

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046329.D
 Acq On : 13 Dec 2021 20:28
 Operator : SY/MD
 Sample : M5062-15ME
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL15ME

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: VU046329.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	74	81	101	rVB	64849	96571	15.76%	1.913%
2	1.916	171	179	201	rVB	34742	66901	10.92%	1.325%
3	2.160	251	255	259	rBV4	506	433	0.07%	0.009%
4	2.424	335	337	341	rBV4	572	328	0.05%	0.006%
5	2.546	364	375	392	rBV	124137	202835	33.10%	4.019%
6	2.784	447	449	452	rBV2	437	336	0.05%	0.007%
7	3.044	519	530	539	rVB5	1898	3817	0.62%	0.076%
8	3.179	557	572	590	rBV2	15029	39341	6.42%	0.779%
9	3.649	712	718	724	rVV2	329	460	0.08%	0.009%
10	4.289	911	917	922	rBV	455	506	0.08%	0.010%
11	4.478	972	976	979	rBV	621	514	0.08%	0.010%
12	4.662	1017	1033	1085	rBV2	28073	148844	24.29%	2.949%
13	5.064	1143	1158	1180	rBV2	96477	246140	40.17%	4.876%
14	5.472	1280	1285	1289	rBV2	266	291	0.05%	0.006%
15	5.723	1342	1363	1384	rBV2	239649	612747	100.00%	12.140%
16	5.983	1434	1444	1456	rVV5	3233	7544	1.23%	0.149%
17	6.105	1478	1482	1489	rVB2	489	521	0.09%	0.010%
18	6.141	1489	1493	1496	rBV	440	372	0.06%	0.007%
19	6.163	1497	1500	1503	rBV	372	320	0.05%	0.006%
20	6.250	1512	1527	1551	rBV	211130	428003	69.85%	8.480%
21	6.526	1606	1613	1623	rVB4	2751	4787	0.78%	0.095%
22	6.604	1623	1637	1642	rBV3	1888	3971	0.65%	0.079%
23	6.690	1650	1664	1685	rBV	131152	270660	44.17%	5.362%
24	6.896	1725	1728	1732	rBV	290	280	0.05%	0.006%
25	7.012	1761	1764	1770	rVV	372	348	0.06%	0.007%
26	7.089	1785	1788	1791	rBV	388	288	0.05%	0.006%
27	7.144	1802	1805	1809	rBV	301	287	0.05%	0.006%
28	7.221	1825	1829	1831	rBV3	473	407	0.07%	0.008%
29	7.491	1907	1913	1918	rVB	320	362	0.06%	0.007%
30	7.568	1924	1937	1959	rBV2	67767	135926	22.18%	2.693%
31	7.697	1971	1977	1980	rBV	250	299	0.05%	0.006%
32	7.793	1998	2007	2019	rVB3	1695	3398	0.55%	0.067%
33	7.899	2027	2040	2058	rBV	258917	485373	79.21%	9.616%
34	8.186	2118	2129	2156	rVB	39806	89847	14.66%	1.780%
35	8.340	2173	2177	2181	rBV	482	428	0.07%	0.008%
36	8.555	2233	2244	2252	rBV3	6146	10048	1.64%	0.199%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046329.D
 Acq On : 13 Dec 2021 20:28
 Operator : SY/MD
 Sample : M5062-15ME
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL15ME

