

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
 Data File : VU046490.D
 Acq On : 19 Dec 2021 13:31
 Operator : SY/MD
 Sample : M5062-13ME
 Misc : 6.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL12ME

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: VU046490.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	55	rBV	2549	3533	0.04%	0.023%
2	1.604	74	82	113	rBV	32612	67804	0.70%	0.434%
3	1.887	158	170	177	rBV	72293	118709	1.23%	0.759%
4	2.141	246	249	253	rBV3	694	692	0.01%	0.004%
5	2.182	258	262	264	rBV4	811	832	0.01%	0.005%
6	2.555	368	378	392	rBV2	79330	148935	1.54%	0.952%
7	2.893	480	483	485	rBV	194	148	0.00%	0.001%
8	2.964	495	505	509	rBV3	1340	2204	0.02%	0.014%
9	3.044	523	530	540	rVB4	1159	2340	0.02%	0.015%
10	3.089	541	544	546	rBV	342	197	0.00%	0.001%
11	3.176	561	571	586	rBV2	2301	5142	0.05%	0.033%
12	3.337	619	621	623	rBV	327	215	0.00%	0.001%
13	3.353	623	626	628	rVV2	447	306	0.00%	0.002%
14	3.404	639	642	644	rBV	137	119	0.00%	0.001%
15	3.436	649	652	655	rBB	152	132	0.00%	0.001%
16	3.485	665	667	670	rBB	171	110	0.00%	0.001%
17	3.690	728	731	735	rBB	168	134	0.00%	0.001%
18	3.867	773	786	800	rBV3	4572	9862	0.10%	0.063%
19	4.060	843	846	847	rBV	275	157	0.00%	0.001%
20	4.073	847	850	852	rVV	323	198	0.00%	0.001%
21	4.121	863	865	869	rBB	235	140	0.00%	0.001%
22	4.292	915	918	920	rBV	152	124	0.00%	0.001%
23	4.665	1017	1034	1084	rBV2	23973	137419	1.42%	0.879%
24	5.067	1140	1159	1195	rVB	90076	214299	2.21%	1.370%
25	5.308	1232	1234	1239	rBV	123	154	0.00%	0.001%
26	5.337	1240	1243	1245	rVB2	248	161	0.00%	0.001%
27	5.404	1261	1264	1267	rBB	170	134	0.00%	0.001%
28	5.722	1343	1363	1394	rBV2	203645	522425	5.40%	3.340%
29	5.832	1394	1397	1402	rVB	153	147	0.00%	0.001%
30	5.980	1434	1443	1450	rBV5	2809	5036	0.05%	0.032%
31	6.250	1512	1527	1560	rBV	169461	349842	3.62%	2.237%
32	6.542	1603	1618	1650	rBV	948351	1782741	18.43%	11.399%
33	6.690	1651	1664	1694	rVB	111427	239384	2.47%	1.531%
34	6.793	1694	1696	1699	rBV	135	115	0.00%	0.001%
35	7.060	1773	1779	1781	rBB	135	165	0.00%	0.001%
36	7.083	1784	1786	1790	rBB	140	120	0.00%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.195	1816	1821	1825	rBB2	299	326	0.00%	0.002%
38	7.259	1838	1841	1843	rBV	176	141	0.00%	0.001%
39	7.314	1856	1858	1862	rBV	152	148	0.00%	0.001%
40	7.430	1891	1894	1897	rBB	122	107	0.00%	0.001%
41	7.568	1925	1937	1969	rBV	52779	120000	1.24%	0.767%
42	7.800	2001	2009	2018	rBV3	492	1083	0.01%	0.007%
43	7.899	2027	2040	2055	rBV	211945	422480	4.37%	2.701%
44	8.137	2112	2114	2116	rBV	246	121	0.00%	0.001%
45	8.185	2116	2129	2160	rVB	25484	82988	0.86%	0.531%
46	8.343	2174	2178	2182	rBB	182	164	0.00%	0.001%
47	8.414	2195	2200	2202	rBB	140	148	0.00%	0.001%
48	8.475	2214	2219	2221	rBV	278	243	0.00%	0.002%
49	8.555	2228	2244	2266	rBV	5456724	9675107	100.00%	61.862%
50	8.886	2344	2347	2352	rBB	142	144	0.00%	0.001%
51	9.047	2394	2397	2399	rBV	128	114	0.00%	0.001%
52	9.211	2444	2448	2450	rBB	155	126	0.00%	0.001%
53	9.375	2497	2499	2501	rVV	153	106	0.00%	0.001%
54	9.430	2501	2516	2538	rVV	188852	478546	4.95%	3.060%
55	9.523	2542	2545	2548	rBV	164	161	0.00%	0.001%
56	9.578	2554	2562	2575	rVB2	1396	2781	0.03%	0.018%
57	9.700	2589	2600	2615	rBV3	7641	15177	0.16%	0.097%
58	9.835	2637	2642	2647	rBB	133	209	0.00%	0.001%
59	9.880	2653	2656	2659	rBV	136	139	0.00%	0.001%
60	9.941	2671	2675	2677	rBV	265	199	0.00%	0.001%
61	10.050	2706	2709	2712	rBV	128	139	0.00%	0.001%
62	10.108	2718	2727	2739	rVB2	3089	5651	0.06%	0.036%
63	10.256	2768	2773	2777	rBV	211	292	0.00%	0.002%
64	10.430	2824	2827	2831	rBB	174	163	0.00%	0.001%
65	10.459	2832	2836	2838	rBV	190	186	0.00%	0.001%
66	10.542	2856	2862	2864	rVV2	270	229	0.00%	0.001%
67	10.623	2883	2887	2891	rBB	142	168	0.00%	0.001%
68	10.668	2891	2901	2909	rBV6	1631	2701	0.03%	0.017%
69	10.777	2922	2935	2956	rVB	181594	306608	3.17%	1.960%
70	10.854	2957	2959	2962	rBV	189	157	0.00%	0.001%
71	10.896	2965	2972	2979	rBV2	442	606	0.01%	0.004%
72	11.005	3002	3006	3012	rVB2	165	203	0.00%	0.001%
73	11.102	3030	3036	3037	rBV	234	226	0.00%	0.001%
74	11.121	3037	3042	3045	rVB4	491	464	0.00%	0.003%
75	11.311	3096	3101	3103	rBV	151	183	0.00%	0.001%
76	11.324	3103	3105	3112	rVB	97	112	0.00%	0.001%

