

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046164.D
 Acq On : 08 Dec 2021 10:33
 Operator : SY/MD
 Sample : VU1208MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK047

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: VU046164.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	75	82	96	rVB	108891	119952	14.41%	1.833%
2	1.919	171	180	193	rVB	79865	100983	12.13%	1.543%
3	2.572	371	383	403	rBV	176606	295691	35.53%	4.519%
4	2.806	446	456	461	rBV3	702	1301	0.16%	0.020%
5	3.054	526	533	542	rVB4	729	1176	0.14%	0.018%
6	3.105	547	549	553	rVV	280	204	0.02%	0.003%
7	3.170	566	569	570	rBV	585	318	0.04%	0.005%
8	3.559	687	690	693	rBB	182	145	0.02%	0.002%
9	3.665	720	723	726	rBB	134	115	0.01%	0.002%
10	3.687	726	730	733	rBV	188	197	0.02%	0.003%
11	3.790	760	762	765	rVB	301	167	0.02%	0.003%
12	3.813	766	769	774	rBV	164	206	0.02%	0.003%
13	3.880	784	790	794	rBV	163	270	0.03%	0.004%
14	4.022	830	834	839	rBV	147	218	0.03%	0.003%
15	4.157	874	876	879	rBB2	266	147	0.02%	0.002%
16	4.186	880	885	888	rBV	147	181	0.02%	0.003%
17	4.231	894	899	904	rBV	173	233	0.03%	0.004%
18	4.308	921	923	929	rBB	152	175	0.02%	0.003%
19	4.382	944	946	949	rBV	248	170	0.02%	0.003%
20	4.398	949	951	954	rVB2	242	140	0.02%	0.002%
21	4.433	957	962	965	rBB2	299	296	0.04%	0.005%
22	4.459	965	970	971	rBV	263	186	0.02%	0.003%
23	4.507	983	985	988	rBB2	277	150	0.02%	0.002%
24	4.526	988	991	992	rBV	230	113	0.01%	0.002%
25	4.568	1002	1004	1008	rBV	262	205	0.02%	0.003%
26	4.642	1012	1027	1069	rBV	69772	226538	27.22%	3.462%
27	4.983	1131	1133	1135	rVB	275	130	0.02%	0.002%
28	5.002	1136	1139	1142	rBV	148	141	0.02%	0.002%
29	5.070	1143	1160	1183	rVV	142485	325247	39.08%	4.970%
30	5.263	1217	1220	1221	rBV	237	135	0.02%	0.002%
31	5.340	1242	1244	1249	rBV	238	210	0.03%	0.003%
32	5.433	1269	1273	1274	rBV	233	156	0.02%	0.002%
33	5.575	1313	1317	1320	rBB	142	145	0.02%	0.002%
34	5.607	1325	1327	1329	rBV	215	124	0.01%	0.002%
35	5.729	1344	1365	1384	rBV2	307820	832226	100.00%	12.718%
36	6.253	1512	1528	1548	rBV	249867	467193	56.14%	7.140%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046164.D
 Acq On : 08 Dec 2021 10:33
 Operator : SY/MD
 Sample : VU1208MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK047

