

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072122\
 Data File : VU049832.D
 Acq On : 21 Jul 2022 16:11
 Operator : SY/MD
 Sample : N3722-08ME
 Misc : 5.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5C41ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	87	rBV	42396	60536	8.10%	1.029%
2	2.514	355	365	380	rVB	132478	211664	28.32%	3.598%
3	2.809	453	457	458	rBV2	292	213	0.03%	0.004%
4	2.867	471	475	480	rBV2	301	321	0.04%	0.005%
5	2.890	480	482	484	rVB2	174	50	0.01%	0.001%
6	2.906	484	487	488	rBV3	397	278	0.04%	0.005%
7	3.022	513	523	542	rBV3	7713	14700	1.97%	0.250%
8	3.173	557	570	589	rBV2	5864	13934	1.86%	0.237%
9	3.250	592	594	598	rVB	416	216	0.03%	0.004%
10	3.272	598	601	603	rBV	288	172	0.02%	0.003%
11	3.356	624	627	628	rBV2	180	107	0.01%	0.002%
12	3.520	676	678	682	rBV2	166	96	0.01%	0.002%
13	3.655	715	720	721	rBV2	525	431	0.06%	0.007%
14	3.729	740	743	746	rBV	147	120	0.02%	0.002%
15	3.790	754	762	764	rBV2	293	413	0.06%	0.007%
16	3.832	773	775	779	rBV2	178	134	0.02%	0.002%
17	3.899	793	796	802	rBV2	202	245	0.03%	0.004%
18	3.941	806	809	812	rBV2	169	125	0.02%	0.002%
19	3.961	812	815	816	rBV2	83	46	0.01%	0.001%
20	4.086	849	854	858	rBV2	147	198	0.03%	0.003%
21	4.131	865	868	875	rBV2	189	202	0.03%	0.003%
22	4.263	905	909	911	rBV2	208	132	0.02%	0.002%
23	4.420	956	958	964	rBV	228	214	0.03%	0.004%
24	4.452	964	968	969	rBV	257	174	0.02%	0.003%
25	4.507	983	985	987	rBV	261	151	0.02%	0.003%
26	4.539	992	995	1000	rVB2	567	465	0.06%	0.008%
27	4.642	1014	1027	1070	rBV	77897	236914	31.69%	4.027%
28	4.899	1104	1107	1109	rBV2	233	122	0.02%	0.002%
29	4.977	1128	1131	1138	rBV2	314	314	0.04%	0.005%
30	5.060	1139	1157	1180	rVV	132998	302493	40.47%	5.142%
31	5.141	1180	1182	1186	rVB2	257	152	0.02%	0.003%
32	5.247	1211	1215	1217	rBV	125	114	0.02%	0.002%
33	5.288	1221	1228	1233	rBV3	778	1297	0.17%	0.022%
34	5.337	1240	1243	1245	rBV	132	79	0.01%	0.001%
35	5.385	1257	1258	1263	rVB2	251	114	0.02%	0.002%
36	5.411	1263	1266	1270	rBV2	172	157	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	5.485	1285	1289	1290	rBV	279	167	0.02%	0.003%
38	5.645	1337	1339	1341	rBV	103	69	0.01%	0.001%
39	5.713	1341	1360	1381	rVV2	297688	747526	100.00%	12.706%
40	5.867	1406	1408	1411	rBV2	155	115	0.02%	0.002%
41	5.896	1415	1417	1421	rVB2	235	115	0.02%	0.002%
42	5.922	1421	1425	1430	rBV2	273	269	0.04%	0.005%
43	5.980	1432	1443	1465	rVB4	7422	17823	2.38%	0.303%
44	6.083	1471	1475	1476	rBV	125	83	0.01%	0.001%
45	6.112	1481	1484	1487	rBV2	188	106	0.01%	0.002%
46	6.173	1499	1503	1512	rBV2	253	288	0.04%	0.005%
47	6.243	1512	1525	1545	rBV	231704	445476	59.59%	7.572%
48	6.369	1560	1564	1570	rVB2	317	372	0.05%	0.006%
49	6.398	1570	1573	1575	rBV	162	83	0.01%	0.001%
50	6.411	1575	1577	1581	rVB3	332	213	0.03%	0.004%
51	6.440	1581	1586	1588	rBV2	262	223	0.03%	0.004%
52	6.526	1605	1613	1626	rVB6	4356	7232	0.97%	0.123%
53	6.604	1626	1637	1650	rBV6	3720	7659	1.02%	0.130%
54	6.687	1650	1663	1687	rVB	178960	356108	47.64%	6.053%
55	6.796	1691	1697	1698	rBV2	606	489	0.07%	0.008%
56	6.854	1713	1715	1718	rBV2	180	104	0.01%	0.002%
57	6.886	1722	1725	1728	rBV	112	60	0.01%	0.001%
58	6.909	1728	1732	1735	rBV	142	130	0.02%	0.002%
59	6.967	1748	1750	1753	rVB2	319	178	0.02%	0.003%
60	7.076	1783	1784	1785	rBV	184	49	0.01%	0.001%
61	7.140	1801	1804	1807	rBV2	141	108	0.01%	0.002%
62	7.195	1811	1821	1822	rBV5	2039	2370	0.32%	0.040%
63	7.279	1845	1847	1851	rVB2	197	125	0.02%	0.002%
64	7.298	1851	1853	1856	rBV3	313	238	0.03%	0.004%
65	7.343	1865	1867	1873	rBV2	158	136	0.02%	0.002%
66	7.475	1903	1908	1910	rBV2	169	151	0.02%	0.003%
67	7.491	1911	1913	1914	rVV2	247	91	0.01%	0.002%
68	7.517	1918	1921	1924	rVB	176	90	0.01%	0.002%
69	7.565	1924	1936	1954	rBV	87652	161916	21.66%	2.752%
70	7.694	1968	1976	1979	rBV5	661	903	0.12%	0.015%
71	7.793	2003	2007	2008	rBV2	302	215	0.03%	0.004%
72	7.896	2021	2039	2056	rBV	299558	527044	70.51%	8.958%
73	8.060	2088	2090	2091	rBV	357	152	0.02%	0.003%
74	8.182	2116	2128	2145	rBV2	58733	109217	14.61%	1.856%
75	8.353	2177	2181	2188	rVB4	791	946	0.13%	0.016%
76	8.388	2188	2192	2194	rBV	159	107	0.01%	0.002%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