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	8.600	2252	2258	2260	rBV2	389	398	0.06%	0.008%
38	8.681	2261	2283	2308	rVV2	92194	282950	46.18%	5.606%
39	8.829	2327	2329	2333	rBV2	385	319	0.05%	0.006%
40	8.928	2354	2360	2362	rBV2	404	438	0.07%	0.009%
41	9.051	2394	2398	2402	rVB	547	440	0.07%	0.009%
42	9.163	2430	2433	2436	rBV	474	366	0.06%	0.007%
43	9.317	2476	2481	2488	rBV2	343	507	0.08%	0.010%
44	9.427	2500	2515	2540	rVV	253916	563630	91.98%	11.167%
45	9.703	2598	2601	2607	rVB4	436	470	0.08%	0.009%
46	9.793	2627	2629	2633	rVV	396	305	0.05%	0.006%
47	9.838	2640	2643	2647	rVB	645	539	0.09%	0.011%
48	9.861	2647	2650	2657	rBV	622	695	0.11%	0.014%
49	9.899	2657	2662	2665	rBV2	447	412	0.07%	0.008%
50	9.964	2680	2682	2688	rVB2	306	281	0.05%	0.006%
51	10.038	2700	2705	2708	rBV	422	369	0.06%	0.007%
52	10.121	2727	2731	2734	rBV	560	529	0.09%	0.010%
53	10.166	2738	2745	2748	rVV2	259	352	0.06%	0.007%
54	10.211	2754	2759	2761	rBV2	463	382	0.06%	0.008%
55	10.404	2813	2819	2822	rBV	486	368	0.06%	0.007%
56	10.613	2879	2884	2889	rBV2	314	383	0.06%	0.008%
57	10.671	2896	2902	2909	rVV4	1235	1558	0.25%	0.031%
58	10.771	2919	2933	2952	rBV	185469	318426	51.97%	6.309%
59	10.890	2967	2970	2979	rVB2	953	1236	0.20%	0.024%
60	11.031	3010	3014	3016	rBV	431	329	0.05%	0.007%
61	11.118	3032	3041	3047	rBV5	1663	2415	0.39%	0.048%
62	11.205	3064	3068	3073	rVB	316	293	0.05%	0.006%
63	11.452	3141	3145	3150	rBV3	1320	1493	0.24%	0.030%
64	11.562	3177	3179	3183	rVB	467	287	0.05%	0.006%
65	11.597	3186	3190	3194	rVB2	368	334	0.05%	0.007%
66	11.636	3199	3202	3210	rVB2	424	480	0.08%	0.010%
67	11.700	3218	3222	3227	rBV5	727	911	0.15%	0.018%
68	11.819	3246	3259	3274	rVB	350040	550354	89.82%	10.904%
69	11.941	3290	3297	3298	rBV2	615	567	0.09%	0.011%
70	11.973	3303	3307	3314	rVB4	1110	1307	0.21%	0.026%
71	12.202	3366	3378	3394	rVB	267670	431400	70.40%	8.547%
72	12.314	3411	3413	3418	rVB2	411	303	0.05%	0.006%
73	12.401	3436	3440	3442	rBV	384	321	0.05%	0.006%
74	12.539	3479	3483	3489	rVB	282	373	0.06%	0.007%
75	12.639	3509	3514	3516	rBV2	489	485	0.08%	0.010%
76	12.774	3548	3556	3564	rVV3	1250	2052	0.33%	0.041%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046329.D
 Acq On : 13 Dec 2021 20:28
 Operator : SY/MD
 Sample : M5062-15ME
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL15ME

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	13.517	3783	3787	3793	rBV2	464	461	0.08%	0.009%
78	13.549	3793	3797	3801	rVB2	497	376	0.06%	0.007%
79	13.584	3804	3808	3811	rBV	400	358	0.06%	0.007%
80	13.661	3829	3832	3835	rVB	449	292	0.05%	0.006%
81	13.716	3846	3849	3855	rVB	342	286	0.05%	0.006%
82	13.980	3927	3931	3934	rBV2	343	288	0.05%	0.006%
83	14.012	3938	3941	3944	rVB2	640	401	0.07%	0.008%
84	14.041	3944	3950	3952	rBV	742	816	0.13%	0.016%
85	14.240	4002	4012	4016	rBV2	445	771	0.13%	0.015%
86	14.317	4032	4036	4039	rBV2	449	359	0.06%	0.007%
87	14.488	4085	4089	4092	rBV	437	358	0.06%	0.007%
88	14.578	4105	4117	4127	rBV3	1121	2165	0.35%	0.043%
89	14.687	4146	4151	4159	rBV2	584	1037	0.17%	0.021%
90	14.909	4217	4220	4226	rVB2	451	487	0.08%	0.010%
91	14.944	4227	4231	4235	rBV2	547	493	0.08%	0.010%
92	15.127	4283	4288	4293	rVB	394	449	0.07%	0.009%
93	15.179	4299	4304	4307	rBV2	321	399	0.07%	0.008%
94	15.320	4345	4348	4350	rBV2	499	313	0.05%	0.006%
95	15.664	4451	4455	4458	rBV2	431	348	0.06%	0.007%
96	15.693	4458	4464	4467	rBV3	491	615	0.10%	0.012%
97	15.944	4538	4542	4548	rBV2	700	731	0.12%	0.014%
98	16.188	4611	4618	4626	rBV4	1317	2136	0.35%	0.042%
99	16.635	4752	4757	4761	rBV3	653	657	0.11%	0.013%
100	16.967	4858	4860	4862	rBV2	467	305	0.05%	0.006%

