

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040721\
 Data File : VU042977.D
 Acq On : 07 Apr 2021 12:30
 Operator : SY/MD
 Sample : VU0407MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK307

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\SFAMULM040721WMA.M

Title : VOC Analysis

Signal : TIC: VU042977.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	75	82	93	rVB	81284	92972	11.89%	1.476%
2	1.909	168	177	194	rVB	63766	89795	11.49%	1.426%
3	2.202	264	268	270	rBV2	486	407	0.05%	0.006%
4	2.572	371	383	404	rVB	152956	254778	32.59%	4.045%
5	3.044	527	530	532	rBV2	369	255	0.03%	0.004%
6	3.173	566	570	571	rBV	605	449	0.06%	0.007%
7	3.350	623	625	626	rBV	338	160	0.02%	0.003%
8	3.359	626	628	632	rVV2	405	331	0.04%	0.005%
9	3.440	649	653	655	rBV	287	261	0.03%	0.004%
10	3.481	663	666	668	rBV	293	174	0.02%	0.003%
11	3.523	675	679	681	rVB2	159	136	0.02%	0.002%
12	3.629	708	712	715	rBB2	330	271	0.03%	0.004%
13	3.652	715	719	722	rBV	324	289	0.04%	0.005%
14	3.690	729	731	734	rBV	239	159	0.02%	0.003%
15	3.768	749	755	758	rBV	330	317	0.04%	0.005%
16	3.819	767	771	773	rBV	192	171	0.02%	0.003%
17	3.883	788	791	796	rVB2	324	313	0.04%	0.005%
18	3.925	802	804	807	rBB2	272	167	0.02%	0.003%
19	3.977	816	820	822	rBV	154	153	0.02%	0.002%
20	3.993	822	825	827	rVB	294	177	0.02%	0.003%
21	4.035	835	838	842	rBV	228	220	0.03%	0.003%
22	4.099	856	858	859	rBV	263	124	0.02%	0.002%
23	4.160	874	877	881	rBB	174	162	0.02%	0.003%
24	4.182	881	884	888	rBB	298	215	0.03%	0.003%
25	4.221	893	896	900	rBV2	260	223	0.03%	0.004%
26	4.311	921	924	926	rBV	152	134	0.02%	0.002%
27	4.501	980	983	985	rBV2	266	181	0.02%	0.003%
28	4.626	1003	1022	1051	rBV	100620	237968	30.44%	3.778%
29	4.915	1110	1112	1118	rVB2	318	302	0.04%	0.005%
30	4.999	1136	1138	1143	rVV	267	227	0.03%	0.004%
31	5.073	1144	1161	1183	rVV	141731	311364	39.83%	4.944%
32	5.179	1191	1194	1198	rVB2	257	162	0.02%	0.003%
33	5.301	1221	1232	1237	rVB3	731	1184	0.15%	0.019%
34	5.324	1237	1239	1243	rVB2	296	219	0.03%	0.003%
35	5.350	1244	1247	1250	rBV	244	184	0.02%	0.003%
36	5.378	1251	1256	1259	rBV4	499	547	0.07%	0.009%