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 BGL12ME

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	11.459	3142	3147	3148	rBV2	604	459	0.00%	0.003%
78	11.700	3219	3222	3227	rVB3	312	243	0.00%	0.002%
79	11.754	3236	3239	3241	rBV	172	141	0.00%	0.001%
80	11.822	3247	3260	3275	rBV	310732	488677	5.05%	3.125%
81	11.944	3292	3298	3302	rBV3	260	300	0.00%	0.002%
82	11.973	3304	3307	3313	rVB2	650	654	0.01%	0.004%
83	12.201	3365	3378	3393	rVV	257897	410474	4.24%	2.625%
84	12.372	3428	3431	3440	rVB	110	131	0.00%	0.001%
85	12.619	3505	3508	3514	rBV	97	113	0.00%	0.001%
86	12.770	3549	3555	3562	rVB2	961	1290	0.01%	0.008%
87	13.848	3886	3890	3897	rVB2	333	329	0.00%	0.002%
88	14.066	3954	3958	3962	rBV	177	161	0.00%	0.001%
89	14.085	3962	3964	3966	rBV	174	117	0.00%	0.001%
90	14.458	4075	4080	4082	rBV	114	126	0.00%	0.001%
91	14.581	4109	4118	4126	rVB2	1312	2268	0.02%	0.015%
92	14.822	4190	4193	4197	rBV	155	122	0.00%	0.001%
93	15.208	4311	4313	4317	rBV	157	120	0.00%	0.001%
94	15.237	4317	4322	4324	rBV	114	126	0.00%	0.001%
95	15.310	4341	4345	4350	rVB2	225	228	0.00%	0.001%
96	15.333	4350	4352	4355	rBV2	140	106	0.00%	0.001%
97	15.413	4372	4377	4378	rBV	193	163	0.00%	0.001%
98	15.487	4396	4400	4403	rBV	373	263	0.00%	0.002%
99	15.674	4455	4458	4460	rBV	135	121	0.00%	0.001%
100	16.327	4659	4661	4664	rVB2	299	120	0.00%	0.001%

Sum of corrected areas: 15639873

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL12ME

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

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL12ME

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
