

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
 Data File : VU046089.D
 Acq On : 04 Dec 2021 13:44
 Operator : SY/MD
 Sample : VU1204MBL01
 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: VU046089.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	92	rBV	103213	114318	15.63%	1.969%
2	1.919	171	180	192	rBV	69577	90893	12.43%	1.565%
3	2.102	235	237	240	rVB	414	203	0.03%	0.003%
4	2.218	268	273	278	rBV3	453	481	0.07%	0.008%
5	2.302	297	299	302	rVB	309	130	0.02%	0.002%
6	2.514	361	365	370	rBV	386	377	0.05%	0.006%
7	2.568	370	382	405	rBV	158664	266262	36.41%	4.585%
8	2.793	444	452	461	rBV2	711	1232	0.17%	0.021%
9	2.961	503	504	511	rVB	216	172	0.02%	0.003%
10	3.051	526	532	538	rBV2	786	1146	0.16%	0.020%
11	3.305	609	611	615	rBV	132	135	0.02%	0.002%
12	3.398	635	640	643	rBV	146	189	0.03%	0.003%
13	3.459	656	659	662	rBV	151	150	0.02%	0.003%
14	3.620	706	709	711	rBV	173	146	0.02%	0.003%
15	3.732	741	744	749	rBB	132	162	0.02%	0.003%
16	3.771	750	756	761	rBB	176	248	0.03%	0.004%
17	3.813	766	769	772	rVB	169	140	0.02%	0.002%
18	3.835	773	776	778	rBV	147	126	0.02%	0.002%
19	3.973	816	819	824	rVB	161	181	0.02%	0.003%
20	4.070	847	849	852	rBV	160	129	0.02%	0.002%
21	4.215	890	894	897	rBB	124	130	0.02%	0.002%
22	4.272	909	912	917	rBV	148	194	0.03%	0.003%
23	4.343	929	934	939	rBV	209	281	0.04%	0.005%
24	4.391	947	949	953	rBB	139	119	0.02%	0.002%
25	4.501	980	983	986	rBB	158	130	0.02%	0.002%
26	4.642	1010	1027	1058	rBV	58118	175194	23.96%	3.017%
27	4.957	1121	1125	1129	rBV2	275	287	0.04%	0.005%
28	5.067	1144	1159	1180	rBV	129190	283628	38.78%	4.884%
29	5.208	1201	1203	1208	rVB	192	139	0.02%	0.002%
30	5.292	1224	1229	1234	rVB2	430	427	0.06%	0.007%
31	5.488	1287	1290	1295	rBV	149	209	0.03%	0.004%
32	5.729	1342	1365	1383	rBV2	272588	731305	100.00%	12.594%
33	6.125	1484	1488	1489	rBV2	336	195	0.03%	0.003%
34	6.253	1512	1528	1550	rBV	257144	485264	66.36%	8.357%
35	6.488	1599	1601	1604	rBV	153	118	0.02%	0.002%
36	6.536	1607	1616	1628	rBV5	2333	5163	0.71%	0.089%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
 Data File : VU046089.D
 Acq On : 04 Dec 2021 13:44
 Operator : SY/MD
 Sample : VU1204MBL01
 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

37	6.597	1628	1635	1637	rVB	135	180	0.02%	0.003%
38	6.694	1647	1665	1686	rBV	164539	320717	43.86%	5.523%
39	6.784	1691	1693	1697	rVB2	302	213	0.03%	0.004%
40	6.806	1697	1700	1703	rBV	292	227	0.03%	0.004%
41	6.822	1703	1705	1710	rVB	299	166	0.02%	0.003%
42	6.906	1728	1731	1737	rBB	168	207	0.03%	0.004%
43	7.102	1789	1792	1797	rBB	155	187	0.03%	0.003%
44	7.141	1801	1804	1807	rVB	166	132	0.02%	0.002%
45	7.166	1810	1812	1815	rBV	172	136	0.02%	0.002%
46	7.243	1833	1836	1842	rVB	187	218	0.03%	0.004%
47	7.317	1857	1859	1864	rBV	135	161	0.02%	0.003%
48	7.568	1924	1937	1956	rVV	94276	161549	22.09%	2.782%
49	7.636	1956	1958	1960	rVV	224	144	0.02%	0.002%
50	7.723	1982	1985	1988	rVB	205	166	0.02%	0.003%
51	7.899	2026	2040	2057	rBV	343590	595741	81.46%	10.260%
52	8.182	2115	2128	2145	rVV	62065	103063	14.09%	1.775%
53	8.272	2152	2156	2159	rVB2	279	233	0.03%	0.004%
54	8.472	2212	2218	2222	rBV	202	298	0.04%	0.005%
55	8.639	2255	2270	2308	rBV	202667	370049	50.60%	6.373%
56	8.822	2322	2327	2331	rBB	171	218	0.03%	0.004%
57	9.112	2412	2417	2421	rBV	165	227	0.03%	0.004%
58	9.150	2426	2429	2431	rVV	215	125	0.02%	0.002%
59	9.176	2434	2437	2439	rVB	264	146	0.02%	0.003%
60	9.282	2468	2470	2474	rVB	175	118	0.02%	0.002%
61	9.324	2480	2483	2486	rBV	164	165	0.02%	0.003%
62	9.420	2499	2513	2546	rVV	355897	589374	80.59%	10.150%
63	9.575	2555	2561	2570	rVB2	588	774	0.11%	0.013%
64	9.697	2592	2599	2606	rVV2	819	1223	0.17%	0.021%
65	10.105	2720	2726	2730	rBV2	580	692	0.09%	0.012%
66	10.484	2838	2844	2851	rVB2	507	689	0.09%	0.012%
67	10.639	2885	2892	2893	rBV	192	256	0.04%	0.004%
68	10.674	2894	2903	2913	rVV3	2490	3240	0.44%	0.056%
69	10.758	2913	2929	2947	rVV	229273	366894	50.17%	6.318%
70	10.857	2957	2960	2962	rBV	260	175	0.02%	0.003%
71	10.922	2977	2980	2984	rVB2	176	128	0.02%	0.002%
72	11.089	3026	3032	3039	rBV2	547	747	0.10%	0.013%
73	11.121	3039	3042	3048	rVB2	342	280	0.04%	0.005%
74	11.465	3140	3149	3158	rVB4	1771	3154	0.43%	0.054%
75	11.581	3181	3185	3189	rVB2	201	214	0.03%	0.004%
76	11.700	3214	3222	3228	rBV3	627	923	0.13%	0.016%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
 Data File : VU046089.D
 Acq On : 04 Dec 2021 13:44
 Operator : SY/MD
 Sample : VU1204MBL01
 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	11.742	3231	3235	3244	rVB	855	1143	0.16%	0.020%
78	11.816	3245	3258	3276	rVB	364031	577321	78.94%	9.942%
79	11.944	3291	3298	3302	rVV2	879	971	0.13%	0.017%
80	11.970	3302	3306	3317	rVB4	1551	2149	0.29%	0.037%
81	12.195	3360	3376	3396	rBV	324385	521255	71.28%	8.977%
82	12.333	3416	3419	3421	rBV	383	210	0.03%	0.004%
83	12.558	3486	3489	3497	rBV	100	145	0.02%	0.002%
