

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043742.D
 Acq On : 14 May 2021 09:47
 Operator : SY/MD
 Sample : VU0514MBL01
 Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK17

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\SFAMULM051421WMA.M
 Title : VOC Analysis

Signal : TIC: VU043742.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	94	rBV	272437	293704	15.31%	2.036%
2	1.912	169	178	195	rVB	184699	244352	12.74%	1.694%
3	2.571	370	383	402	rBV	415544	681500	35.52%	4.724%
4	2.681	414	417	420	rBV2	322	198	0.01%	0.001%
5	2.700	420	423	426	rBV2	269	171	0.01%	0.001%
6	2.751	437	439	442	rVB2	363	165	0.01%	0.001%
7	2.793	446	452	454	rBV2	884	796	0.04%	0.006%
8	2.944	496	499	500	rBV2	308	194	0.01%	0.001%
9	2.960	500	504	508	rVV3	478	468	0.02%	0.003%
10	3.057	524	534	542	rBV4	2843	4838	0.25%	0.034%
11	3.121	548	554	559	rVB4	333	363	0.02%	0.003%
12	3.198	559	578	590	rBV4	1363	3777	0.20%	0.026%
13	3.362	626	629	633	rVB	395	266	0.01%	0.002%
14	3.398	633	640	643	rBV2	266	241	0.01%	0.002%
15	3.555	687	689	691	rBV	276	169	0.01%	0.001%
16	3.681	725	728	731	rVB	282	189	0.01%	0.001%
17	3.748	745	749	752	rBV2	279	219	0.01%	0.002%
18	3.764	752	754	759	rVB2	318	232	0.01%	0.002%
19	3.796	759	764	769	rBV2	236	303	0.02%	0.002%
20	3.851	776	781	789	rBV2	213	316	0.02%	0.002%
21	4.028	831	836	838	rBV	217	230	0.01%	0.002%
22	4.494	977	981	984	rBV	220	193	0.01%	0.001%
23	4.530	988	992	997	rVV2	265	348	0.02%	0.002%
24	4.626	1005	1022	1050	rBV	215553	511292	26.65%	3.544%
25	4.883	1097	1102	1106	rBV3	211	212	0.01%	0.001%
26	4.938	1114	1119	1123	rVB2	322	306	0.02%	0.002%
27	4.960	1123	1126	1129	rBV2	308	245	0.01%	0.002%
28	5.073	1143	1161	1187	rVV	340668	733632	38.24%	5.086%
29	5.169	1190	1191	1194	rVB2	490	207	0.01%	0.001%
30	5.224	1204	1208	1212	rBV3	410	403	0.02%	0.003%
31	5.282	1223	1226	1227	rBV	433	252	0.01%	0.002%
32	5.295	1227	1230	1232	rBV	486	307	0.02%	0.002%
33	5.343	1241	1245	1248	rBV2	185	165	0.01%	0.001%
34	5.385	1252	1258	1265	rVB2	630	769	0.04%	0.005%
35	5.526	1297	1302	1305	rBV	220	205	0.01%	0.001%
36	5.648	1336	1340	1344	rBV2	227	242	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043742.D
 Acq On : 14 May 2021 09:47
 Operator : SY/MD
 Sample : VU0514MBL01
 Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK17

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\SFAMULM051421WMA.M
 Title : VOC Analysis

