

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
 Data File : VU046094.D
 Acq On : 04 Dec 2021 15:36
 Operator : SY/MD
 Sample : M4942-06
 Misc : 5.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKQ8

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: VU046094.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	97	rBV	128572	174967	13.53%	1.824%
2	1.861	156	162	169	rBV2	2568	3011	0.23%	0.031%
3	1.916	170	179	198	rVV	74134	131504	10.17%	1.371%
4	2.546	363	375	389	rBV	234378	382724	29.59%	3.991%
5	3.031	520	526	529	rBV5	1360	1705	0.13%	0.018%
6	3.179	555	572	595	rBV	10823	29479	2.28%	0.307%
7	3.334	617	620	621	rBV2	205	120	0.01%	0.001%
8	3.404	639	642	645	rVB2	252	206	0.02%	0.002%
9	3.437	649	652	656	rBB	196	177	0.01%	0.002%
10	3.523	676	679	682	rBV	153	152	0.01%	0.002%
11	3.633	710	713	716	rVB	174	140	0.01%	0.001%
12	3.768	750	755	757	rBV	137	141	0.01%	0.001%
13	4.002	825	828	831	rBB	187	147	0.01%	0.002%
14	4.022	831	834	839	rBB	144	168	0.01%	0.002%
15	4.044	840	841	845	rBV	208	137	0.01%	0.001%
16	4.128	865	867	871	rBV	130	137	0.01%	0.001%
17	4.186	881	885	889	rBB	138	165	0.01%	0.002%
18	4.404	948	953	955	rBB	139	139	0.01%	0.001%
19	4.658	1014	1032	1085	rBV2	61593	290642	22.47%	3.031%
20	5.064	1141	1158	1187	rVB	205978	495201	38.28%	5.163%
21	5.208	1202	1203	1205	rBV	308	129	0.01%	0.001%
22	5.292	1226	1229	1235	rBB3	363	340	0.03%	0.004%
23	5.337	1240	1243	1247	rVB	194	173	0.01%	0.002%
24	5.372	1250	1254	1258	rBV	142	189	0.01%	0.002%
25	5.456	1277	1280	1283	rBB	270	170	0.01%	0.002%
26	5.629	1331	1334	1338	rBB	165	157	0.01%	0.002%
27	5.723	1341	1363	1386	rBV2	508339	1293548	100.00%	13.488%
28	5.835	1397	1398	1404	rVV2	223	122	0.01%	0.001%
29	5.867	1405	1408	1414	rVB2	286	309	0.02%	0.003%
30	5.980	1433	1443	1468	rBV2	5043	14254	1.10%	0.149%
31	6.105	1479	1482	1489	rBV2	290	357	0.03%	0.004%
32	6.250	1511	1527	1551	rBV	253810	521878	40.34%	5.442%
33	6.488	1598	1601	1605	rBV	141	169	0.01%	0.002%
34	6.526	1605	1613	1627	rVV4	3408	8052	0.62%	0.084%
35	6.600	1630	1636	1649	rVV6	2329	5398	0.42%	0.056%
36	6.690	1649	1664	1689	rVV	280006	572518	44.26%	5.970%

