Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

New pentose dimers with bicyclic moieties from pretreated biomass

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Table 1. Comparison of water fractions from 2-butanone extraction of LfHP 1 and LfHP2.

Retention time (min)	Ions, *m/z* $[M- H^+]^-$	Source	Compounds
0.34	281.08670, 413.12897, 545.17053	LfHP 1	Pentoses DP2, DP 3, DP 4.
0.34	281.0864, 413.12854, 545.17017	LfHP 2	Pentoses DP2, DP 3, DP 4.
0.47	281.08667, 413.12878, 545.17102, 677.21277	LfHP 1	Pentoses DP2, DP 3, DP 4, DP 5
0.47	281.0849, 413.12857, 545.17041, 677.21246	LfHP 2	Pentoses DP2, DP 3, DP 4, DP 5
0.61	545.17047, 677.21411, 809.25598	LfHP 1	Pentoses DP 4, DP 5, DP6.
0.58	545.17053, 677.21307, 809.25549	LfHP 2	Pentoses DP 4, DP 5, DP6.
0.89	677.21252, 809.25641, 941.29730	LfHP 1	Pentoses DP 5, DP 6, DP 7.
0.88	677.21240, 809.25648, 941.29651	LfHP 2	Pentoses DP 5, DP 6, DP 7.
1.15	455.13885, 809.25500, 941.29755	LfHP 1	Pentoses + 1 acetyl, DP 3. Pentoses DP 6, DP 7.
1.15	455.13895, 809.25488, 941.29688	LfHP 1	Pentoses + 1 acetyl, DP 3. Pentoses DP 6, DP 7.
1.34	941.29785, 1073.33887	LfHP 1	Pentoses DP 7, DP 8.
1.34	941.29651, 1073.33862	LfHP 2	Pentoses DP 7, DP 8.
1.48	587.18073, 941.29657	LfHP 1	Pentoses + 1 acetyl, DP 4. Pentose DP 7.
1.48	587.18073, 941.29669	LfHP 2	Pentoses + 1 acetyl, DP 4. Pentose DP 7.
1.70	941.29742, 1073.34097, 1205.38257	LfHP 1	Pentoses DP 7, DP 8, DP 9
1.70	587.18115, 719.22363, 851.26581, 983.30768	LfHP 2	Pentoses + 1 acetyl, DP 4, DP 5, DP 6, DP 7
1.78	587.18103, 719.22339, 851.26563, 983.30780, 1115.35010, 1247.39148, 1379.43311	LfHP 1	Pentoses + 1 acetyl, DP 4, DP 5, DP 6, DP 7, DP 8, DP 9, DP 10
1.78	587.18109, 719.22333, 851.26569, 983.30768, 1115.34949, 1247.39160, 1379.43335	LfHP 2	Pentoses + 1 acetyl, DP 4, DP 5, DP 6, DP 7, DP 8, DP 9, DP 10
1.96	629.19171, 761.23376, 893.27631, 1025.31848, 1157.36035, 1289.40210, 1421.44312	LfHP 1	Pentoses + 2 acetyl, DP 4, DP 5, DP 6, DP 7, DP 8, DP 9.
1.96	629.19183, 761.23413, 893.27649, 1025.31824, 1157.36023, 1289.40283, 1421.44348	LfHP 2	Pentoses + 2 acetyl, DP 4, DP 5, DP 6, DP 7, DP 8, DP 9.

Table 2. Comparison of 2-butanone fractions from 2-butanone extraction of LfHP 1 and LfHP2. Please refer to ref 14 for structures of compounds marked in italic. Compounds marked with * were subjected to fragmentation and showed the same fragmentation pattern in LfHP 1 and LfHP 2.

Retention time (min)	Ions, *m/z* $[M- H^+]^-$	Source	Compounds
2.85	163.03880*	LfHP 1	Compound **1**
2.85	163.03870*	LfHP 2	Compound **1**
3.04	181.04932	LfHP 1	Not determined
3.04	181.04929	LfHP 2	Not determined
3.20	*265.07108, 325.09229*, 457.13498, 589,17682	LfHP 1	Pentose + feruloyl, DP 2, DP 3.
3.20	*265.07068, 325.09167*, 457.13583, 589,17706	LfHP 2	Pentose + feruloyl, DP 2, DP 3.
3.28	*265.07095, 327.08679, 357.09720, 387.10751**	LfHP 1	
3.28	*265.07071, 327.08627, 357.09689*, *387.10736**	LfHP 2	
3.35	*327.08643, 357.09790, 387.10760**	LfHP 1	
3.35	*327.08630, 357.09698, 387.10760**	LfHP 2	
3.41	*327.08655, 387.10889**	LfHP 1	
3.40	*327.08624, 387.09686**	LfHP 2	
3.52	*357.09763, 387.10760**, 601.17664	LfHP 1	Pentose + 1 acetyl + cumaroyl, DP 3
3.52	*307.04510*, 357.09689, 387.10736**, 601.17670	LfHP 2	Pentose + 1 acetyl + cumaroyl, DP 3
3.63	*187. 09630*, *307.04520*, 323.11258, *387.10849**, 631.18738	LfHP 1	Pentose + 1 acetyl + feruloyl, DP 3
3.63	*187. 09613, 307.04489** 323.11227, *387.10745**, 631.18695	LfHP 2	Pentose + 1 acetyl + feruloyl, DP 3
3.75	*239.12767, 275.09158, 305.10199, 387.10757**	LfHP 1	
3.75	*239.12756, 275.09137, 305.10172, 387.10721**	LfHP 2	
3.89	425.08713	LfHP 1	Not determined
3.89	425.08713	LfHP 2	Not determined
4.21	*371.11252, 383.11255 401.12302,*	LfHP 1	
4.21	*371.11218, 383.11212 401.12259,*	LfHP 2	
4.58	*301.07056*	LfHP 1	
4.58	*301.07047*	LfHP 2	