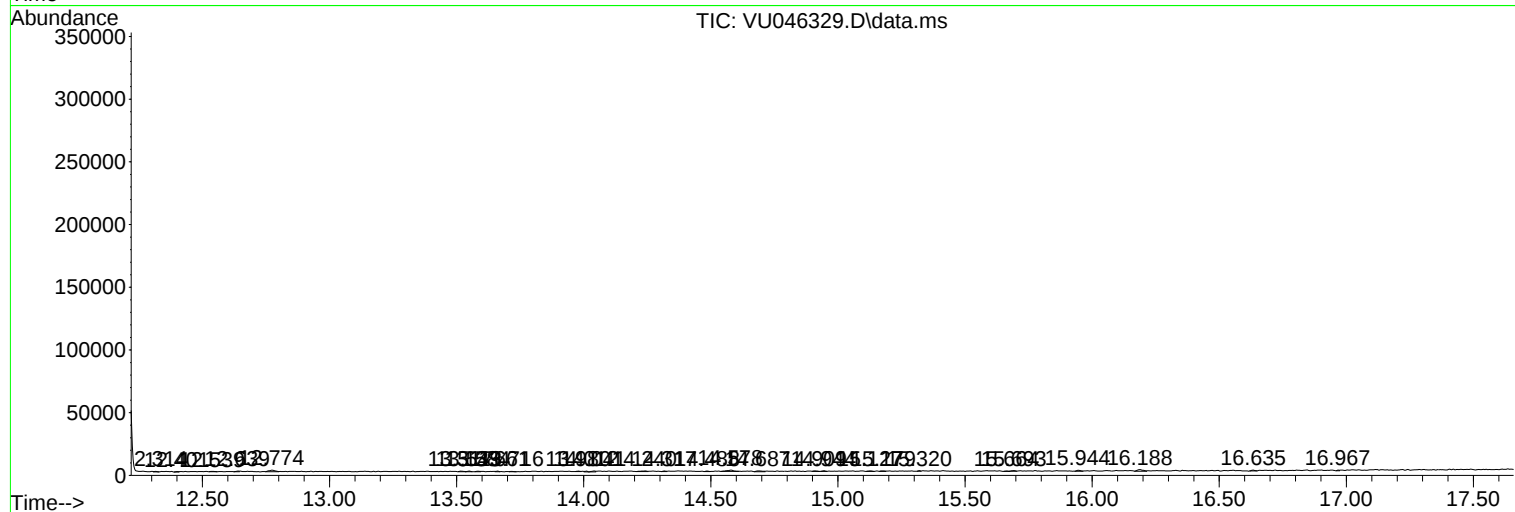
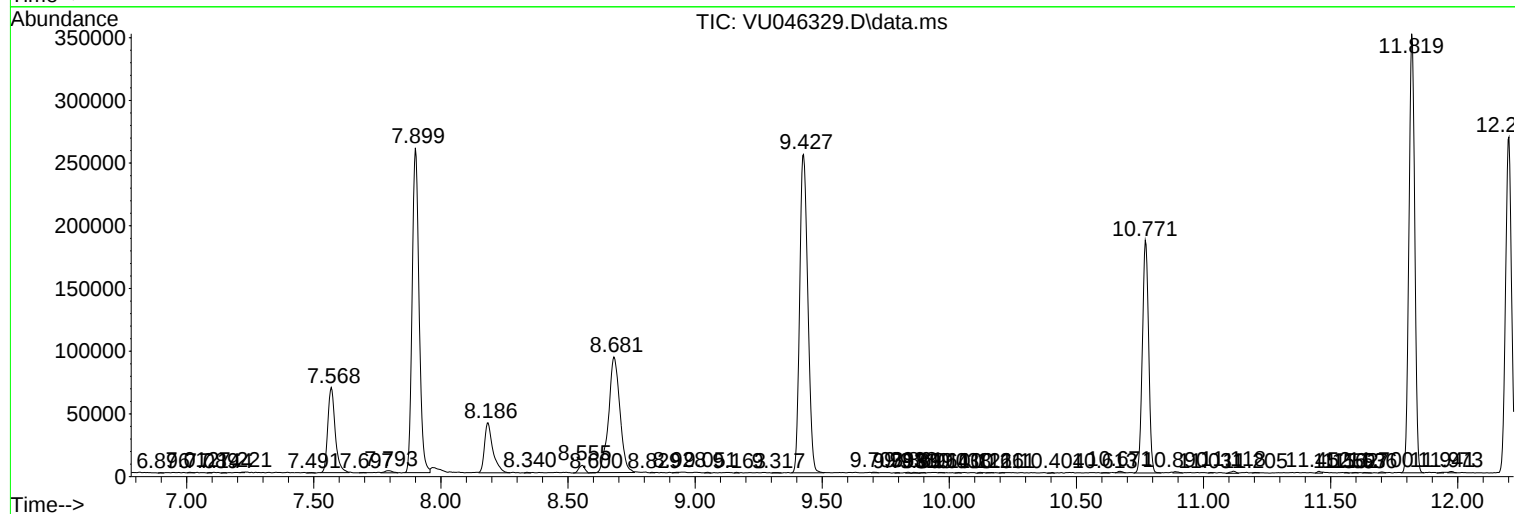
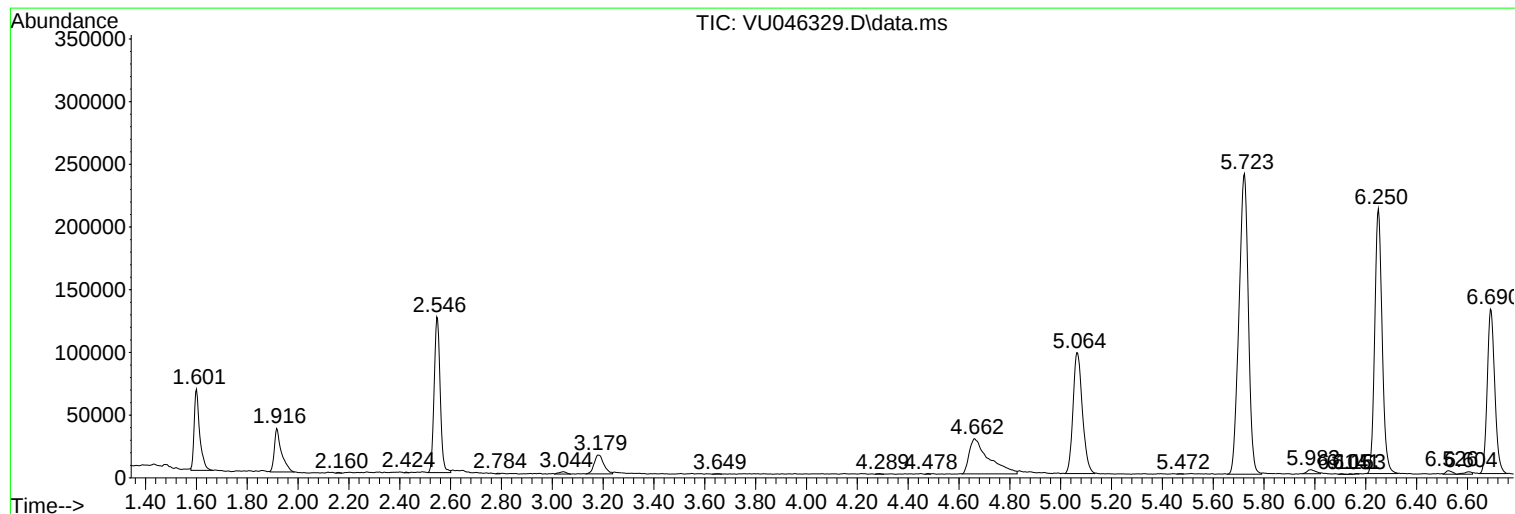
Sum of corrected areas: 5047491

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046329.D
Acq On : 13 Dec 2021 20:28
Operator : SY/MD
Sample : M5062-15ME
Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL15ME

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\VU121321\
Data File : VU046329.D
Acq On : 13 Dec 2021 20:28
Operator : SY/MD
Sample : M5062-15ME
Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL15ME

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\VU121321\
Data File : VU046329.D
Acq On : 13 Dec 2021 20:28
Operator : SY/MD
Sample : M5062-15ME
Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL15ME

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