84	12.594	3497	3500	3504	rVB	192	118	0.02%	0.002%
85	12.635	3510	3513	3515	rBV2	179	127	0.02%	0.002%
86	12.886	3588	3591	3599	rBV	154	178	0.02%	0.003%
87	12.999	3623	3626	3631	rBV3	330	266	0.04%	0.005%
88	13.147	3670	3672	3677	rBV2	178	155	0.02%	0.003%
89	13.221	3689	3695	3703	rBV3	1507	1920	0.26%	0.033%
90	13.844	3881	3889	3897	rBV2	2416	3183	0.44%	0.055%
91	14.089	3956	3965	3981	rVB	5069	8045	1.10%	0.139%
92	14.333	4032	4041	4048	rVB2	3202	4431	0.61%	0.076%
93	14.571	4111	4115	4117	rBV	201	191	0.03%	0.003%
94	15.095	4273	4278	4282	rBV2	274	366	0.05%	0.006%
95	15.214	4313	4315	4318	rBV2	201	154	0.02%	0.003%
96	15.333	4350	4352	4358	rVB2	240	209	0.03%	0.004%
97	15.462	4390	4392	4395	rBV2	199	137	0.02%	0.002%
98	15.623	4438	4442	4446	rBV2	226	281	0.04%	0.005%
99	16.294	4648	4651	4658	rVB	409	305	0.04%	0.005%
100	16.635	4756	4757	4762	rBV2	472	298	0.04%	0.005%

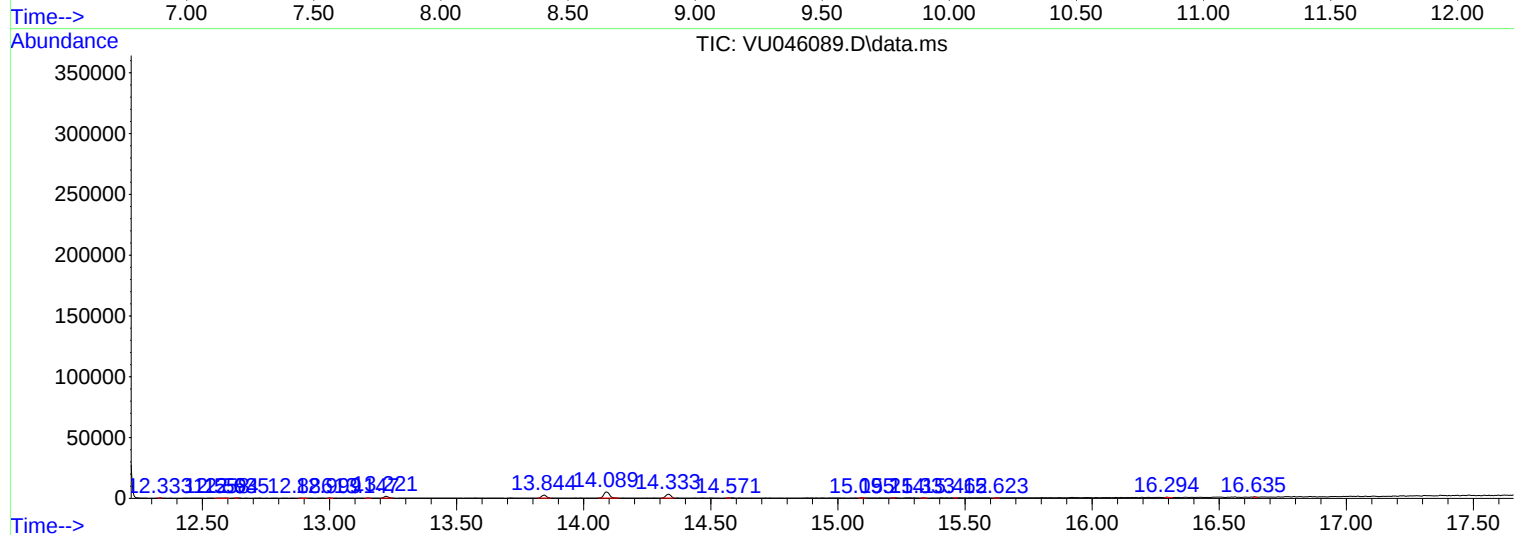
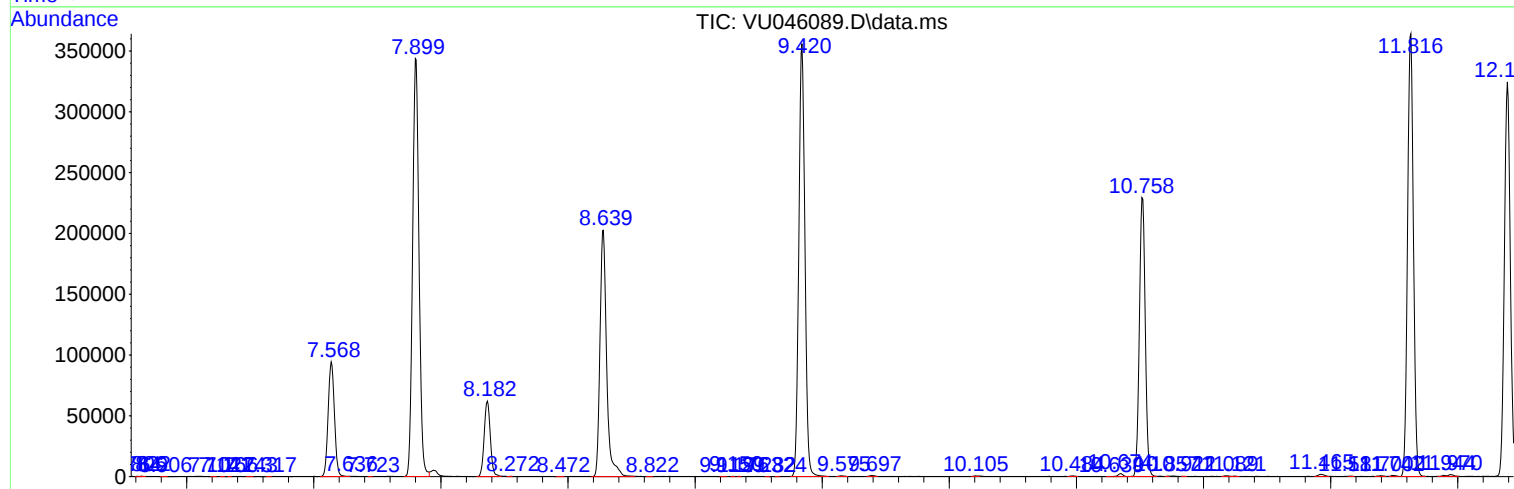
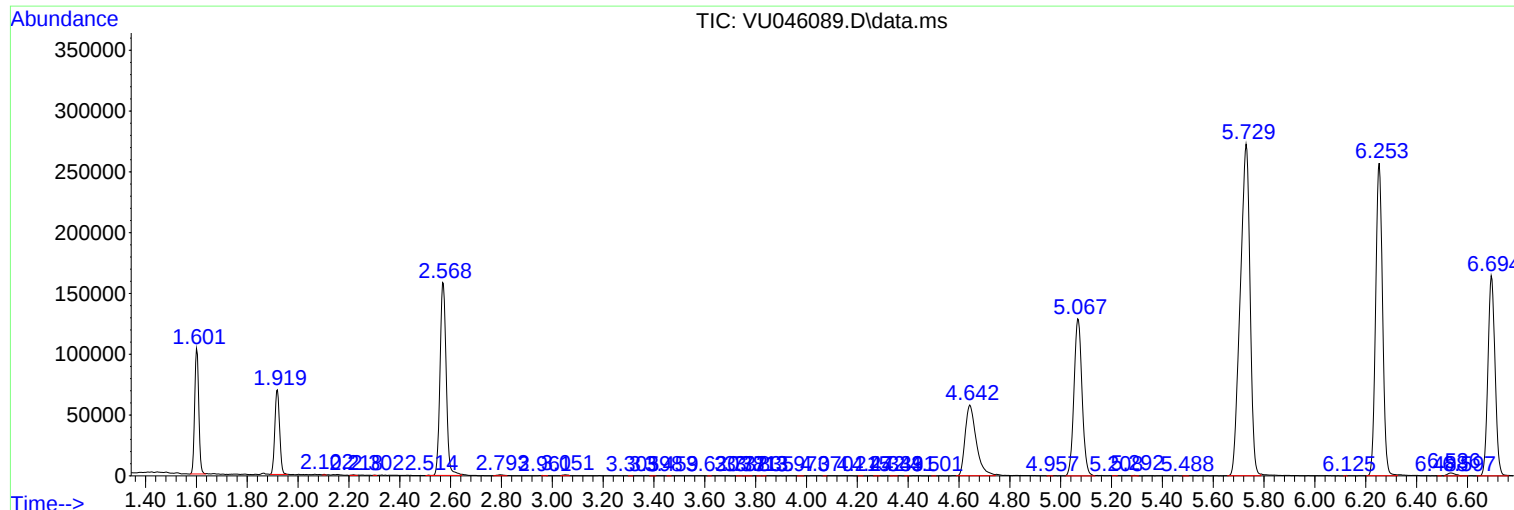
Sum of corrected areas: 5806710

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
Data File : VU046089.D
Acq On : 04 Dec 2021 13:44
Operator : SY/MD
Sample : VU1204MBL01
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\VU120421\
Data File : VU046089.D
Acq On : 04 Dec 2021 13:44
Operator : SY/MD
Sample : VU1204MBL01
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\VU120421\
Data File : VU046089.D
Acq On : 04 Dec 2021 13:44
Operator : SY/MD
Sample : VU1204MBL01
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

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