

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
 Data File : VU046499.D
 Acq On : 19 Dec 2021 16:53
 Operator : SY/MD
 Sample : M5062-07ME
 Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL06ME

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: VU046499.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	40	46	53	rBV	2659	3340	0.66%	0.061%
2	1.604	74	82	113	rVB	33826	66254	13.07%	1.215%
3	1.887	160	170	220	rBV2	95820	232504	45.87%	4.264%
4	2.166	254	257	262	rBV3	607	505	0.10%	0.009%
5	2.192	262	265	269	rBV2	252	224	0.04%	0.004%
6	2.218	269	273	275	rBV3	335	286	0.06%	0.005%
7	2.250	281	283	285	rBV2	562	283	0.06%	0.005%
8	2.565	369	381	398	rBV3	108505	229148	45.21%	4.203%
9	2.761	440	442	449	rVB3	216	166	0.03%	0.003%
10	2.848	467	469	473	rBV2	140	124	0.02%	0.002%
11	2.967	494	506	516	rBV4	1847	3808	0.75%	0.070%
12	3.041	523	529	533	rBV3	444	563	0.11%	0.010%
13	3.128	554	556	560	rBB	178	140	0.03%	0.003%
14	3.179	567	572	573	rBV2	392	298	0.06%	0.005%
15	3.260	595	597	600	rBV	140	117	0.02%	0.002%
16	3.282	601	604	608	rVB	187	182	0.04%	0.003%
17	3.305	609	611	614	rBV	137	115	0.02%	0.002%
18	3.366	626	630	633	rBB	167	160	0.03%	0.003%
19	3.498	667	671	674	rBB	150	156	0.03%	0.003%
20	3.867	767	786	807	rBV	138423	327567	64.62%	6.008%
21	4.665	1017	1034	1052	rBV	24784	99141	19.56%	1.818%
22	5.006	1138	1140	1143	rVV	333	166	0.03%	0.003%
23	5.067	1143	1159	1188	rVV	88043	205488	40.54%	3.769%
24	5.163	1188	1189	1193	rVB	354	164	0.03%	0.003%
25	5.311	1226	1235	1246	rBB2	1214	2506	0.49%	0.046%
26	5.584	1318	1320	1324	rBB	142	117	0.02%	0.002%
27	5.723	1343	1363	1387	rBV3	196834	506876	100.00%	9.296%
28	5.980	1432	1443	1460	rBV5	2527	6503	1.28%	0.119%
29	6.041	1460	1462	1468	rVB2	495	425	0.08%	0.008%
30	6.166	1498	1501	1504	rBB2	272	177	0.03%	0.003%
31	6.250	1513	1527	1558	rBV	176920	344024	67.87%	6.310%
32	6.543	1605	1618	1636	rBV	137751	258344	50.97%	4.738%
33	6.690	1651	1664	1691	rVB	111586	225858	44.56%	4.142%
34	7.182	1814	1817	1819	rBV2	280	202	0.04%	0.004%
35	7.398	1879	1884	1888	rBB2	429	458	0.09%	0.008%
36	7.568	1925	1937	1966	rVB	53662	111118	21.92%	2.038%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
 Data File : VU046499.D
 Acq On : 19 Dec 2021 16:53
 Operator : SY/MD
 Sample : M5062-07ME
 Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL06ME

