

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046450.D
 Acq On : 17 Dec 2021 03:03
 Operator : SY/MD
 Sample : M5121-04 20X
 Misc : 5.71g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL53

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: VU046450.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	105	rVB	59296	75950	14.82%	1.842%
2	1.919	172	180	203	rVB	39946	58606	11.44%	1.421%
3	2.572	370	383	404	rBV	106425	177165	34.58%	4.297%
4	2.842	463	467	470	rBB	165	156	0.03%	0.004%
5	2.867	471	475	477	rBV	126	111	0.02%	0.003%
6	2.903	483	486	488	rBV	236	157	0.03%	0.004%
7	2.941	496	498	500	rBV	132	97	0.02%	0.002%
8	2.993	510	514	516	rBB	159	130	0.03%	0.003%
9	3.022	520	523	526	rBB	132	113	0.02%	0.003%
10	3.057	526	534	541	rBB	1096	1679	0.33%	0.041%
11	3.099	542	547	550	rBB	132	135	0.03%	0.003%
12	3.118	550	553	555	rBB	132	92	0.02%	0.002%
13	3.189	561	575	590	rBB	7892	17954	3.50%	0.435%
14	3.289	603	606	608	rBV	140	121	0.02%	0.003%
15	3.388	635	637	639	rBV	130	93	0.02%	0.002%
16	3.761	750	753	755	rBB	136	95	0.02%	0.002%
17	3.797	761	764	767	rBB	148	120	0.02%	0.003%
18	4.028	833	836	839	rBB	170	132	0.03%	0.003%
19	4.488	977	979	981	rBV	129	96	0.02%	0.002%
20	4.552	997	999	1002	rBB	141	97	0.02%	0.002%
21	4.633	1011	1024	1052	rBV2	48798	127160	24.82%	3.084%
22	4.813	1077	1080	1082	rBV2	281	208	0.04%	0.005%
23	5.067	1144	1159	1184	rBV	94619	204757	39.96%	4.966%
24	5.208	1199	1203	1205	rBV	216	138	0.03%	0.003%
25	5.340	1242	1244	1247	rVB2	211	104	0.02%	0.003%
26	5.375	1253	1255	1260	rVB	226	148	0.03%	0.004%
27	5.729	1344	1365	1386	rBV2	191450	512382	100.00%	12.426%
28	5.916	1420	1423	1425	rBB	138	97	0.02%	0.002%
29	6.060	1465	1468	1470	rBB	142	97	0.02%	0.002%
30	6.128	1487	1489	1491	rBV	120	88	0.02%	0.002%
31	6.250	1512	1527	1549	rBV	177424	333686	65.12%	8.092%
32	6.526	1611	1613	1616	rBV2	533	494	0.10%	0.012%
33	6.694	1651	1665	1686	rBB	120084	229375	44.77%	5.563%
34	6.784	1691	1693	1697	rBB	120	88	0.02%	0.002%
35	6.809	1698	1701	1703	rBV	243	160	0.03%	0.004%
36	6.867	1717	1719	1723	rBB	138	116	0.02%	0.003%