37	5.735	1344	1367	1393	rBV2	717283	1918408	100.00%	13.299%
38	6.050	1458	1465	1471	rBV3	638	852	0.04%	0.006%
39	6.185	1501	1507	1510	rVB3	319	299	0.02%	0.002%
40	6.256	1510	1529	1552	rBV	574433	1073673	55.97%	7.443%
41	6.536	1605	1616	1625	rVB4	3737	6679	0.35%	0.046%
42	6.700	1650	1667	1690	rBV	444246	865633	45.12%	6.001%
43	6.816	1698	1703	1711	rVB6	1488	2310	0.12%	0.016%
44	6.877	1718	1722	1724	rBV2	720	503	0.03%	0.003%
45	7.044	1767	1774	1779	rBV	730	1042	0.05%	0.007%
46	7.185	1813	1818	1825	rVB4	734	1053	0.05%	0.007%
47	7.311	1850	1857	1865	rVB2	241	363	0.02%	0.003%
48	7.353	1865	1870	1873	rBV	300	260	0.01%	0.002%
49	7.491	1907	1913	1918	rBV2	108	170	0.01%	0.001%
50	7.571	1925	1938	1955	rBV	235356	411406	21.45%	2.852%
51	7.742	1988	1991	1996	rVB3	284	237	0.01%	0.002%
52	7.825	2014	2017	2019	rBV2	238	178	0.01%	0.001%
53	7.906	2025	2042	2056	rBV	875130	1486654	77.49%	10.306%
54	7.976	2058	2064	2075	rVB	13253	21994	1.15%	0.152%
55	8.121	2107	2109	2112	rVB2	371	221	0.01%	0.002%
56	8.185	2116	2129	2146	rBV	166932	277325	14.46%	1.923%
57	8.288	2158	2161	2166	rVB4	358	350	0.02%	0.002%
58	8.359	2181	2183	2186	rVB3	292	203	0.01%	0.001%
59	8.385	2186	2191	2196	rVB4	395	296	0.02%	0.002%
60	8.472	2214	2218	2221	rBV2	217	228	0.01%	0.002%
61	8.639	2255	2270	2304	rBV	598627	1070155	55.78%	7.419%
62	8.857	2336	2338	2342	rVB2	312	199	0.01%	0.001%
63	8.877	2342	2344	2349	rVB2	318	244	0.01%	0.002%
64	8.909	2349	2354	2356	rBV3	425	373	0.02%	0.003%
65	8.941	2361	2364	2370	rVB3	638	512	0.03%	0.004%
66	9.423	2500	2514	2535	rBV	807946	1311503	68.36%	9.092%
67	9.578	2558	2562	2567	rBV2	558	449	0.02%	0.003%
68	9.607	2569	2571	2575	rBV	305	203	0.01%	0.001%
69	9.697	2593	2599	2600	rBV2	1102	1010	0.05%	0.007%
70	9.806	2626	2633	2638	rBV2	200	264	0.01%	0.002%
71	9.999	2689	2693	2699	rBV2	187	219	0.01%	0.002%
72	10.095	2717	2723	2725	rBV2	348	362	0.02%	0.003%
73	10.259	2771	2774	2778	rBV	223	168	0.01%	0.001%
74	10.426	2822	2826	2829	rVV2	263	213	0.01%	0.001%
75	10.491	2843	2846	2850	rVB2	286	225	0.01%	0.002%
76	10.674	2896	2903	2912	rBV4	5050	7741	0.40%	0.054%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043742.D
 Acq On : 14 May 2021 09:47
 Operator : SY/MD
 Sample : VU0514MBL01
 Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK17

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\SFAMULM051421WMA.M

Title : VOC Analysis

77	10.764	2917	2931	2951	rBV	606744	991799	51.70%	6.875%
78	10.838	2951	2954	2958	rVB3	410	312	0.02%	0.002%
79	10.877	2958	2966	2971	rBV6	1108	1976	0.10%	0.014%
80	11.005	3001	3006	3011	rVB3	371	378	0.02%	0.003%
81	11.211	3067	3070	3075	rVB2	428	396	0.02%	0.003%
82	11.465	3141	3149	3160	rVB3	3228	4925	0.26%	0.034%
83	11.700	3215	3222	3229	rBV3	2020	2653	0.14%	0.018%
84	11.819	3246	3259	3285	rBV	756496	1178041	61.41%	8.167%
85	11.947	3293	3299	3303	rBV6	1678	1945	0.10%	0.013%
86	12.021	3318	3322	3325	rBV2	274	259	0.01%	0.002%
87	12.082	3336	3341	3342	rBV2	413	329	0.02%	0.002%
88	12.121	3351	3353	3356	rVB	361	189	0.01%	0.001%
89	12.198	3363	3377	3396	rBV	805273	1288645	67.17%	8.933%
90	12.378	3430	3433	3436	rBV2	270	207	0.01%	0.001%
91	12.404	3436	3441	3443	rBV4	459	385	0.02%	0.003%
92	12.555	3484	3488	3490	rBV3	356	284	0.01%	0.002%
93	12.886	3587	3591	3594	rBV2	190	191	0.01%	0.001%
94	13.098	3654	3657	3661	rBV	328	332	0.02%	0.002%
95	13.140	3668	3670	3671	rBV	334	165	0.01%	0.001%
96	13.233	3691	3699	3706	rBV3	816	1309	0.07%	0.009%
97	13.339	3727	3732	3735	rBV3	346	325	0.02%	0.002%
98	13.764	3861	3864	3868	rBV3	336	220	0.01%	0.002%
99	13.848	3887	3890	3900	rVB6	1251	1409	0.07%	0.010%
100	14.095	3962	3967	3978	rVB3	1902	2819	0.15%	0.020%

