

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046454.D
 Acq On : 17 Dec 2021 04:34
 Operator : SY/MD
 Sample : M5121-09 20X
 Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL54

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: VU046454.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	100	rBV	61998	78598	14.68%	1.784%
2	1.919	171	180	203	rBV	46224	67326	12.58%	1.528%
3	2.195	263	266	271	rBV	250	237	0.04%	0.005%
4	2.572	371	383	402	rBV	110237	184318	34.43%	4.184%
5	2.871	473	476	481	rBB2	257	228	0.04%	0.005%
6	2.896	481	484	487	rBB	179	136	0.03%	0.003%
7	3.051	526	532	542	rVB2	1024	1628	0.30%	0.037%
8	3.189	562	575	591	rBB2	6861	15860	2.96%	0.360%
9	3.530	678	681	684	rBB	137	115	0.02%	0.003%
10	3.755	748	751	756	rBB	143	138	0.03%	0.003%
11	3.806	763	767	770	rBB	126	113	0.02%	0.003%
12	4.636	1011	1025	1048	rBV	50131	133123	24.87%	3.022%
13	5.067	1144	1159	1179	rVV	98322	211426	39.49%	4.799%
14	5.247	1211	1215	1218	rBB	127	136	0.03%	0.003%
15	5.571	1311	1316	1319	rBV	137	194	0.04%	0.004%
16	5.729	1343	1365	1390	rBV2	198695	535380	100.00%	12.153%
17	6.250	1513	1527	1543	rBV	182341	348540	65.10%	7.912%
18	6.427	1579	1582	1585	rBB	134	114	0.02%	0.003%
19	6.530	1610	1614	1619	rBB	583	561	0.10%	0.013%
20	6.694	1651	1665	1687	rBB	123800	238993	44.64%	5.425%
21	7.044	1772	1774	1778	rBB	141	121	0.02%	0.003%
22	7.182	1812	1817	1821	rBV2	369	378	0.07%	0.009%
23	7.568	1925	1937	1954	rBB	64623	111135	20.76%	2.523%
24	7.700	1976	1978	1980	rBB	327	126	0.02%	0.003%
25	7.787	1999	2005	2007	rBV2	454	491	0.09%	0.011%
26	7.899	2027	2040	2056	rBV	242841	417919	78.06%	9.486%
27	8.179	2115	2127	2148	rBB	45392	74750	13.96%	1.697%
28	8.266	2149	2154	2159	rBB2	289	385	0.07%	0.009%
29	8.298	2160	2164	2167	rBB	263	227	0.04%	0.005%
30	8.472	2214	2218	2219	rBV	322	242	0.05%	0.005%
31	8.636	2257	2269	2288	rBV	160450	266355	49.75%	6.046%
32	8.793	2312	2318	2323	rBB	178	265	0.05%	0.006%
33	8.919	2349	2357	2365	rBB4	933	1490	0.28%	0.034%
34	9.079	2403	2407	2409	rBV	129	115	0.02%	0.003%
35	9.202	2442	2445	2450	rBV	140	196	0.04%	0.004%
36	9.285	2467	2471	2475	rBB	136	141	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046454.D
 Acq On : 17 Dec 2021 04:34
 Operator : SY/MD
 Sample : M5121-09 20X
 Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL54