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

37	7.047	1772	1775	1777	rBV	229	131	0.03%	0.003%
38	7.137	1801	1803	1806	rBB	121	88	0.02%	0.002%
39	7.176	1813	1815	1819	rBV	303	237	0.05%	0.006%
40	7.449	1898	1900	1902	rBV	128	87	0.02%	0.002%
41	7.568	1924	1937	1951	rBV	62389	104091	20.32%	2.524%
42	7.649	1959	1962	1965	rBB	130	113	0.02%	0.003%
43	7.668	1966	1968	1971	rBV	132	117	0.02%	0.003%
44	7.713	1980	1982	1985	rBB	130	93	0.02%	0.002%
45	7.784	2000	2004	2007	rBV	476	512	0.10%	0.012%
46	7.841	2020	2022	2027	rBV	127	155	0.03%	0.004%
47	7.899	2027	2040	2055	rBV	232685	395830	77.25%	9.600%
48	8.044	2083	2085	2088	rBV	116	103	0.02%	0.002%
49	8.179	2117	2127	2145	rBB	42192	70404	13.74%	1.707%
50	8.266	2151	2154	2156	rBV	173	135	0.03%	0.003%
51	8.304	2163	2166	2169	rBB	143	120	0.02%	0.003%
52	8.346	2175	2179	2181	rBB	229	152	0.03%	0.004%
53	8.472	2213	2218	2219	rBV	469	355	0.07%	0.009%
54	8.636	2257	2269	2293	rBV	149783	249206	48.64%	6.044%
55	8.874	2339	2343	2345	rBV	135	141	0.03%	0.003%
56	8.912	2349	2355	2365	rVB3	1177	1850	0.36%	0.045%
57	9.009	2381	2385	2391	rBB	177	206	0.04%	0.005%
58	9.044	2392	2396	2399	rBB	130	134	0.03%	0.003%
59	9.115	2414	2418	2421	rBV	225	214	0.04%	0.005%
60	9.185	2438	2440	2443	rBV	159	129	0.03%	0.003%
61	9.343	2487	2489	2492	rBB	136	94	0.02%	0.002%
62	9.420	2499	2513	2536	rVV	267601	437496	85.38%	10.610%
63	9.520	2542	2544	2547	rBB	234	111	0.02%	0.003%
64	9.542	2548	2551	2553	rBV	152	129	0.03%	0.003%
65	9.655	2582	2586	2589	rBV	190	208	0.04%	0.005%
66	9.694	2595	2598	2603	rBV2	516	521	0.10%	0.013%
67	9.732	2607	2610	2612	rBB	137	94	0.02%	0.002%
68	9.748	2613	2615	2618	rBB	130	90	0.02%	0.002%
69	9.767	2618	2621	2624	rBB	150	122	0.02%	0.003%
70	9.790	2625	2628	2630	rBV	128	114	0.02%	0.003%
71	9.835	2639	2642	2644	rBB	121	88	0.02%	0.002%
72	9.880	2653	2656	2658	rBV	141	117	0.02%	0.003%
73	9.928	2666	2671	2676	rBB	191	222	0.04%	0.005%
74	9.960	2677	2681	2682	rBV	170	148	0.03%	0.004%
75	10.153	2735	2741	2745	rBV	170	267	0.05%	0.006%
76	10.388	2809	2814	2818	rBV	159	217	0.04%	0.005%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
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77	10.549	2862	2864	2867	rBB	147	100	0.02%	0.002%
78	10.568	2867	2870	2873	rBV	168	153	0.03%	0.004%
79	10.674	2894	2903	2910	rBV4	1897	2664	0.52%	0.065%
80	10.758	2917	2929	2946	rVB	168334	269199	52.54%	6.529%
81	10.867	2960	2963	2966	rBV2	321	259	0.05%	0.006%
82	10.928	2979	2982	2985	rVB2	198	120	0.02%	0.003%
83	11.404	3128	3130	3132	rBV	147	103	0.02%	0.002%
84	11.462	3141	3148	3159	rBV5	1251	1769	0.35%	0.043%
85	11.542	3170	3173	3175	rBV	146	132	0.03%	0.003%
86	11.700	3214	3222	3229	rVB4	1203	1895	0.37%	0.046%
87	11.751	3230	3238	3242	rBV2	433	645	0.13%	0.016%
88	11.812	3245	3257	3272	rBV	290396	450960	88.01%	10.937%
89	12.195	3363	3376	3392	rVB	236531	380247	74.21%	9.222%
90	12.401	3437	3440	3444	rVB	216	162	0.03%	0.004%
91	12.629	3509	3511	3514	rBV	157	121	0.02%	0.003%
92	12.825	3568	3572	3577	rBV2	202	195	0.04%	0.005%
93	13.140	3667	3670	3671	rBV2	324	173	0.03%	0.004%
94	13.221	3690	3695	3703	rVB2	846	1063	0.21%	0.026%
95	13.841	3882	3888	3896	rVB3	2822	4178	0.82%	0.101%
96	14.092	3961	3966	3973	rBV	540	790	0.15%	0.019%
97	15.211	4310	4314	4319	rVB4	802	736	0.14%	0.018%
98	15.606	4432	4437	4439	rBV2	335	338	0.07%	0.008%
99	15.722	4471	4473	4476	rBV	519	360	0.07%	0.009%
100	15.867	4516	4518	4519	rBV	461	209	0.04%	0.005%

Sum of corrected areas: 4123409

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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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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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