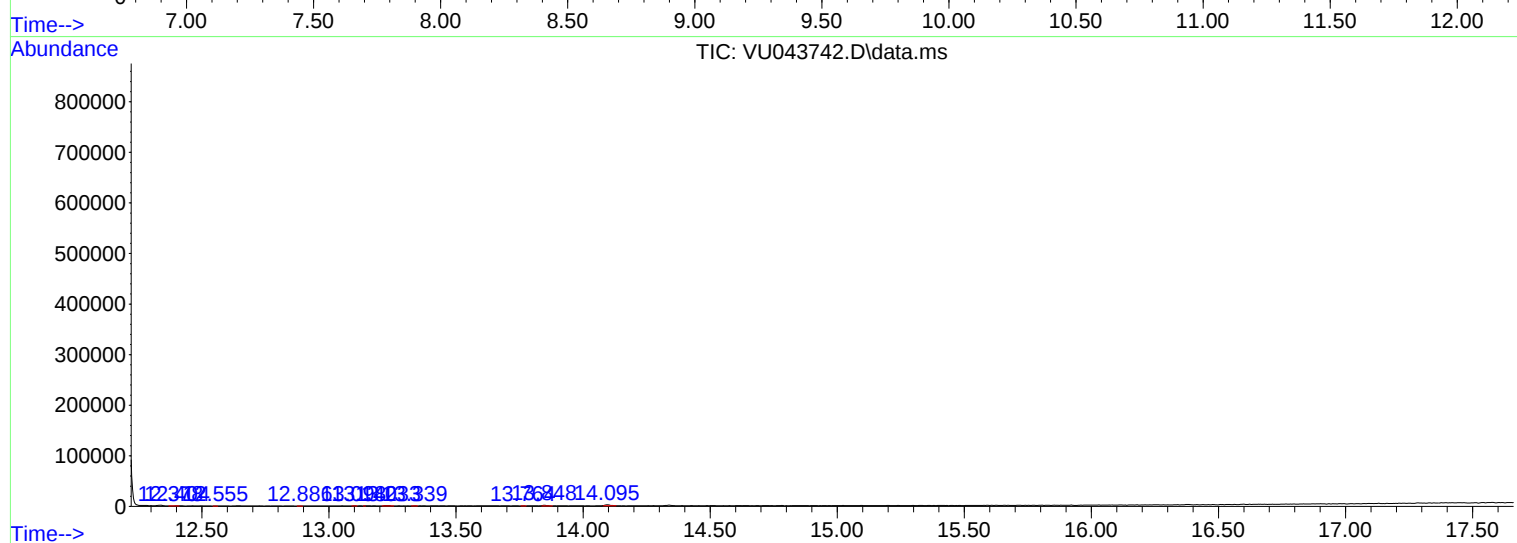
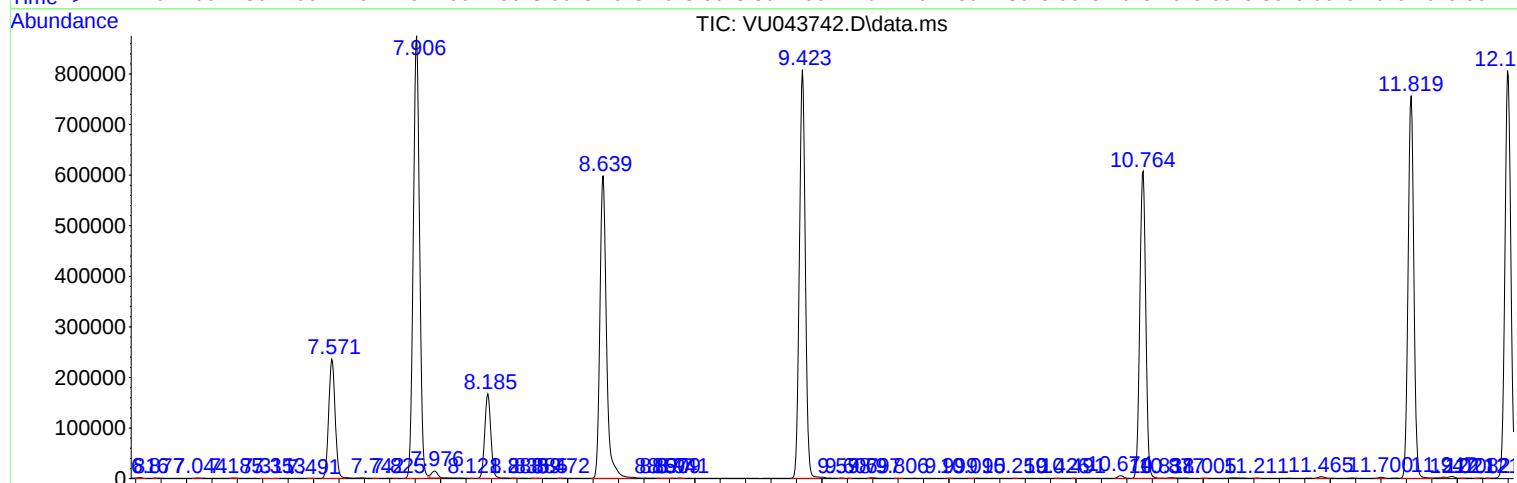
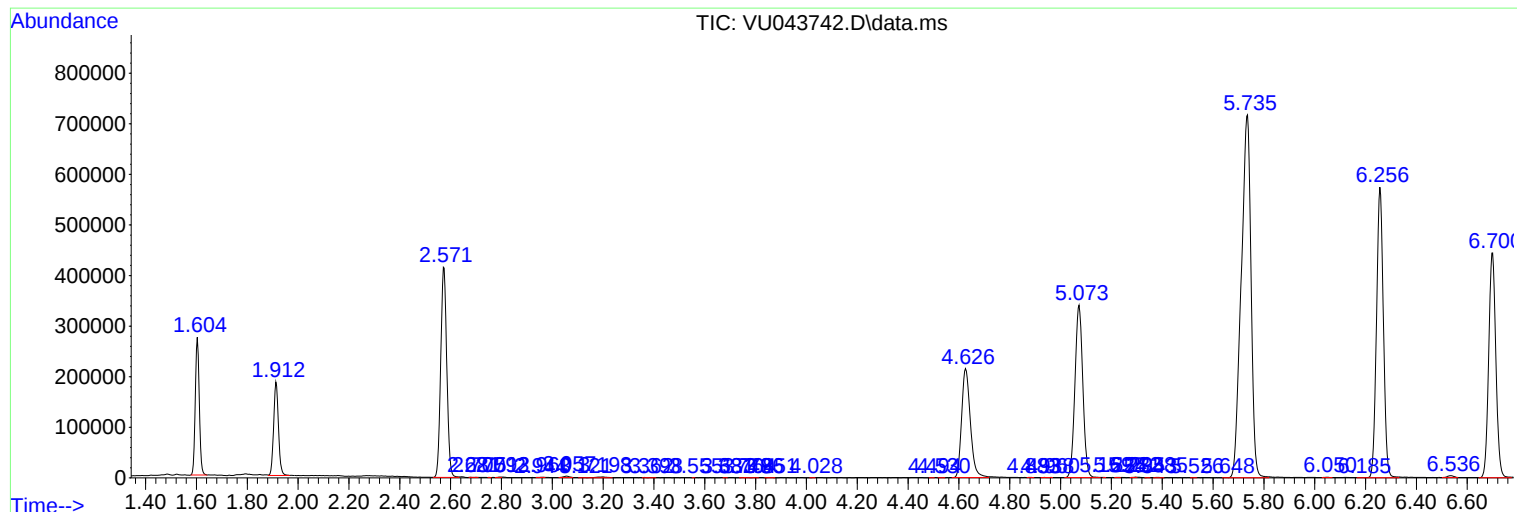
Sum of corrected areas: 14425139

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043742.D
Acq On : 14 May 2021 09:47
Operator : SY/MD
Sample : VU0514MBL01
Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043742.D
Acq On : 14 May 2021 09:47
Operator : SY/MD
Sample : VU0514MBL01
Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043742.D
Acq On : 14 May 2021 09:47
Operator : SY/MD
Sample : VU0514MBL01
Misc : 5.0g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 55 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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