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	7.796	2006	2008	2010	rVB	251	136	0.03%	0.002%
38	7.899	2027	2040	2056	rBV	211733	395954	78.12%	7.262%
39	8.186	2114	2129	2160	rBB2	27546	79245	15.63%	1.453%
40	8.407	2195	2198	2203	rBB	122	130	0.03%	0.002%
41	8.488	2220	2223	2228	rVV2	262	219	0.04%	0.004%
42	8.552	2228	2243	2262	rVB	230940	398081	78.54%	7.301%
43	8.694	2262	2287	2311	rBV3	85356	294086	58.02%	5.394%
44	8.825	2326	2328	2331	rVB	384	261	0.05%	0.005%
45	8.845	2331	2334	2337	rBV	181	178	0.04%	0.003%
46	9.063	2398	2402	2405	rBB	130	134	0.03%	0.002%
47	9.112	2414	2417	2420	rBV	116	129	0.03%	0.002%
48	9.227	2450	2453	2456	rBB	151	129	0.03%	0.002%
49	9.266	2462	2465	2470	rBV	145	197	0.04%	0.004%
50	9.340	2485	2488	2490	rBV	141	122	0.02%	0.002%
51	9.362	2492	2495	2497	rVV2	292	256	0.05%	0.005%
52	9.427	2501	2515	2542	rVB2	185685	472531	93.22%	8.666%
53	9.694	2594	2598	2599	rBV2	304	162	0.03%	0.003%
54	9.764	2616	2620	2627	rBB	154	219	0.04%	0.004%
55	9.812	2632	2635	2638	rBB	131	117	0.02%	0.002%
56	9.832	2639	2641	2644	rBV	138	119	0.02%	0.002%
57	9.954	2674	2679	2682	rBB	138	141	0.03%	0.003%
58	10.086	2717	2720	2724	rBB	193	187	0.04%	0.003%
59	10.118	2728	2730	2733	rVB	183	122	0.02%	0.002%
60	10.169	2744	2746	2749	rBV	137	116	0.02%	0.002%
61	10.343	2796	2800	2803	rBV	134	163	0.03%	0.003%
62	10.417	2816	2823	2826	rBB	140	197	0.04%	0.004%
63	10.452	2830	2834	2836	rBV	153	158	0.03%	0.003%
64	10.546	2860	2863	2867	rVB	394	354	0.07%	0.006%
65	10.674	2897	2903	2908	rBV4	808	981	0.19%	0.018%
66	10.777	2920	2935	2951	rVB	176694	303748	59.93%	5.571%
67	10.861	2959	2961	2964	rBV	167	141	0.03%	0.003%
68	10.899	2968	2973	2981	rBV2	432	698	0.14%	0.013%
69	10.954	2986	2990	2992	rBV	159	156	0.03%	0.003%
70	10.980	2996	2998	3002	rBV	120	128	0.03%	0.002%
71	11.070	3020	3026	3028	rBV2	151	162	0.03%	0.003%
72	11.115	3037	3040	3046	rVB3	378	419	0.08%	0.008%
73	11.237	3073	3078	3081	rBV	188	220	0.04%	0.004%
74	11.324	3102	3105	3107	rBV	149	123	0.02%	0.002%
75	11.340	3107	3110	3113	rVB	181	150	0.03%	0.003%
76	11.359	3114	3116	3119	rBV	153	133	0.03%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
 Data File : VU046499.D
 Acq On : 19 Dec 2021 16:53
 Operator : SY/MD
 Sample : M5062-07ME
 Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL06ME

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	11.455	3140	3146	3147	rBV	373	303	0.06%	0.006%
78	11.465	3147	3149	3151	rVV	168	114	0.02%	0.002%
79	11.697	3217	3221	3223	rBV	313	303	0.06%	0.006%
80	11.822	3247	3260	3277	rBV	297015	472215	93.16%	8.661%
81	11.886	3277	3280	3287	rVB2	177	159	0.03%	0.003%
82	11.941	3293	3297	3299	rBV	167	154	0.03%	0.003%
83	11.973	3305	3307	3314	rVB3	538	438	0.09%	0.008%
84	12.201	3364	3378	3393	rBV	247169	393446	77.62%	7.216%
85	12.314	3406	3413	3417	rBV	113	130	0.03%	0.002%
86	12.642	3512	3515	3520	rVB	228	142	0.03%	0.003%
87	12.774	3549	3556	3563	rVB3	830	1244	0.25%	0.023%
88	14.098	3963	3968	3978	rVB2	232	341	0.07%	0.006%
89	14.578	4109	4117	4124	rVB3	1334	1974	0.39%	0.036%
90	15.420	4376	4379	4383	rVB2	172	118	0.02%	0.002%
91	15.439	4383	4385	4387	rBV	183	130	0.03%	0.002%
92	15.481	4395	4398	4403	rBV2	268	202	0.04%	0.004%
93	15.610	4435	4438	4444	rBV2	195	240	0.05%	0.004%
94	15.671	4455	4457	4460	rBV	237	178	0.04%	0.003%
95	15.729	4472	4475	4478	rBV	228	178	0.04%	0.003%
96	15.848	4510	4512	4515	rVB2	200	116	0.02%	0.002%
97	15.909	4529	4531	4534	rBV2	216	181	0.04%	0.003%
98	16.179	4611	4615	4627	rVB5	645	1151	0.23%	0.021%
99	17.063	4887	4890	4894	rBV2	445	276	0.05%	0.005%
100	17.327	4970	4972	4975	rBV2	503	308	0.06%	0.006%

