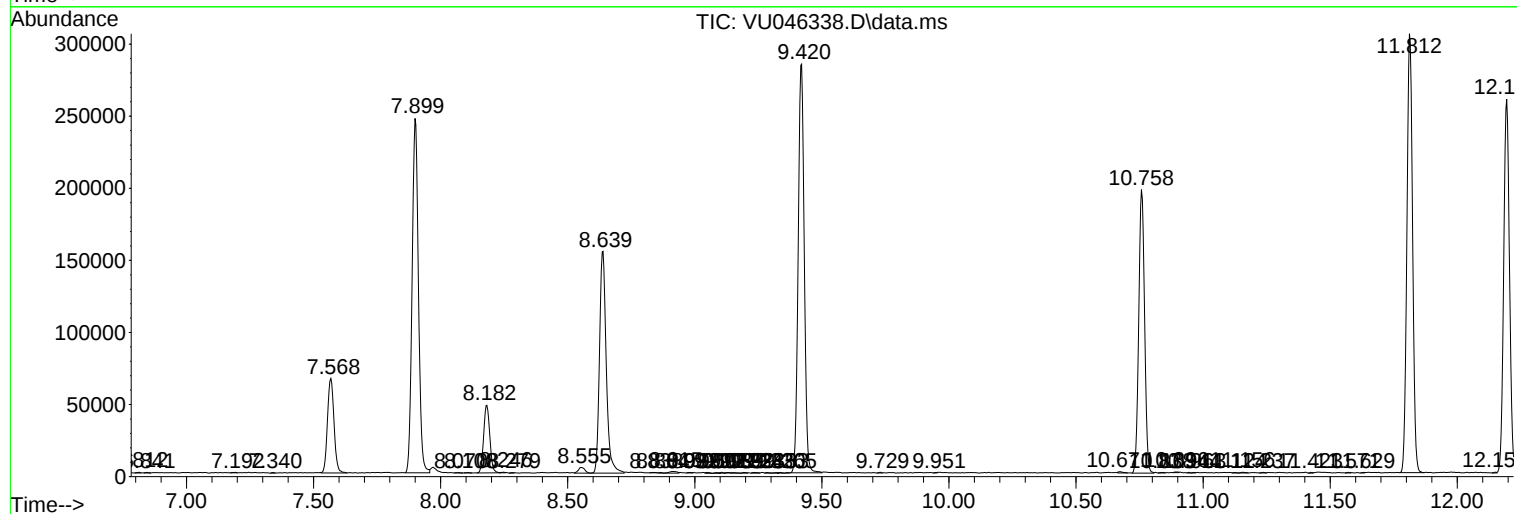
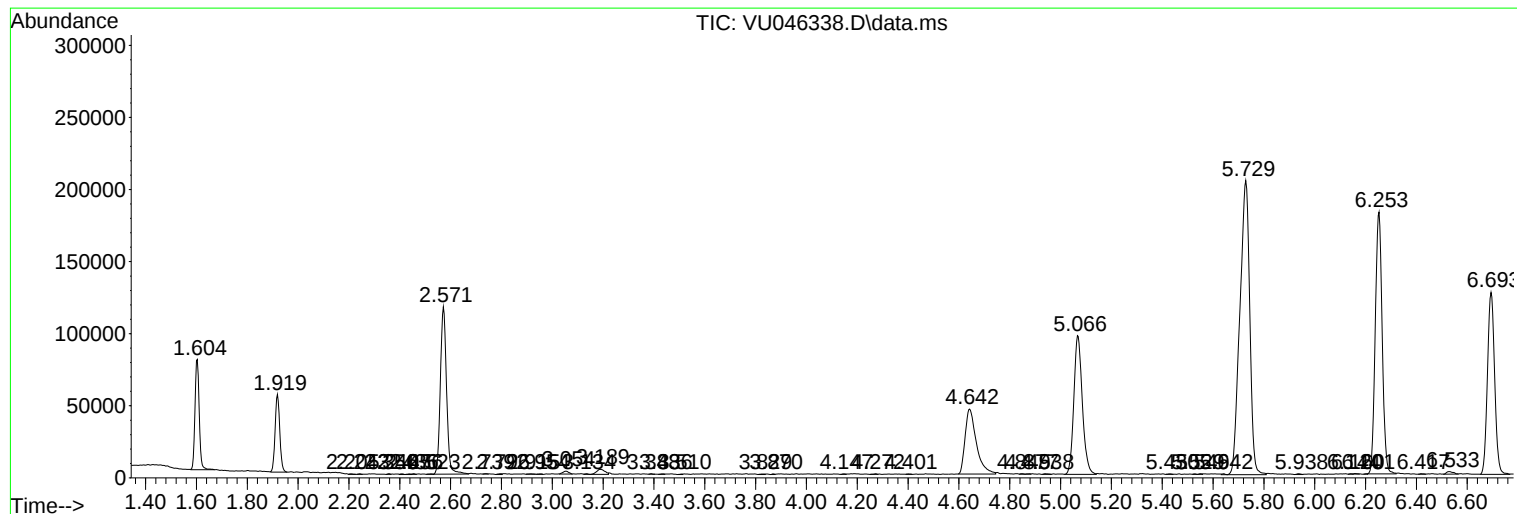
Sum of corrected areas: 4465261

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046338.D
Acq On : 13 Dec 2021 23:49
Operator : SY/MD
Sample : M5062-04 20X
Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046338.D
Acq On : 13 Dec 2021 23:49
Operator : SY/MD
Sample : M5062-04 20X
Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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\VU121321\
Data File : VU046338.D
Acq On : 13 Dec 2021 23:49
Operator : SY/MD
Sample : M5062-04 20X
Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
------------------	----	---------	-------	----------	---	----	------	------