Supporting Information

Comparison of the structural characteristics of cellulolytic enzyme lignin preparations isolated from wheat straw stem and leaf

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Table of Contents

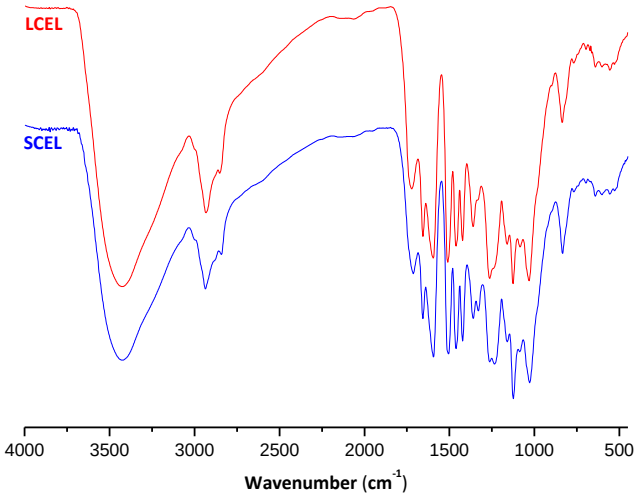

Figure S1. FTIR spectra of LCEL and SCEL.

Table S1. Assignment of the $^{1}H-^{13}C$correlation peaks in the 2D HSQC spectra of SCEL and LCEL.

label	chemical shifts δ_C/δ_H (ppm)	assignment
$-OCH_3$	55.4/3.74	C–H in methoxyls
A_{γ}	59.5/3.40 and 3.72	$C_{\gamma}-H_{\gamma}$ in γ-hydroxylated β–O–4' substructures
$A_{\alpha(G)}$	70.1/4.74	$C_{\alpha}-H_{\alpha}$ in β–O–4' substructures linked to a G-units
$A_{\alpha(S)}$	71.7/4.87	Cα−Hα in β–O–4' substructures linked to a S-unit
$A_{\beta(G)}$	83.7/4.29	$C_{\beta}-H_{\beta}$ in β–O–4' substructures linked to a G-units
$A_{\beta(S)}$	85.8/4.12	$C_{\beta}-H_{\beta}$ in β–O–4' substructures linked to a S-unit
B_{β}	53.0/3.45	$C_{\beta}-H_{\beta}$ in phenylcoumaran substructures
B_{γ}	62.5/3.66	$C_{\gamma}-H_{\gamma}$ in phenylcoumaran substructures
B_{α}	86.8/5.45	$C_{\alpha}-H_{\alpha}$ in phenylcoumaran substructures
C_{β}	53.5/3.07	$C_{\beta}-H_{\beta}$ in $\beta-\beta$' resinol substructures
C_{γ}	71.0/3.82 and 4.19	$C_{\gamma}-H_{\gamma}$ in $\beta-\beta$' resinol substructures
C_{α}	84.7/4.67	$C_{\alpha}-H_{\alpha}$ in $\beta-\beta$' resinol substructures
F_{α}	81.2/5.05	$C_{\alpha}-H_{\alpha}$ in spirodienone substructures
$H_{3,5}$	114.4/6.70	$C_{3,5}-H_{3,5}$ in *p*-hydroxyphenyl units
I_{γ}	61.3/4.10	$C_{\gamma}-H_{\gamma}$ in cinnamyl alcohol end-groups
I_{β}	128.3/6.23	$C_{\beta}-H_{\beta}$ in cinnamyl alcohol end-groups
I_{α}	128.2/6.46	$C_{\alpha}-H_{\alpha}$ in cinnamyl alcohol end-groups
J_{β}	126.1/6.77	$C_{\beta}-H_{\beta}$ in cinnamyl aldehyde end-groups
PCA_{β}	113.5/6.28	$C_{\beta}-H_{\beta}$ in *p*-coumarate
$PCA_{3,5}$	115.3/6.79	$C_{3,5}-H_{3,5}$ in *p*-coumarate
$PCA_{2,6}$	129.9/7.47	$C_{2,6}-H_{2,6}$ in *p*-coumarate
PCA_{α}	144.7/7.41	$C_{\alpha}-H_{\alpha}$ in *p*-coumarate
FA_2	110.9/7.35	C_2-H_2 in ferulate
FA_{β}	113.3/6.28	$C_{\beta}-H_{\beta}$ in ferulate
FA_6	122.4/7.17	C_6-H_6 in ferulate
$H_{2,6}$	127.5/7.19	$C_{2,6}-H_{2,6}$ in *p*-hydroxyphenyl units
G_2	110.8/6.98	C_2-H_2 in guaiacyl units
G_5	115.1/6.70 and 6.95	C_5-H_5 in guaiacyl units
G_6	118.8/6.79	C_6-H_6 in guaiacyl units
$S_{2,6}$	103.9/6.70	$C_{2,6}-H_{2,6}$ in etherified syringyl units
$S'_{2,6}$	106.2/7.33	$C_{2,6}-H_{2,6}$, C(α)=O in syringyl units
A'_{γ}	63.5/3.82 and 4.32	$C_{\gamma}-H_{\gamma}$ in γ-acylated β–O–4 substructures
$A'_{\beta(G)}$	81.4/4.41	$C_{\beta}-H_{\beta}$ in γ-acylated β–O–4 substructures
$T_{2',6'}$	103.9/7.32	$C_{2',6'}-H_{2',6'}$ in tricin
T_8	93.9/6.58	C_8-H_8 in tricin
T_6	98.6/6.23	C_6-H_6 in tricin
T_3	104.5/7.05	C_3-H_3 in tricin

Table S2. Positions and assignments of absorption peaks in CELs.

wavenumber (cm^{-1})		assignment
SCEL	LCEL	
3426	3425	stretching vibration of –OH (phenolic and alcoholic hydroxyl)
2936	2933	C–H stretching vibration in the aromatic methoxyl
2842	2851	the C–H stretching in methyl and methylene of the side chains
1713	1722	stretching vibration of non-conjugate C=O
1656	1656	stretching vibration of conjugate C=O
1594	1595	stretching vibration of benzene ring
1505	1510	stretching vibration of benzene ring
1462	1462	bending vibration of C–H (CH_2, CH_3)
1422	1423	stretching vibration of benzene ring
1360	1361	in-plane bending vibrations of phenolic O–H
1330	1331	stretching vibration of C–O in S-unit
1263	1264	stretching vibration of C–O in G-unit
1235	1234	vibrations of aryl–O in aryl–OH and aryl–O–CH_3
1160	1161	stretching vibration of phenolic acid ester
1125	1126	in-plane bending vibration of C–H in benzene ring of S-unit
1086	1085	bending vibration of C–H and C–O
1028	1032	stretching vibration of C–O (alcoholic hydroxyl and alkyl ether)
835	837	out-of plane bending vibration of C–H in benzene ring (S/H)