

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046104.D
 Acq On : 06 Dec 2021 11:41
 Operator : SY/MD
 Sample : VU1206MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK049

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: VU046104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	74	81	96	rVB	107545	118144	14.00%	1.676%
2	1.919	171	180	192	rVB	75637	96829	11.47%	1.373%
3	2.089	230	233	235	rBV2	406	269	0.03%	0.004%
4	2.237	274	279	281	rBV2	297	237	0.03%	0.003%
5	2.353	311	315	316	rBV2	344	246	0.03%	0.003%
6	2.571	371	383	407	rBV	185033	308777	36.59%	4.379%
7	2.748	434	438	440	rBV2	168	149	0.02%	0.002%
8	2.796	444	453	464	rBV2	1595	2459	0.29%	0.035%
9	2.960	498	504	511	rBV	216	353	0.04%	0.005%
10	3.054	524	533	540	rBV3	2049	3361	0.40%	0.048%
11	3.247	590	593	595	rBV	174	146	0.02%	0.002%
12	3.353	623	626	633	rVB3	347	398	0.05%	0.006%
13	3.510	672	675	681	rVB	175	220	0.03%	0.003%
14	3.539	681	684	688	rBV	171	189	0.02%	0.003%
15	3.813	764	769	772	rBB	145	171	0.02%	0.002%
16	3.915	797	801	804	rBV	143	175	0.02%	0.002%
17	3.983	817	822	824	rBV	132	155	0.02%	0.002%
18	4.047	838	842	848	rBV	179	263	0.03%	0.004%
19	4.542	992	996	1000	rBV	132	182	0.02%	0.003%
20	4.639	1010	1026	1055	rBV	72370	203766	24.15%	2.890%
21	4.935	1116	1118	1121	rBV	226	155	0.02%	0.002%
22	5.066	1143	1159	1183	rBV	146757	328555	38.93%	4.660%
23	5.211	1201	1204	1206	rBV	185	144	0.02%	0.002%
24	5.314	1233	1236	1239	rVB	165	134	0.02%	0.002%
25	5.565	1311	1314	1318	rBB	148	152	0.02%	0.002%
26	5.652	1338	1341	1342	rBV	237	136	0.02%	0.002%
27	5.729	1342	1365	1389	rVV2	313573	843866	100.00%	11.968%
28	5.890	1413	1415	1417	rBV	281	146	0.02%	0.002%
29	5.902	1417	1419	1423	rVV2	271	176	0.02%	0.002%
30	5.941	1426	1431	1433	rBV	273	225	0.03%	0.003%
31	6.047	1461	1464	1467	rVV2	337	267	0.03%	0.004%
32	6.115	1483	1485	1488	rBV2	271	169	0.02%	0.002%
33	6.131	1488	1490	1495	rVB	381	227	0.03%	0.003%
34	6.160	1496	1499	1502	rBV	154	147	0.02%	0.002%
35	6.253	1513	1528	1547	rBV	313228	590719	70.00%	8.378%
36	6.536	1607	1616	1628	rBV6	2889	6018	0.71%	0.085%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046104.D
 Acq On : 06 Dec 2021 11:41
 Operator : SY/MD
 Sample : VU1206MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK049