77	8.427	2201	2204	2207	rVB	191	116	0.02%	0.002%
78	8.446	2207	2210	2214	rBV2	120	116	0.02%	0.002%
79	8.501	2222	2227	2230	rBV	223	282	0.04%	0.005%
80	8.552	2241	2243	2244	rBV	158	58	0.01%	0.001%
81	8.648	2259	2273	2300	rBV2	242222	529767	70.87%	9.005%
82	8.877	2342	2344	2346	rBV2	123	71	0.01%	0.001%
83	8.909	2352	2354	2355	rBV2	196	65	0.01%	0.001%
84	9.021	2386	2389	2394	rBV2	214	210	0.03%	0.004%
85	9.311	2476	2479	2483	rBV	184	167	0.02%	0.003%
86	9.356	2492	2493	2494	rVB	309	60	0.01%	0.001%
87	9.365	2494	2496	2497	rBV	267	54	0.01%	0.001%
88	9.420	2500	2513	2532	rBV	324030	567700	75.94%	9.650%
89	9.636	2577	2580	2586	rBV2	190	210	0.03%	0.004%
90	10.099	2720	2724	2725	rBV2	297	218	0.03%	0.004%
91	10.562	2866	2868	2874	rBV2	267	224	0.03%	0.004%
92	10.603	2878	2881	2882	rBV2	277	140	0.02%	0.002%
93	10.761	2917	2930	2946	rBV	282125	465208	62.23%	7.907%
94	11.092	3024	3033	3035	rBV3	535	715	0.10%	0.012%
95	11.224	3068	3074	3077	rBV2	217	292	0.04%	0.005%
96	11.719	3225	3228	3230	rBV2	287	197	0.03%	0.003%
97	11.816	3246	3258	3276	rBV	351067	549117	73.46%	9.334%
98	11.896	3281	3283	3290	rVB4	652	517	0.07%	0.009%
99	12.195	3364	3376	3390	rBV	325850	531377	71.08%	9.032%
100	12.925	3598	3603	3606	rBV2	414	460	0.06%	0.008%

Sum of corrected areas: 5883180

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Instrument :
MSVOA_U
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F5C41ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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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Instrument :
MSVOA_U
ClientSampleId :
F5C41ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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
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