Whole Plant Cell Wall NMR with Ionic Liquids: A Powerful Tool in Biofuel Research

Marcus Foston[1,2,*], Reichel Samuel[3], Jian He[2], and Arthur J. Ragauskas[1,3,4]

[1]*BioEnergy Science Center*

[2]*Washington University in St. Louis, Department of Energy, Environmental & Chemical Engineering, St. Louis, MO, USA*

[3]*Georgia Institute of Technology, School of Chemistry and Biochemistry, Institute of Paper Science and Technology, Atlanta, GA, USA*

[4]*Department of Chemical and Biomolecular Engineering, Department of Forestry, Wildlife, and Fisheries, University of Tennessee, Knoxville, TN, USA*

Supplementary Table 1 Represents the typical chemical shift assignments of 1D ^{13}C NMR spectra of biomass in DMSO-d_6.

Assignments	^{13}C Chemical Shift (ppm)
C=O in φ-COOH	179-173
C=O in φ-COOR	167-168
C=O in Ar-C=C-COOR	168-166
H_4	164-158
$G_{3/4}$, $S_{3/5}$, and C_α in Cinnamate	157-140
$S_{1/4}$ and G_1	140-123
G_6	123-117
$H_{3/5}$, G_5, C_β in Cinnamate	117-113
G_2	113-110
$S_{2,6}$	110-106
C_1 in Cellulose and Hemicellulose	105-98
$C_{2,3,4,5}$ in Cellulose, $C_{2,3,4}$ in Hemicellulose, and Lignin Side Chains	94-65
C_6 in Cellulose, C_5 in Hemicellulose, and Lignin Side Chains	65-58
Methoxy	57-54
Acetate-Methyl	22-20