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 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	6.533	1607	1615	1627	rBV5	3451	7015	0.84%	0.107%
38	6.694	1652	1665	1693	rBV	187538	363182	43.64%	5.550%
39	6.838	1707	1710	1715	rBV3	190	173	0.02%	0.003%
40	6.899	1725	1729	1732	rBV	159	172	0.02%	0.003%
41	7.018	1763	1766	1769	rBB	151	126	0.02%	0.002%
42	7.041	1770	1773	1774	rBV	349	205	0.02%	0.003%
43	7.076	1782	1784	1787	rBV	262	205	0.02%	0.003%
44	7.182	1812	1817	1819	rBV2	265	246	0.03%	0.004%
45	7.224	1827	1830	1834	rBV	273	236	0.03%	0.004%
46	7.308	1854	1856	1859	rBV	148	124	0.01%	0.002%
47	7.407	1881	1887	1889	rBV	142	195	0.02%	0.003%
48	7.475	1906	1908	1910	rBV	234	133	0.02%	0.002%
49	7.510	1917	1919	1921	rBV	148	108	0.01%	0.002%
50	7.568	1925	1937	1952	rBV	109205	187969	22.59%	2.873%
51	7.761	1993	1997	1999	rBV	155	130	0.02%	0.002%
52	7.796	2004	2008	2014	rVB	437	576	0.07%	0.009%
53	7.845	2019	2023	2026	rBB	181	169	0.02%	0.003%
54	7.903	2026	2041	2057	rBV	393739	689091	82.80%	10.531%
55	8.140	2111	2115	2116	rBV	174	137	0.02%	0.002%
56	8.182	2116	2128	2145	rVV	72999	123010	14.78%	1.880%
57	8.411	2196	2199	2203	rBV	188	190	0.02%	0.003%
58	8.462	2212	2215	2220	rVV2	335	268	0.03%	0.004%
59	8.513	2227	2231	2233	rBB	160	133	0.02%	0.002%
60	8.636	2257	2269	2298	rBV	244717	444934	53.46%	6.799%
61	8.909	2350	2354	2356	rBV	763	656	0.08%	0.010%
62	8.976	2372	2375	2378	rBV	153	158	0.02%	0.002%
63	9.015	2384	2387	2389	rBV	237	163	0.02%	0.002%
64	9.095	2409	2412	2417	rBV2	258	267	0.03%	0.004%
65	9.166	2431	2434	2439	rVB2	436	360	0.04%	0.006%
66	9.243	2453	2458	2460	rBV2	242	225	0.03%	0.003%
67	9.304	2469	2477	2480	rBV	191	308	0.04%	0.005%
68	9.362	2488	2495	2499	rBV	211	362	0.04%	0.006%
69	9.420	2499	2513	2546	rVV	351402	589276	70.81%	9.005%
70	9.578	2554	2562	2570	rVB3	747	1340	0.16%	0.020%
71	9.693	2592	2598	2609	rVB3	1116	1745	0.21%	0.027%
72	9.738	2609	2612	2614	rBV2	200	162	0.02%	0.002%
73	9.845	2643	2645	2649	rVB	303	212	0.03%	0.003%
74	9.870	2649	2653	2657	rBV	205	255	0.03%	0.004%
75	10.115	2720	2729	2736	rVB6	1101	1729	0.21%	0.026%
76	10.218	2757	2761	2763	rBV	154	159	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046164.D
 Acq On : 08 Dec 2021 10:33
 Operator : SY/MD
 Sample : VU1208MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK047

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	10.555	2864	2866	2869	rBV	198	127	0.02%	0.002%
78	10.674	2893	2903	2910	rVB3	1721	2305	0.28%	0.035%
79	10.758	2916	2929	2945	rBV	276588	444330	53.39%	6.790%
80	10.867	2959	2963	2967	rBV3	342	329	0.04%	0.005%
81	11.002	3003	3005	3007	rVB	265	125	0.02%	0.002%
82	11.092	3026	3033	3039	rBV2	887	1212	0.15%	0.019%
83	11.153	3050	3052	3056	rVB	266	122	0.01%	0.002%
84	11.462	3139	3148	3159	rBV5	2169	3636	0.44%	0.056%
85	11.690	3216	3219	3220	rBV5	559	275	0.03%	0.004%
86	11.751	3232	3238	3245	rVB4	1350	1716	0.21%	0.026%
87	11.812	3245	3257	3275	rBV	385190	617468	74.19%	9.436%
88	11.893	3280	3282	3286	rBV2	279	214	0.03%	0.003%
89	11.938	3294	3296	3297	rBV2	297	113	0.01%	0.002%
90	12.195	3362	3376	3397	rVB	410146	655467	78.76%	10.017%
91	12.327	3416	3417	3421	rVB2	213	110	0.01%	0.002%
92	12.822	3567	3571	3574	rBV2	170	125	0.02%	0.002%
93	12.912	3597	3599	3604	rBV	225	109	0.01%	0.002%
94	13.224	3688	3696	3704	rVB5	2119	2974	0.36%	0.045%
95	13.336	3729	3731	3735	rBV	218	116	0.01%	0.002%
96	13.844	3881	3889	3898	rVB3	3328	4501	0.54%	0.069%
97	13.986	3931	3933	3938	rBV	175	137	0.02%	0.002%
98	14.089	3958	3965	3979	rVB2	6585	10472	1.26%	0.160%
99	14.330	4032	4040	4051	rBV3	4166	6128	0.74%	0.094%
100	14.790	4180	4183	4188	rBV2	285	260	0.03%	0.004%