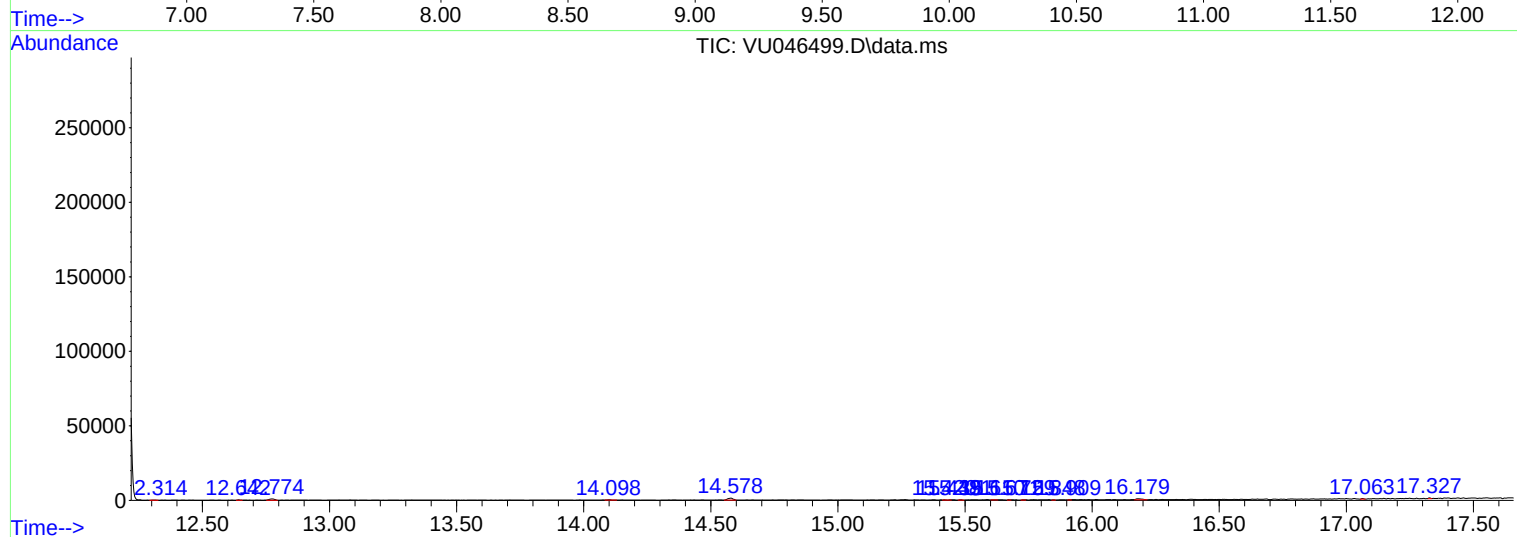
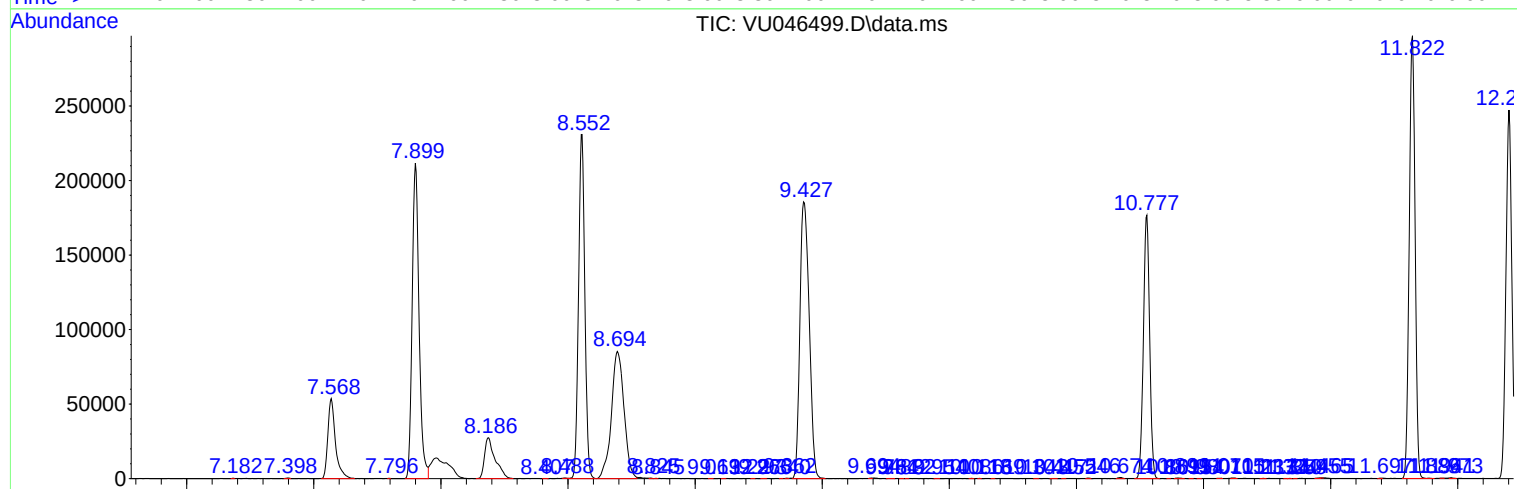
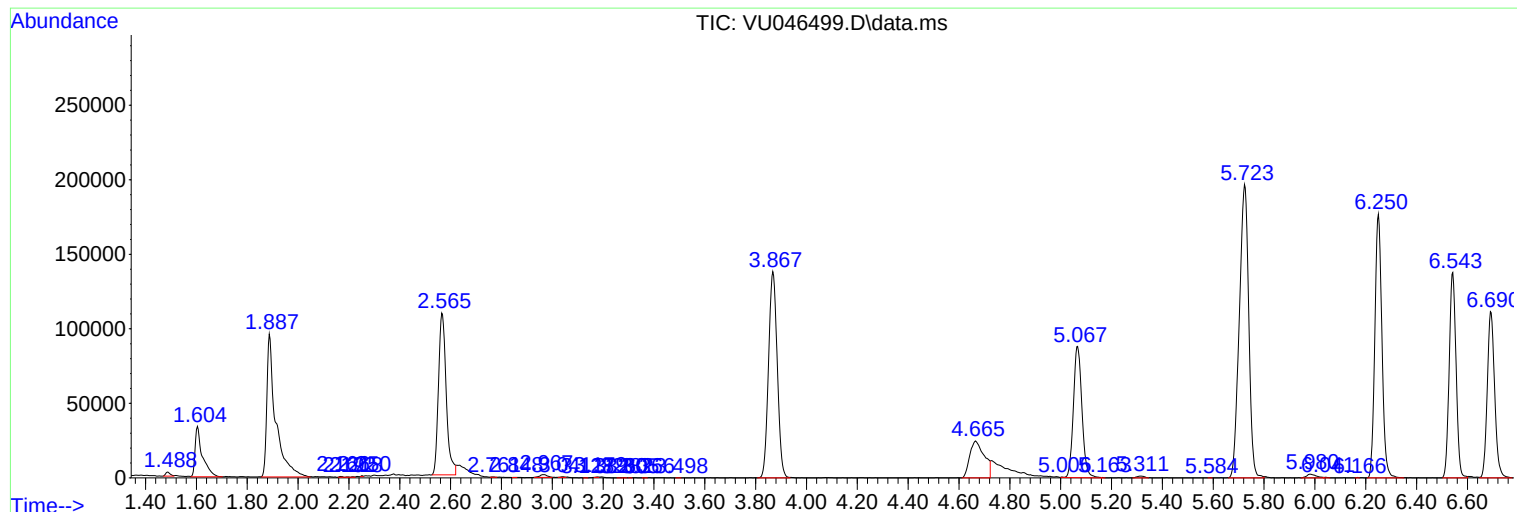
Sum of corrected areas: 5452450

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
Data File : VU046499.D
Acq On : 19 Dec 2021 16:53
Operator : SY/MD
Sample : M5062-07ME
Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL06ME

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\VU121921\
Data File : VU046499.D
Acq On : 19 Dec 2021 16:53
Operator : SY/MD
Sample : M5062-07ME
Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL06ME

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\VU121921\
Data File : VU046499.D
Acq On : 19 Dec 2021 16:53
Operator : SY/MD
Sample : M5062-07ME
Misc : 6.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL06ME

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