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

37	6.813	1693	1702	1709	rBV3	605	940	0.07%	0.010%
38	6.871	1717	1720	1723	rBV	191	177	0.01%	0.002%
39	6.912	1728	1733	1736	rBV	178	222	0.02%	0.002%
40	7.018	1763	1766	1769	rBV	186	166	0.01%	0.002%
41	7.044	1771	1774	1779	rVV2	181	205	0.02%	0.002%
42	7.115	1793	1796	1798	rBV	152	127	0.01%	0.001%
43	7.131	1799	1801	1803	rVV	248	123	0.01%	0.001%
44	7.144	1803	1805	1809	rVB	263	154	0.01%	0.002%
45	7.173	1809	1814	1817	rBV2	251	261	0.02%	0.003%
46	7.195	1817	1821	1826	rVB2	266	291	0.02%	0.003%
47	7.231	1826	1832	1837	rBB3	517	676	0.05%	0.007%
48	7.340	1862	1866	1870	rBV	186	227	0.02%	0.002%
49	7.452	1898	1901	1903	rBV	245	156	0.01%	0.002%
50	7.478	1907	1909	1914	rVB	167	163	0.01%	0.002%
51	7.568	1923	1937	1967	rVV	165313	318072	24.59%	3.317%
52	7.793	1997	2007	2018	rVB4	1337	2856	0.22%	0.030%
53	7.835	2018	2020	2023	rBV	153	127	0.01%	0.001%
54	7.899	2024	2040	2057	rBV	610176	1137682	87.95%	11.863%
55	8.076	2092	2095	2097	rBV	154	127	0.01%	0.001%
56	8.182	2116	2128	2157	rBV	97644	212177	16.40%	2.212%
57	8.362	2181	2184	2187	rBV	154	167	0.01%	0.002%
58	8.478	2213	2220	2226	rVV2	339	590	0.05%	0.006%
59	8.552	2237	2243	2250	rBV	221	363	0.03%	0.004%
60	8.681	2258	2283	2317	rBV	204371	646917	50.01%	6.745%
61	8.951	2358	2367	2378	rVB3	1128	2282	0.18%	0.024%
62	9.337	2479	2487	2493	rVB3	893	1092	0.08%	0.011%
63	9.362	2493	2495	2498	rVB	217	144	0.01%	0.002%
64	9.423	2499	2514	2538	rBV	307198	668449	51.68%	6.970%
65	9.575	2550	2561	2575	rBV	10898	19518	1.51%	0.204%
66	9.626	2575	2577	2581	rVB2	272	177	0.01%	0.002%
67	9.697	2587	2599	2616	rBV	34824	69775	5.39%	0.728%
68	9.758	2616	2618	2622	rVB2	397	232	0.02%	0.002%
69	9.957	2677	2680	2682	rBV2	301	162	0.01%	0.002%
70	9.989	2686	2690	2693	rBV	233	158	0.01%	0.002%
71	10.018	2693	2699	2706	rBV4	1834	2429	0.19%	0.025%
72	10.044	2706	2707	2712	rVB	265	173	0.01%	0.002%
73	10.112	2717	2728	2740	rBV4	6726	12286	0.95%	0.128%
74	10.166	2740	2745	2747	rBV2	459	468	0.04%	0.005%
75	10.253	2756	2772	2782	rVB2	3643	6133	0.47%	0.064%
76	10.311	2785	2790	2791	rBV3	545	407	0.03%	0.004%

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77	10.349	2798	2802	2810	rVB5	1198	1525	0.12%	0.016%
78	10.394	2812	2816	2823	rVB4	1653	2146	0.17%	0.022%
79	10.459	2831	2836	2839	rBV2	457	495	0.04%	0.005%
80	10.491	2844	2846	2851	rVB3	466	357	0.03%	0.004%
81	10.530	2856	2858	2859	rBV	371	168	0.01%	0.002%
82	10.558	2859	2867	2875	rBV5	2540	4417	0.34%	0.046%
83	10.674	2894	2903	2914	rVB3	5895	10282	0.79%	0.107%
84	10.719	2914	2917	2918	rBV	844	504	0.04%	0.005%
85	10.774	2920	2934	2949	rVV	385039	662864	51.24%	6.912%
86	11.005	3000	3006	3018	rBV5	3055	6132	0.47%	0.064%
87	11.208	3060	3069	3072	rBV7	1934	2633	0.20%	0.027%
88	11.250	3075	3082	3084	rBV5	1062	1241	0.10%	0.013%
89	11.372	3116	3120	3126	rBV5	2447	2852	0.22%	0.030%
90	11.417	3128	3134	3141	rVV2	7866	11258	0.87%	0.117%
91	11.468	3142	3150	3169	rVB4	13992	32023	2.48%	0.334%
92	11.578	3175	3184	3190	rBV5	3920	6880	0.53%	0.072%
93	11.700	3215	3222	3232	rBV9	5267	9070	0.70%	0.095%
94	11.819	3247	3259	3271	rBV	440316	707894	54.72%	7.381%
95	12.070	3334	3337	3338	rBV2	1057	658	0.05%	0.007%
96	12.198	3364	3377	3391	rVB	633270	1038302	80.27%	10.826%
97	14.089	3960	3965	3975	rVB	10437	14379	1.11%	0.150%
98	15.224	4307	4318	4328	rBV2	19232	33768	2.61%	0.352%
99	15.716	4470	4471	4474	rBV3	810	397	0.03%	0.004%
100	16.410	4682	4687	4692	rVB4	4100	4602	0.36%	0.048%

Sum of corrected areas: 9590523

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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 Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc