

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046153.D
 Acq On : 07 Dec 2021 20:41
 Operator : SY/MD
 Sample : M4887-07ME
 Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A4ME

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: VU046153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	41	44	52	rVB2	4258	4390	0.27%	0.041%
2	1.601	72	81	98	rVB	183693	238768	14.43%	2.230%
3	1.919	170	180	197	rBV	104956	178401	10.78%	1.666%
4	2.549	364	376	393	rBV	291586	474242	28.66%	4.430%
5	3.041	522	529	537	rVV5	1478	2623	0.16%	0.025%
6	3.183	559	573	595	rBV	10179	27134	1.64%	0.253%
7	3.279	601	603	606	rVB2	221	121	0.01%	0.001%
8	3.330	617	619	622	rVB2	319	159	0.01%	0.001%
9	3.366	628	630	635	rVB2	273	184	0.01%	0.002%
10	3.588	694	699	700	rBV	213	215	0.01%	0.002%
11	3.623	706	710	714	rBB	197	200	0.01%	0.002%
12	3.883	788	791	797	rVB	170	185	0.01%	0.002%
13	3.919	798	802	804	rBV	124	138	0.01%	0.001%
14	3.961	812	815	817	rBV	146	126	0.01%	0.001%
15	3.996	823	826	829	rBV	167	171	0.01%	0.002%
16	4.179	880	883	887	rBV	187	206	0.01%	0.002%
17	4.488	975	979	984	rBB	155	202	0.01%	0.002%
18	4.517	984	988	990	rBV	171	176	0.01%	0.002%
19	4.655	1013	1031	1090	rBV	80074	397626	24.03%	3.714%
20	5.063	1141	1158	1188	rVV	262721	638142	38.57%	5.961%
21	5.227	1206	1209	1211	rBV	138	121	0.01%	0.001%
22	5.266	1215	1221	1224	rBV	195	260	0.02%	0.002%
23	5.340	1241	1244	1247	rBV	147	154	0.01%	0.001%
24	5.594	1320	1323	1326	rBV	148	144	0.01%	0.001%
25	5.723	1341	1363	1397	rBV2	652586	1654639	100.00%	15.456%
26	5.845	1400	1401	1403	rVV2	291	123	0.01%	0.001%
27	5.871	1406	1409	1414	rVV2	216	206	0.01%	0.002%
28	5.980	1433	1443	1458	rBV4	5707	14869	0.90%	0.139%
29	6.147	1492	1495	1500	rVB	305	259	0.02%	0.002%
30	6.250	1512	1527	1552	rBV	155351	318562	19.25%	2.976%
31	6.369	1561	1564	1567	rBV	129	133	0.01%	0.001%
32	6.481	1595	1599	1601	rBV	161	161	0.01%	0.002%
33	6.533	1604	1615	1626	rBV4	5687	11873	0.72%	0.111%
34	6.591	1630	1633	1634	rBV2	1015	534	0.03%	0.005%
35	6.690	1649	1664	1692	rVB	356086	733219	44.31%	6.849%
36	6.793	1692	1696	1697	rBV2	416	267	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046153.D
 Acq On : 07 Dec 2021 20:41
 Operator : SY/MD
 Sample : M4887-07ME
 Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A4ME

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	6.806	1697	1700	1701	rBV2	357	164	0.01%	0.002%
38	6.851	1710	1714	1717	rBV2	356	254	0.02%	0.002%
39	6.938	1738	1741	1746	rBV	164	204	0.01%	0.002%
40	6.999	1757	1760	1766	rBB	180	219	0.01%	0.002%
41	7.092	1787	1789	1793	rVB	372	237	0.01%	0.002%
42	7.134	1796	1802	1806	rBV	178	288	0.02%	0.003%
43	7.182	1813	1817	1818	rBV	517	343	0.02%	0.003%
44	7.308	1854	1856	1858	rBV2	258	162	0.01%	0.002%
45	7.395	1878	1883	1886	rBB	147	147	0.01%	0.001%
46	7.417	1887	1890	1893	rBB	159	129	0.01%	0.001%
47	7.440	1894	1897	1900	rBV	145	148	0.01%	0.001%
48	7.507	1914	1918	1920	rBV	159	166	0.01%	0.002%
49	7.568	1922	1937	1965	rVV	200141	398872	24.11%	3.726%
50	7.687	1971	1974	1979	rVB3	310	277	0.02%	0.003%
51	7.710	1979	1981	1983	rBV3	256	130	0.01%	0.001%
52	7.790	1997	2006	2018	rVB5	2786	5146	0.31%	0.048%
53	7.899	2025	2040	2057	rBV	766675	1420156	85.83%	13.266%
54	8.182	2116	2128	2159	rVB	118064	269040	16.26%	2.513%
55	8.353	2178	2181	2183	rBV	168	146	0.01%	0.001%
56	8.443	2206	2209	2211	rVV	159	122	0.01%	0.001%
57	8.462	2211	2215	2216	rVV	321	183	0.01%	0.002%
58	8.478	2216	2220	2226	rVB2	299	362	0.02%	0.003%
59	8.555	2233	2244	2255	rBV2	20605	34955	2.11%	0.327%
60	8.681	2259	2283	2316	rBV	260172	854590	51.65%	7.983%
61	8.944	2357	2365	2367	rBV3	613	708	0.04%	0.007%
62	9.025	2386	2390	2398	rVB	124	148	0.01%	0.001%
63	9.423	2498	2514	2534	rBV	182923	405975	24.54%	3.792%
64	9.571	2554	2560	2568	rBV	349	541	0.03%	0.005%
65	9.694	2590	2598	2599	rBV	1245	1031	0.06%	0.010%
66	9.780	2622	2625	2628	rVB	204	148	0.01%	0.001%
67	10.047	2703	2708	2712	rBV	272	330	0.02%	0.003%
68	10.102	2720	2725	2726	rBV	226	204	0.01%	0.002%
69	10.224	2760	2763	2766	rBV2	172	160	0.01%	0.001%
70	10.378	2806	2811	2813	rBV	209	152	0.01%	0.001%
71	10.539	2855	2861	2866	rVV3	569	639	0.04%	0.006%
72	10.613	2880	2884	2893	rVB	154	170	0.01%	0.002%
73	10.668	2893	2901	2910	rBV3	3906	6140	0.37%	0.057%
74	10.771	2918	2933	2949	rBV	503837	852424	51.52%	7.963%
75	10.864	2957	2962	2963	rBV2	554	409	0.02%	0.004%
76	11.147	3048	3050	3052	rBV2	357	165	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046153.D
 Acq On : 07 Dec 2021 20:41
 Operator : SY/MD
 Sample : M4887-07ME
 Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A4ME

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	11.201	3064	3067	3069	rBV2	279	163	0.01%	0.002%
78	11.455	3136	3146	3159	rBV4	3360	6070	0.37%	0.057%
79	11.574	3179	3183	3191	rVV3	654	781	0.05%	0.007%
80	11.697	3213	3221	3230	rVB3	1488	2301	0.14%	0.021%
81	11.819	3247	3259	3272	rBV	271128	424856	25.68%	3.969%
82	11.915	3285	3289	3290	rBV	289	194	0.01%	0.002%
83	11.941	3290	3297	3302	rVV4	1442	2376	0.14%	0.022%
84	11.973	3302	3307	3315	rVB3	3327	4186	0.25%	0.039%
85	12.079	3336	3340	3345	rBV2	225	259	0.02%	0.002%
86	12.198	3359	3377	3392	rVV	806126	1302375	78.71%	12.166%
87	12.330	3413	3418	3425	rVB2	1090	1306	0.08%	0.012%
88	12.401	3435	3440	3446	rBV4	730	836	0.05%	0.008%
89	12.594	3496	3500	3505	rVB2	187	182	0.01%	0.002%
90	12.639	3508	3514	3519	rBV2	524	581	0.04%	0.005%
91	12.771	3549	3555	3564	rBV2	634	738	0.04%	0.007%
92	13.147	3665	3672	3678	rVB3	437	707	0.04%	0.007%
93	13.825	3880	3883	3888	rVB	254	212	0.01%	0.002%
94	14.578	4113	4117	4125	rVB	1049	1179	0.07%	0.011%
95	14.639	4133	4136	4141	rBV2	312	333	0.02%	0.003%
96	14.809	4187	4189	4192	rBV	255	174	0.01%	0.002%
97	14.848	4197	4201	4202	rBV2	204	144	0.01%	0.001%
98	15.115	4282	4284	4290	rVB	346	220	0.01%	0.002%
99	15.886	4522	4524	4536	rVB	338	209	0.01%	0.002%
100	15.931	4536	4538	4540	rBV	274	132	0.01%	0.001%

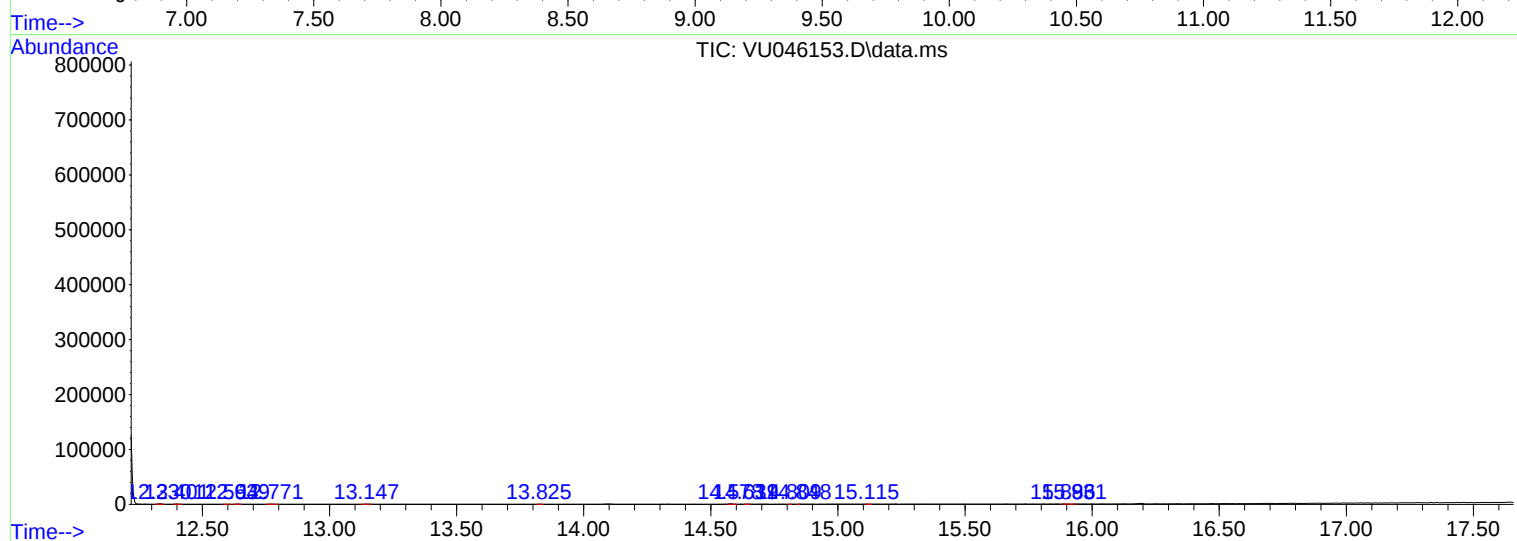
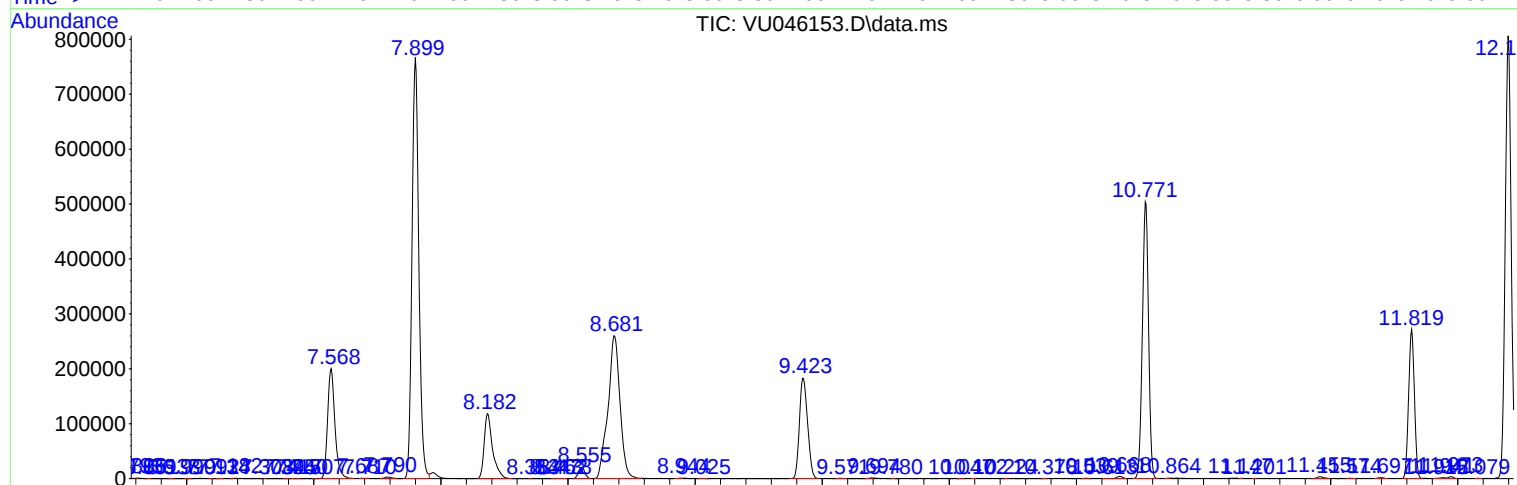
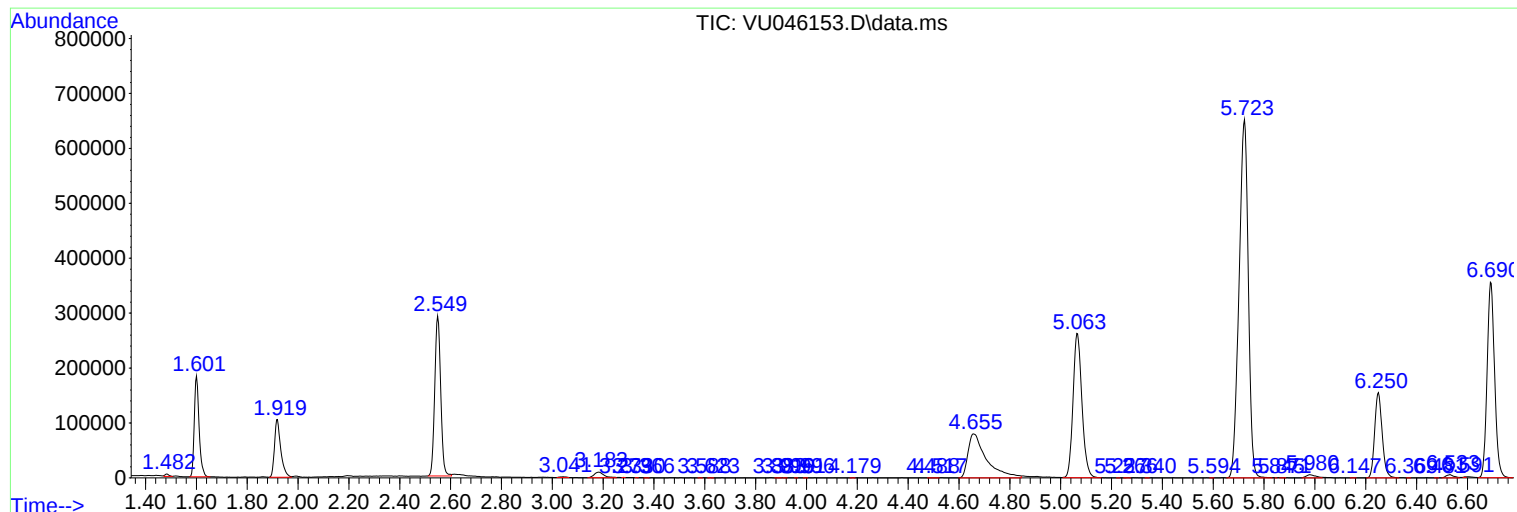
Sum of corrected areas: 10705231

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046153.D
Acq On : 07 Dec 2021 20:41
Operator : SY/MD
Sample : M4887-07ME
Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A4ME

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\VU120721\
Data File : VU046153.D
Acq On : 07 Dec 2021 20:41
Operator : SY/MD
Sample : M4887-07ME
Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A4ME

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\VU120721\
Data File : VU046153.D
Acq On : 07 Dec 2021 20:41
Operator : SY/MD
Sample : M4887-07ME
Misc : 5.93g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A4ME

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
------------------	----	---------	-------	----------	---	----	------	------