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	6.616	1639	1641	1644	rBV	276	201	0.02%	0.003%
38	6.693	1648	1665	1682	rBV	190240	366729	43.46%	5.201%
39	6.812	1696	1702	1703	rBV3	418	305	0.04%	0.004%
40	6.867	1715	1719	1723	rBV	295	274	0.03%	0.004%
41	6.944	1740	1743	1748	rBB	157	179	0.02%	0.003%
42	7.044	1769	1774	1780	rVV2	300	428	0.05%	0.006%
43	7.173	1810	1814	1815	rBV	178	145	0.02%	0.002%
44	7.182	1815	1817	1821	rVV	233	156	0.02%	0.002%
45	7.201	1821	1823	1827	rVB	154	131	0.02%	0.002%
46	7.234	1828	1833	1836	rBV	218	248	0.03%	0.004%
47	7.295	1846	1852	1856	rBV	166	275	0.03%	0.004%
48	7.423	1890	1892	1895	rVB	219	128	0.02%	0.002%
49	7.568	1925	1937	1954	rBV	112480	195543	23.17%	2.773%
50	7.677	1968	1971	1976	rBV2	203	187	0.02%	0.003%
51	7.793	2001	2007	2016	rBV3	994	1571	0.19%	0.022%
52	7.845	2019	2023	2027	rBV	159	218	0.03%	0.003%
53	7.902	2027	2041	2057	rBV	405914	709286	84.05%	10.059%
54	8.182	2117	2128	2146	rBV	77443	128983	15.28%	1.829%
55	8.304	2163	2166	2170	rBV	286	245	0.03%	0.003%
56	8.635	2256	2269	2310	rBV	239259	424880	50.35%	6.026%
57	8.886	2345	2347	2352	rBV	213	133	0.02%	0.002%
58	8.976	2372	2375	2377	rBV	180	151	0.02%	0.002%
59	9.166	2427	2434	2441	rVV2	508	683	0.08%	0.010%
60	9.420	2498	2513	2541	rBV	443241	737583	87.41%	10.461%
61	9.578	2554	2562	2570	rVB2	968	1518	0.18%	0.022%
62	9.642	2579	2582	2587	rVB2	250	227	0.03%	0.003%
63	9.697	2591	2599	2608	rVB3	1515	2277	0.27%	0.032%
64	10.108	2718	2727	2728	rBV2	1692	1592	0.19%	0.023%
65	10.484	2838	2844	2854	rVB	1274	1628	0.19%	0.023%
66	10.674	2896	2903	2911	rBV3	2452	3024	0.36%	0.043%
67	10.761	2917	2930	2945	rBV	270592	431083	51.08%	6.114%
68	10.832	2949	2952	2957	rVB2	772	584	0.07%	0.008%
69	11.031	3010	3014	3017	rBV	210	146	0.02%	0.002%
70	11.092	3026	3033	3040	rBV3	1694	2247	0.27%	0.032%
71	11.468	3139	3150	3162	rBV3	3215	5208	0.62%	0.074%
72	11.584	3181	3186	3191	rVB2	464	380	0.05%	0.005%
73	11.610	3191	3194	3201	rBV	111	146	0.02%	0.002%
74	11.696	3215	3221	3230	rBV	744	889	0.11%	0.013%
75	11.751	3230	3238	3246	rVB3	1979	2976	0.35%	0.042%
76	11.815	3246	3258	3274	rBV	506498	798023	94.57%	11.318%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046104.D
 Acq On : 06 Dec 2021 11:41
 Operator : SY/MD
 Sample : VU1206MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK049

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	11.922	3286	3291	3293	rBV	389	323	0.04%	0.005%
78	11.934	3293	3295	3296	rBV2	300	131	0.02%	0.002%
79	11.976	3303	3308	3315	rVB5	1658	1945	0.23%	0.028%
80	12.069	3335	3337	3341	rBV2	173	142	0.02%	0.002%
81	12.195	3362	3376	3393	rBV	417225	672683	79.71%	9.540%
82	12.333	3413	3419	3425	rVB3	664	494	0.06%	0.007%
83	12.397	3434	3439	3441	rBV3	250	211	0.03%	0.003%
84	12.632	3510	3512	3514	rBV2	274	172	0.02%	0.002%
85	12.690	3526	3530	3532	rBV2	189	134	0.02%	0.002%
86	13.002	3622	3627	3632	rVB2	873	964	0.11%	0.014%
87	13.092	3652	3655	3659	rBV	237	169	0.02%	0.002%
88	13.153	3670	3674	3677	rVB2	265	167	0.02%	0.002%
89	13.224	3688	3696	3706	rVB4	3483	5180	0.61%	0.073%
90	13.844	3881	3889	3899	rBV2	5654	8012	0.95%	0.114%
91	14.037	3946	3949	3952	rBV2	195	132	0.02%	0.002%
92	14.089	3956	3965	3974	rVV	11263	16390	1.94%	0.232%
93	14.333	4031	4041	4051	rVV3	6076	9289	1.10%	0.132%
94	14.892	4211	4215	4219	rBV	367	367	0.04%	0.005%
95	15.150	4293	4295	4297	rBV	237	155	0.02%	0.002%
96	15.227	4311	4319	4330	rVB2	2682	4179	0.50%	0.059%
97	15.407	4372	4375	4376	rBV2	729	469	0.06%	0.007%
98	15.658	4449	4453	4459	rBV3	388	460	0.05%	0.007%
99	16.137	4599	4602	4604	rBV2	420	222	0.03%	0.003%
100	16.230	4629	4631	4633	rBV2	468	262	0.03%	0.004%