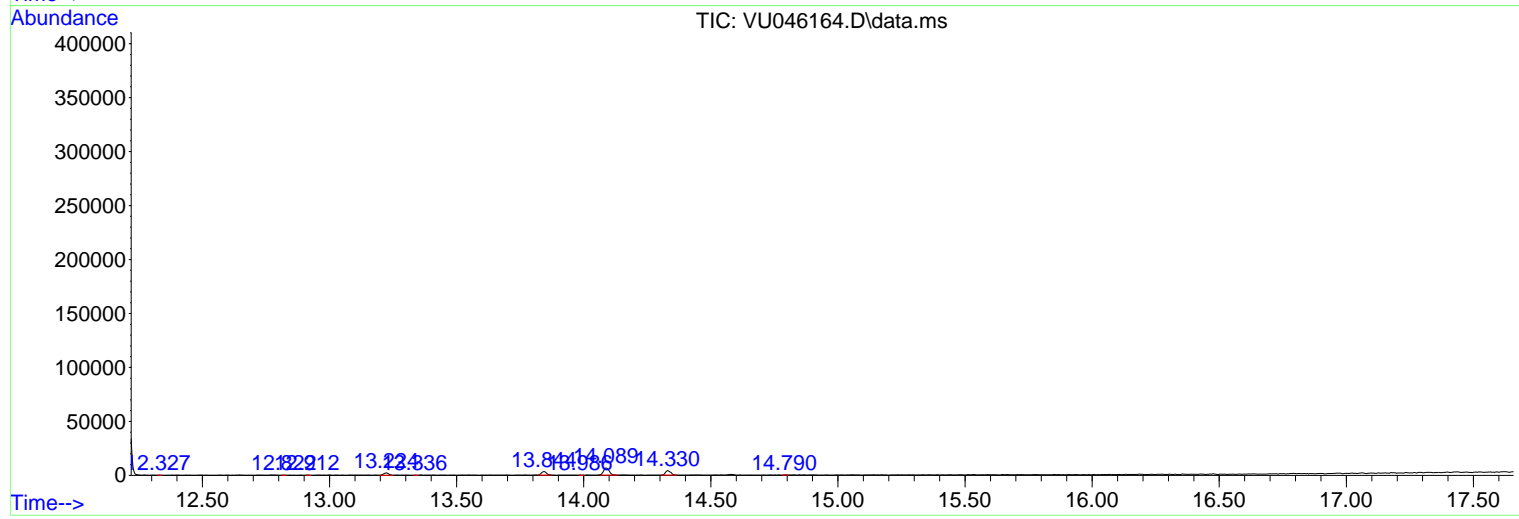
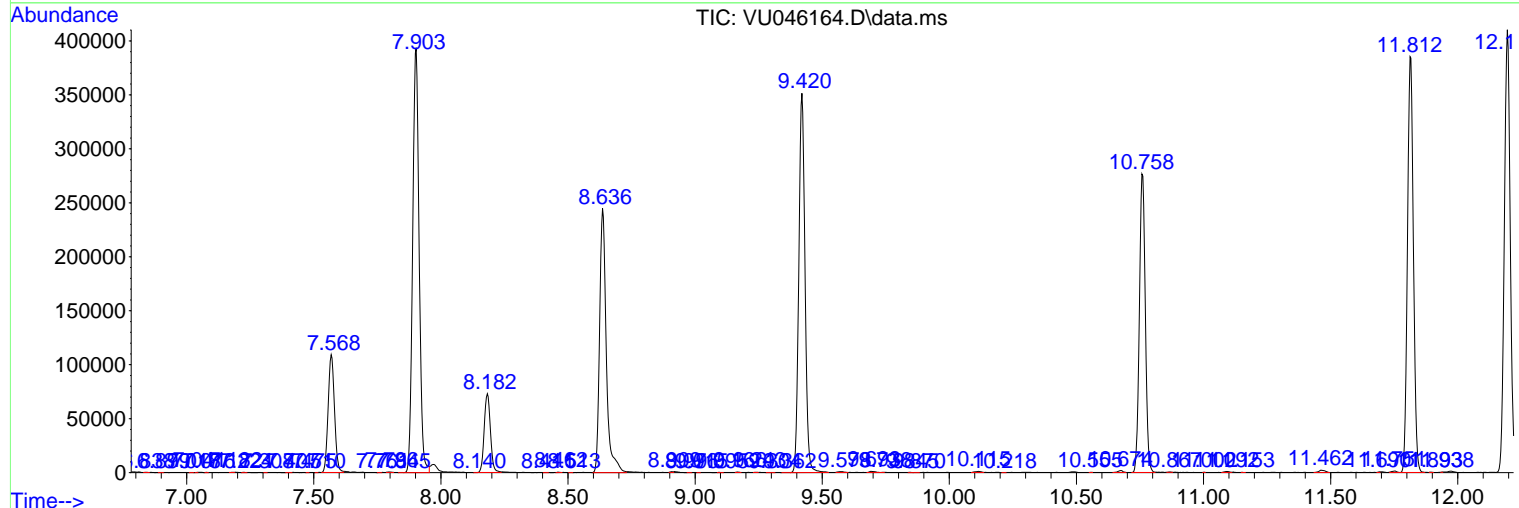
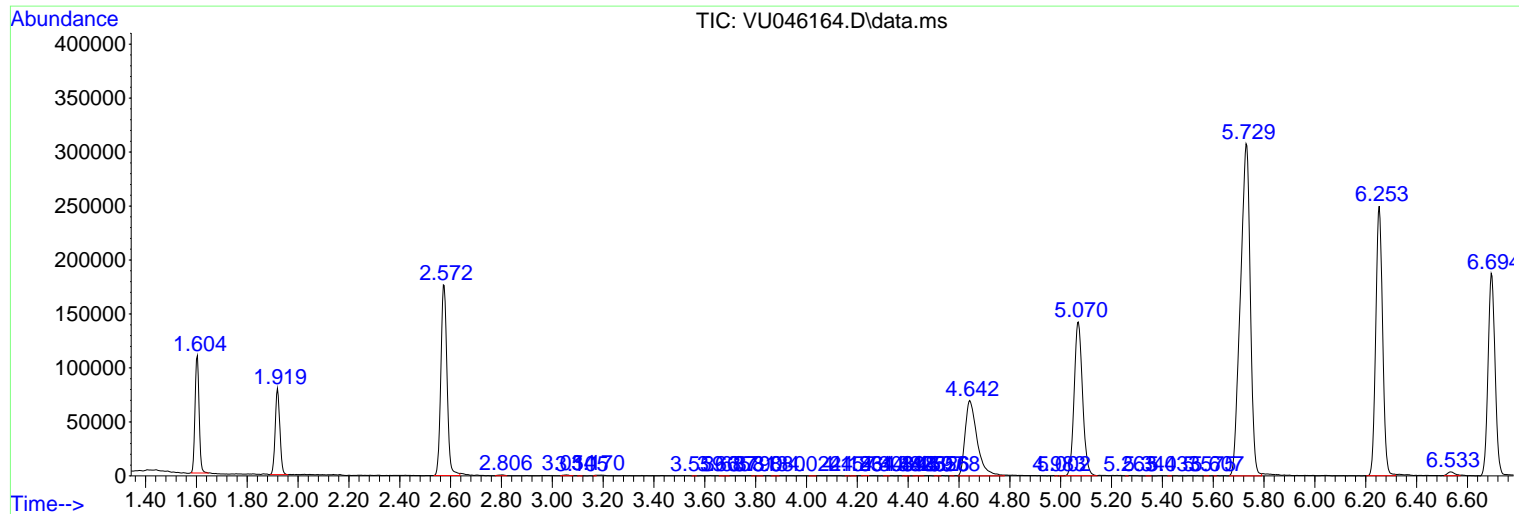
Sum of corrected areas: 6543659

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046164.D
 Acq On : 08 Dec 2021 10:33
 Operator : SY/MD
 Sample : VU1208MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
ClientSampleId :
 VBLK047

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\VU120821\
Data File : VU046164.D
Acq On : 08 Dec 2021 10:33
Operator : SY/MD
Sample : VU1208MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK047

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\VU120821\
Data File : VU046164.D
Acq On : 08 Dec 2021 10:33
Operator : SY/MD
Sample : VU1208MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK047

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--		
					#	RT	Resp Conc
