

Table S-3 Assignments of the lignin ^{13}C - ^1H correlation peaks in the HSQC spectra of control and fungal-treated wheat straw. (t) tentative assignment.

label	$\delta_{\text{C}}/\delta_{\text{H}}$ (ppm)	Assignment ^a
A $_{\alpha}$ (G)	70.9/4.70	C $_{\alpha}$ -H $_{\alpha}$ in β -O-4' substructures linked to G-unit
A $_{\alpha}$ (S)	71.8/4.82	C $_{\alpha}$ -H $_{\alpha}$ in β -O-4' substructures linked to S-unit
A $_{\beta}$ (G)	83.5/4.25	C $_{\beta}$ -H $_{\beta}$ in β -O-4' substructures linked to G-unit
A $_{\beta}$ (S)	85.9/4.09	C $_{\beta}$ -H $_{\beta}$ in β -O-4' substructures linked to S-unit
C $_{\alpha}$	84.9/4.64	C $_{\alpha}$ -H $_{\alpha}$ in resinol substructures
B $_{\alpha}$	86.9/5.42	C $_{\alpha}$ -H $_{\alpha}$ in phenylcoumaran substructures
T $_{8}$	94.1/6.56	C $_{8}$ -H $_{8}$ in triclin
T $_{6}$	98.8/6.20	C $_{6}$ -H $_{6}$ in triclin
Smod $_{2,6}$	103.5/6.97	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in S-unit derivative (t)
S $_{2,6}$	103.6/6.68	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in S-unit
T $_{2'6'}$	104.0/7.31	C $_{2'}$ -H $_{2'}$ and C $_{6'}$ -H $_{6'}$ in triclin
T $_{3}$	104.6/6.99	C $_{3}$ -H $_{3}$ in triclin
Sox $_{2,6}$	106.4/7.32	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in C $_{\alpha}$ -oxidized (C $_{\alpha}$ =O) S-unit
Sox $_{2,6}$	106.5/7.18	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in C $_{\alpha}$ -oxidized (C $_{\alpha}$ OOH) S-unit
Sald $_{2,6}$	106.3/7.03	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in cinnamaldehyde end-group S-unit
G $_{2}$	110.5/6.94	C $_{2}$ -H $_{2}$ in G-unit
FA $_{2}$	110.9/7.32	C $_{2}$ -H $_{2}$ in ferulate
GoxI $_{2}$	111.4/7.53	C $_{2}$ -H $_{2}$ in C $_{\alpha}$ -oxidized G-unit
GoxII $_{2}$	112.4/7.42	C $_{2}$ -H $_{2}$ in C $_{\alpha}$ -oxidized G-unit (t)
Gmod $_{2}$	112.7/6.76	C $_{2}$ -H $_{2}$ in G-unit derivative (t)
FA $_{\beta}$ /pCA $_{\beta}$	113.9/6.51	C $_{\beta}$ -H $_{\beta}$ in ferulate/ <i>p</i> -coumarate
H $_{3,5}$ /FA $_{5}$	114.5/6.69	C $_{3}$ -H $_{3}$ and C $_{5}$ -H $_{5}$ in H-unit, C $_{5}$ -H $_{5}$ in FA
G $_{5}$ /G $_{6}$ /pCA $_{3,5}$	115.1/6.94 and 115.3/6.72	C $_{5}$ -H $_{5}$ and C $_{6}$ -H $_{6}$ in G-unit, C $_{3}$ -H $_{3}$ and C $_{5}$ -H $_{5}$ of pCA
G $_{5}$	118.9/6.77	C $_{5}$ -H $_{5}$ in G-unit
GoxI $_{6}$	122.8/7.49	C $_{6}$ -H $_{6}$ in C $_{\alpha}$ -oxidized G-unit
FA $_{6}$	123.1/7.12	C $_{6}$ -H $_{6}$ in ferulate
GoxII $_{6}$	125.8/7.40	C $_{2}$ -H $_{2}$ in C $_{\alpha}$ -oxidized G-unit (t)
H $_{2,6}$ /PHE $_{3,5}$	127.7/7.17	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in H-unit, C $_{3}$ -H $_{3}$ and C $_{5}$ -H $_{5}$ in phenylalanine
PHE $_{2,6}$	129.0/7.20	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in phenylalanine
pCA $_{2,6}$	130.1/7.48	C $_{2}$ -H $_{2}$ and C $_{6}$ -H $_{6}$ in <i>p</i> -coumarate
FA $_{\alpha}$ /pCA $_{\alpha}$	145.0/7.56	C $_{\alpha}$ -H $_{\alpha}$ in ferulate/ <i>p</i> -coumarate

^a: assignment by comparison with literature (1-9).

References

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