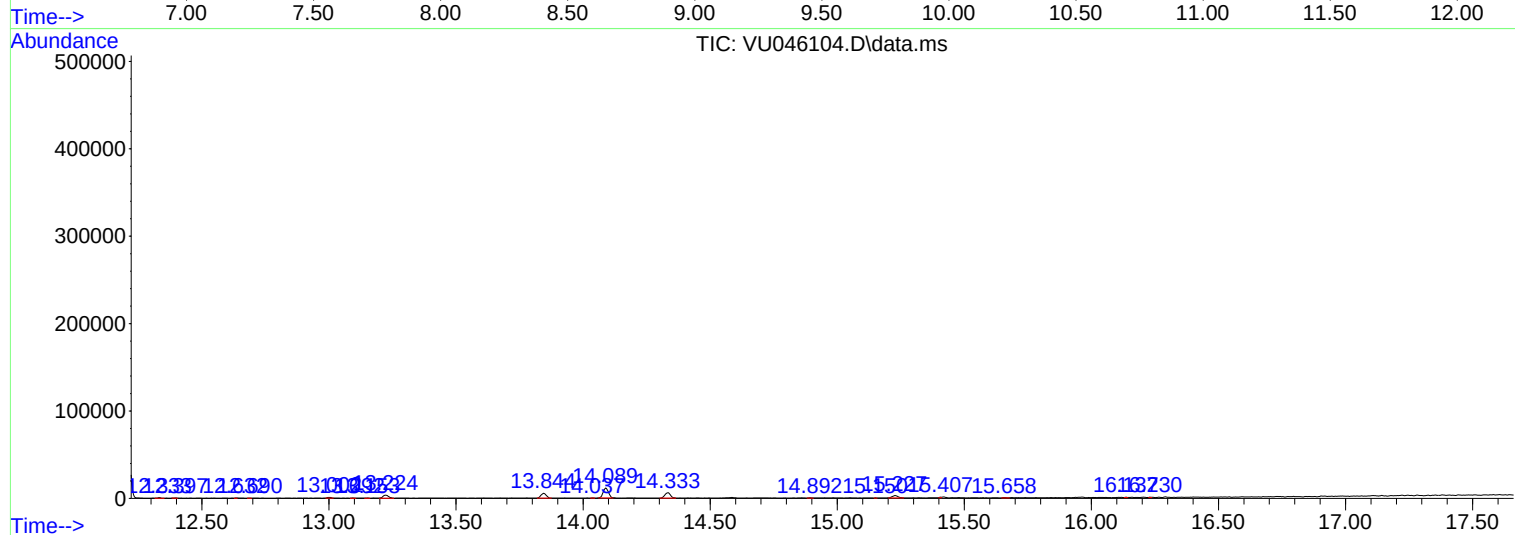
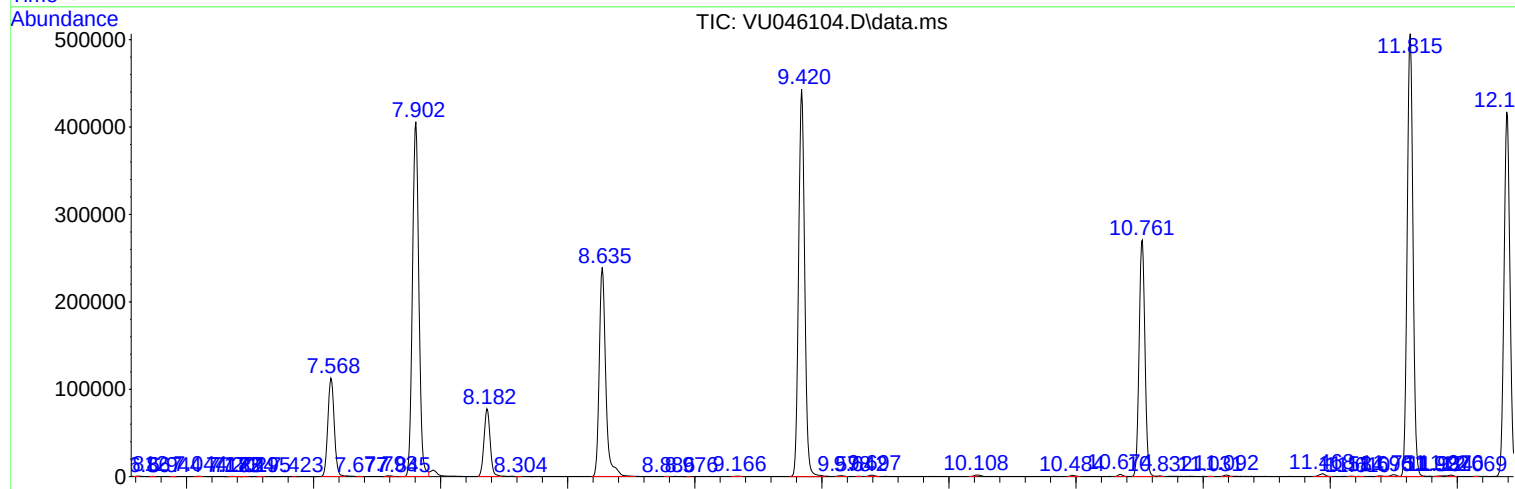
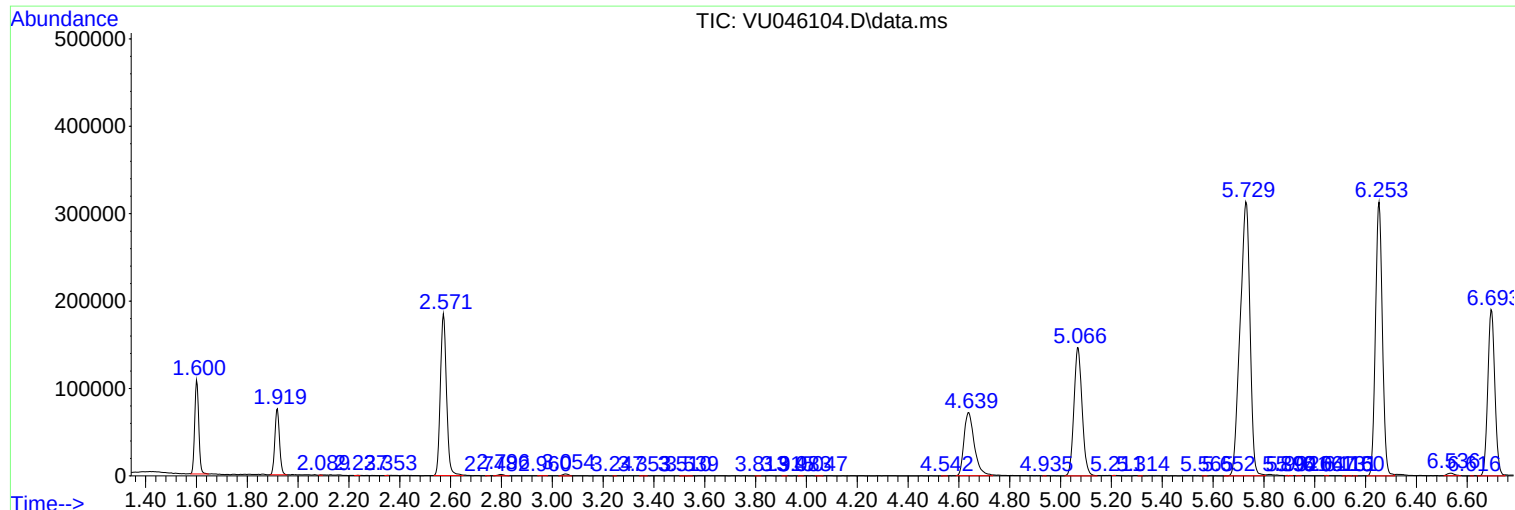
Sum of corrected areas: 7050987

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046104.D
Acq On : 06 Dec 2021 11:41
Operator : SY/MD
Sample : VU1206MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK049

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\VU120621\
Data File : VU046104.D
Acq On : 06 Dec 2021 11:41
Operator : SY/MD
Sample : VU1206MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK049

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\VU120621\
Data File : VU046104.D
Acq On : 06 Dec 2021 11:41
Operator : SY/MD
Sample : VU1206MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK049

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	--Internal Standard--			
					#	RT	Resp	Conc