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	9.311	2476	2479	2484	rBV	162	214	0.04%	0.005%
38	9.359	2490	2494	2499	rBB	173	218	0.04%	0.005%
39	9.417	2499	2512	2532	rBV	277382	457411	85.44%	10.383%
40	9.575	2558	2561	2566	rBV	256	237	0.04%	0.005%
41	9.652	2582	2585	2588	rBV	183	162	0.03%	0.004%
42	9.694	2591	2598	2602	rBV2	343	533	0.10%	0.012%
43	9.716	2602	2605	2614	rVB2	420	611	0.11%	0.014%
44	9.790	2625	2628	2631	rBV	141	150	0.03%	0.003%
45	9.883	2654	2657	2660	rBB	155	126	0.02%	0.003%
46	9.960	2678	2681	2686	rBB	149	170	0.03%	0.004%
47	10.025	2698	2701	2702	rBV	320	175	0.03%	0.004%
48	10.118	2726	2730	2735	rBV3	723	732	0.14%	0.017%
49	10.253	2763	2772	2778	rBV5	1486	2246	0.42%	0.051%
50	10.356	2797	2804	2812	rBV4	841	1019	0.19%	0.023%
51	10.388	2812	2814	2815	rBV4	499	240	0.04%	0.005%
52	10.449	2829	2833	2835	rBV	152	123	0.02%	0.003%
53	10.459	2835	2836	2840	rVB	318	178	0.03%	0.004%
54	10.491	2842	2846	2849	rBV	146	166	0.03%	0.004%
55	10.552	2862	2865	2868	rBV2	172	167	0.03%	0.004%
56	10.674	2895	2903	2911	rBV4	2081	2845	0.53%	0.065%
57	10.758	2916	2929	2949	rBV	179392	283962	53.04%	6.446%
58	10.870	2958	2964	2967	rBV2	386	498	0.09%	0.011%
59	10.964	2989	2993	2996	rVB3	370	294	0.05%	0.007%
60	11.002	2997	3005	3007	rBV3	580	639	0.12%	0.015%
61	11.063	3018	3024	3026	rBV3	1161	1102	0.21%	0.025%
62	11.124	3034	3043	3046	rBV4	1486	1991	0.37%	0.045%
63	11.176	3056	3059	3061	rBV3	346	194	0.04%	0.004%
64	11.240	3076	3079	3080	rBV2	303	175	0.03%	0.004%
65	11.279	3088	3091	3092	rBV2	600	343	0.06%	0.008%
66	11.301	3096	3098	3099	rBV	495	184	0.03%	0.004%
67	11.574	3174	3183	3191	rBV3	1964	3152	0.59%	0.072%
68	11.639	3198	3203	3209	rVB6	1411	1676	0.31%	0.038%
69	11.700	3214	3222	3231	rVB6	2756	4261	0.80%	0.097%
70	11.745	3231	3236	3237	rBV2	867	753	0.14%	0.017%
71	11.812	3245	3257	3271	rBV	323135	498668	93.14%	11.319%
72	12.079	3333	3340	3342	rBV2	699	822	0.15%	0.019%
73	12.195	3364	3376	3390	rVB	258344	420072	78.46%	9.535%
74	12.333	3411	3419	3428	rBV7	1577	2718	0.51%	0.062%
75	12.472	3454	3462	3464	rBV4	922	1064	0.20%	0.024%
76	12.877	3587	3588	3590	rBV4	340	133	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046454.D
 Acq On : 17 Dec 2021 04:34
 Operator : SY/MD
 Sample : M5121-09 20X
 Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL54

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	13.005	3626	3628	3630	rBV2	323	141	0.03%	0.003%
78	13.256	3704	3706	3707	rBV2	233	124	0.02%	0.003%
79	13.304	3718	3721	3725	rBV2	536	463	0.09%	0.011%
80	13.513	3783	3786	3787	rBV	409	256	0.05%	0.006%
81	13.529	3787	3791	3793	rVV4	622	415	0.08%	0.009%
82	13.542	3793	3795	3797	rVV	526	264	0.05%	0.006%
83	13.587	3799	3809	3817	rBV6	2500	4234	0.79%	0.096%
84	13.726	3850	3852	3855	rVB2	284	139	0.03%	0.003%
85	13.745	3855	3858	3859	rBV	379	191	0.04%	0.004%
86	14.028	3943	3946	3950	rBV2	417	347	0.06%	0.008%
87	14.195	3988	3998	4007	rBV5	2858	5130	0.96%	0.116%
88	14.340	4040	4043	4045	rBV	341	207	0.04%	0.005%
89	14.378	4052	4055	4056	rBV2	382	210	0.04%	0.005%
90	14.404	4060	4063	4064	rBV2	487	284	0.05%	0.006%
91	14.494	4088	4091	4095	rBV2	496	463	0.09%	0.011%
92	14.645	4132	4138	4144	rBV4	1068	1347	0.25%	0.031%
93	14.751	4168	4171	4175	rVB3	408	248	0.05%	0.006%
94	14.825	4191	4194	4197	rBV2	420	361	0.07%	0.008%
95	14.979	4240	4242	4244	rVV	272	120	0.02%	0.003%
96	15.031	4253	4258	4264	rBV3	354	451	0.08%	0.010%
97	15.086	4273	4275	4277	rBV	386	198	0.04%	0.004%
98	15.208	4307	4313	4324	rVB6	2551	4150	0.78%	0.094%
99	15.365	4357	4362	4364	rBV2	534	496	0.09%	0.011%
100	15.973	4546	4551	4559	rBV5	2198	3273	0.61%	0.074%