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 Title : VOC Analysis

37	5.478	1285	1287	1291	rBV	138	145	0.02%	0.002%
38	5.501	1291	1294	1297	rVV2	207	155	0.02%	0.002%
39	5.542	1303	1307	1308	rBV	175	150	0.02%	0.002%
40	5.568	1312	1315	1319	rVB	379	301	0.04%	0.005%
41	5.633	1331	1335	1338	rBV2	267	275	0.04%	0.004%
42	5.732	1344	1366	1386	rBV2	282555	781820	100.00%	12.413%
43	5.874	1408	1410	1416	rVB3	360	369	0.05%	0.006%
44	6.022	1453	1456	1458	rBV	248	179	0.02%	0.003%
45	6.070	1468	1471	1477	rVB2	184	196	0.03%	0.003%
46	6.256	1514	1529	1547	rBV	254727	475144	60.77%	7.544%
47	6.440	1584	1586	1592	rBV2	204	209	0.03%	0.003%
48	6.539	1607	1617	1625	rVB4	2600	4367	0.56%	0.069%
49	6.697	1651	1666	1685	rBV2	186782	363733	46.52%	5.775%
50	6.793	1694	1696	1699	rVB2	476	212	0.03%	0.003%
51	6.813	1699	1702	1705	rVB2	504	389	0.05%	0.006%
52	6.883	1722	1724	1728	rVB	239	134	0.02%	0.002%
53	6.954	1743	1746	1750	rBV	155	183	0.02%	0.003%
54	7.108	1791	1794	1798	rVB	244	187	0.02%	0.003%
55	7.173	1811	1814	1816	rBV	208	173	0.02%	0.003%
56	7.324	1858	1861	1864	rBV2	289	271	0.03%	0.004%
57	7.362	1870	1873	1874	rBV	192	129	0.02%	0.002%
58	7.391	1878	1882	1887	rBB2	285	296	0.04%	0.005%
59	7.417	1887	1890	1891	rBV	251	128	0.02%	0.002%
60	7.491	1910	1913	1918	rBV2	300	311	0.04%	0.005%
61	7.571	1926	1938	1951	rBV	110811	191746	24.53%	3.044%
62	7.684	1966	1973	1975	rBV2	289	273	0.03%	0.004%
63	7.745	1988	1992	1995	rBB	193	174	0.02%	0.003%
64	7.771	1995	2000	2003	rBV	297	347	0.04%	0.006%
65	7.793	2004	2007	2016	rVB2	1116	1325	0.17%	0.021%
66	7.906	2027	2042	2057	rBV	361236	614947	78.66%	9.764%
67	8.054	2086	2088	2091	rBV2	242	174	0.02%	0.003%
68	8.185	2117	2129	2149	rBV	77922	131992	16.88%	2.096%
69	8.385	2187	2191	2194	rVB2	178	136	0.02%	0.002%
70	8.491	2221	2224	2227	rVB	224	153	0.02%	0.002%
71	8.552	2239	2243	2244	rBV	230	193	0.02%	0.003%
72	8.562	2244	2246	2249	rVB	340	187	0.02%	0.003%
73	8.639	2257	2270	2309	rBV	294832	532043	68.05%	8.447%
74	8.816	2322	2325	2328	rVB2	230	181	0.02%	0.003%
75	8.841	2330	2333	2336	rBV	301	177	0.02%	0.003%
76	9.423	2501	2514	2533	rBV	358034	590959	75.59%	9.383%

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77	9.697	2595	2599	2606	rBV3	656	902	0.12%	0.014%
78	9.890	2656	2659	2662	rVB	202	146	0.02%	0.002%
79	10.102	2722	2725	2727	rBV3	461	300	0.04%	0.005%
80	10.677	2898	2904	2911	rVB3	2250	2884	0.37%	0.046%
81	10.764	2919	2931	2948	rBV	267533	438144	56.04%	6.957%
82	10.825	2948	2950	2953	rBV	493	277	0.04%	0.004%
83	10.931	2981	2983	2986	rBV	276	187	0.02%	0.003%
84	10.980	2996	2998	3000	rBV	227	125	0.02%	0.002%
85	11.054	3018	3021	3023	rBV	218	148	0.02%	0.002%
86	11.118	3039	3041	3043	rBV2	393	175	0.02%	0.003%
87	11.381	3121	3123	3127	rBV2	285	192	0.02%	0.003%
88	11.459	3142	3147	3149	rBV5	1258	1195	0.15%	0.019%
89	11.523	3162	3167	3171	rBV2	266	308	0.04%	0.005%
90	11.597	3183	3190	3194	rBV2	329	325	0.04%	0.005%
91	11.703	3218	3223	3227	rVB3	836	870	0.11%	0.014%
92	11.819	3247	3259	3276	rBV	354169	560828	71.73%	8.904%
93	12.201	3363	3378	3396	rBV	360941	588087	75.22%	9.337%
94	12.394	3435	3438	3440	rBV	239	171	0.02%	0.003%
95	12.407	3440	3442	3444	rVV	362	212	0.03%	0.003%
96	12.433	3446	3450	3451	rBV	237	164	0.02%	0.003%
97	12.558	3484	3489	3495	rVB	324	347	0.04%	0.006%
98	13.224	3691	3696	3703	rBV4	1522	1939	0.25%	0.031%
99	14.095	3961	3967	3978	rVB	4614	6869	0.88%	0.109%
100	14.340	4037	4043	4051	rVB5	2816	3901	0.50%	0.062%

Sum of corrected areas: 6298310

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM040721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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Instrument :
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TIC Integration Parameters: LSCINT.P

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