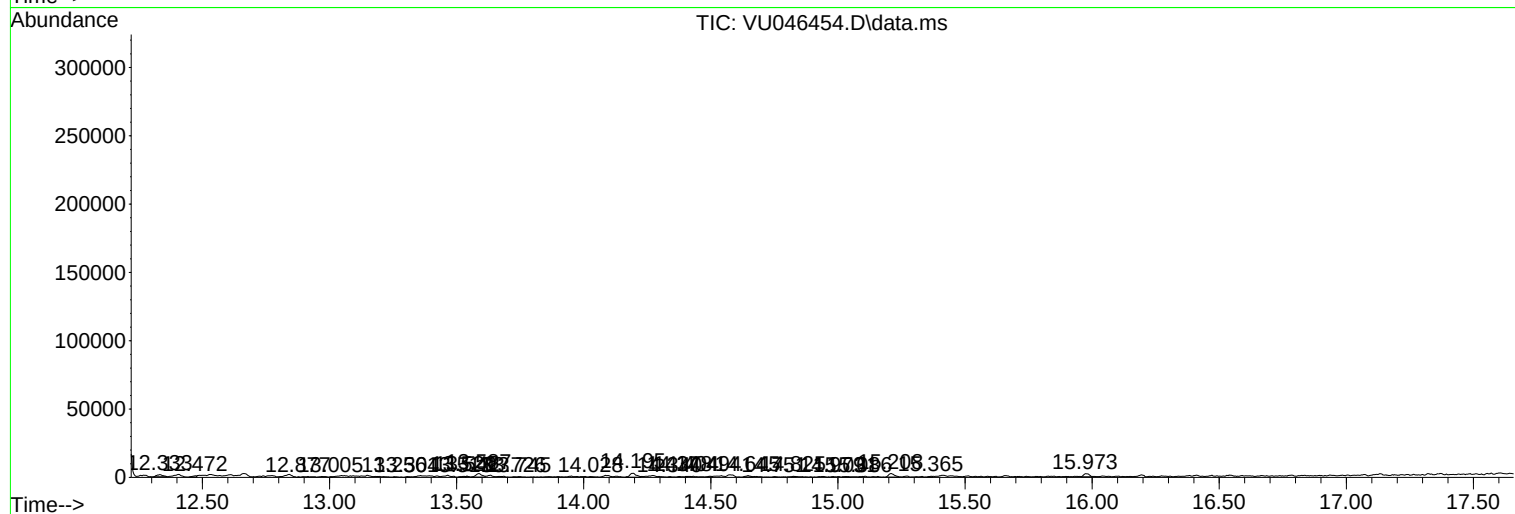
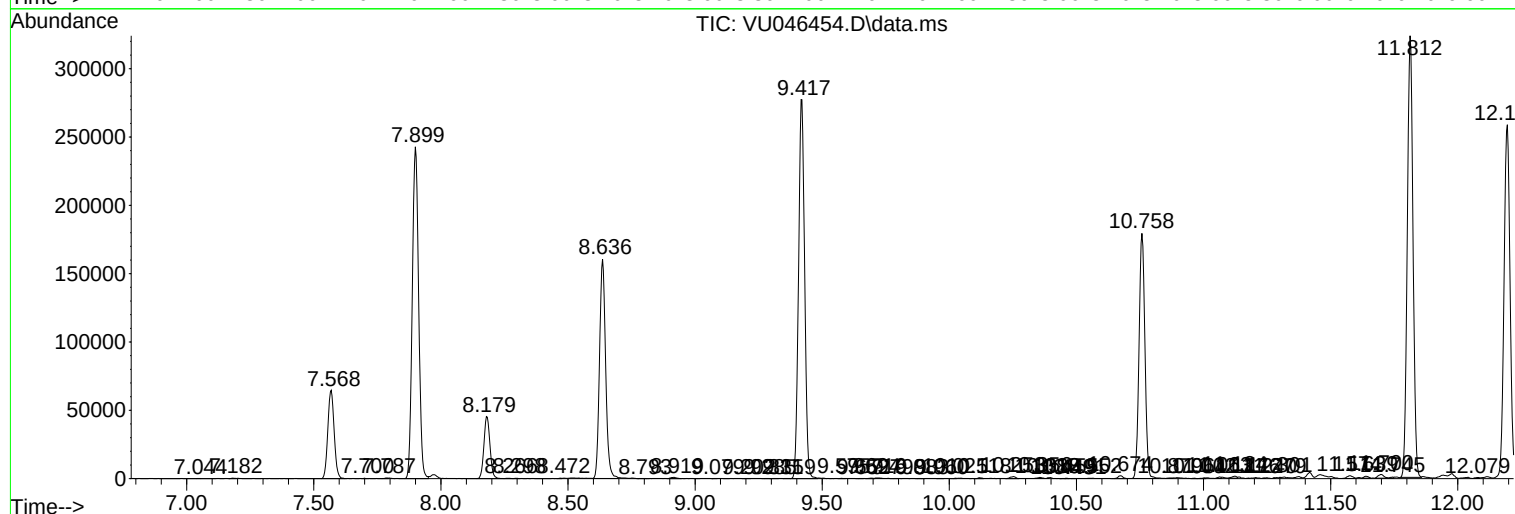
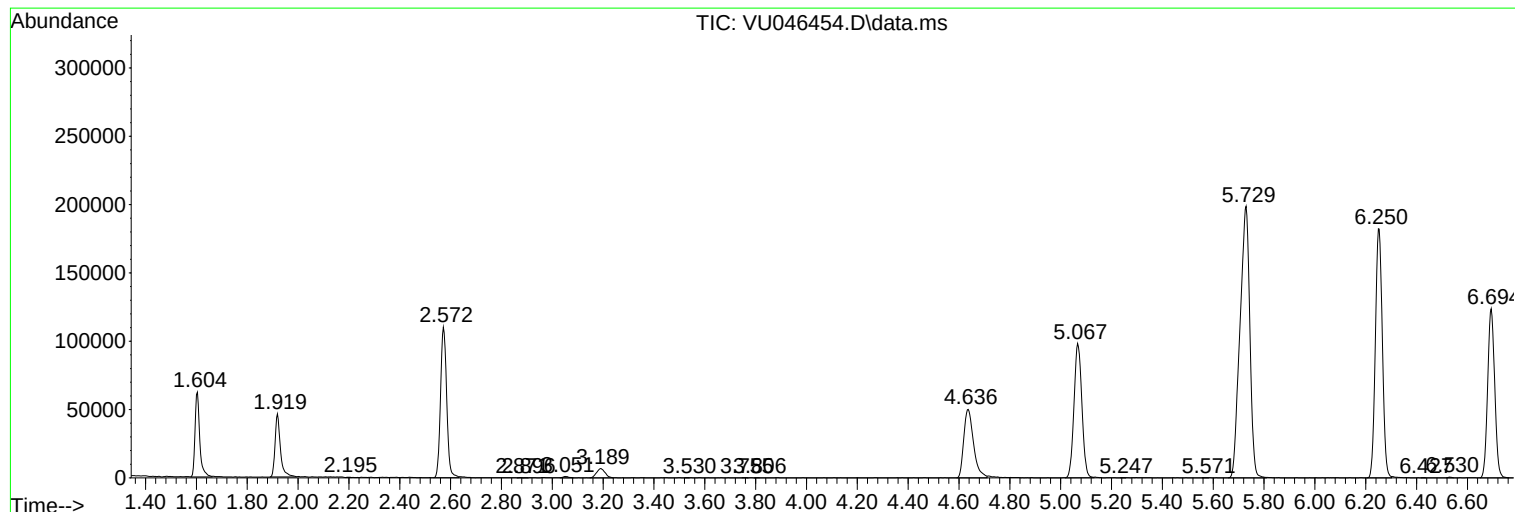
Sum of corrected areas: 4405436

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
Data File : VU046454.D
Acq On : 17 Dec 2021 04:34
Operator : SY/MD
Sample : M5121-09 20X
Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL54

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\VU121621\
Data File : VU046454.D
Acq On : 17 Dec 2021 04:34
Operator : SY/MD
Sample : M5121-09 20X
Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL54

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\VU121621\
Data File : VU046454.D
Acq On : 17 Dec 2021 04:34
Operator : SY/MD
Sample : M5121-09 20X
Misc : 5.69g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL54

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