Supplementary Table 1. Annotation of the 2D 1H-13C HSQC-NMR spectral peaks.

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| --- | --- | --- | --- | --- | --- | --- |
| ROI　No. | 1H-chemical shift (ppm) | | 13C-chemical shift (ppm) | | Annotation | |
| downfield | upfield | downfield | upfield | Large category | Small category |
| ROI.1 | 7.68 | 7.63 | 130.97 | 129.93 | Lignin. aromatic | *p*-Coumarate |
| ROI.2 | 7.64 | 7.57 | 130.89 | 129.80 | Lignin. aromatic | *p*-Coumarate |
| ROI.3 | 7.57 | 7.51 | 130.82 | 129.82 | Lignin. aromatic | *p*-Coumarate |
| ROI.4 | 7.51 | 7.46 | 130.83 | 129.84 | Lignin. aromatic | *p*-Coumarate |
| ROI.5 | 7.13 | 7.03 | 117.02 | 115.27 | Lignin. aromatic | Guaiacyl |
| ROI.6 | 7.05 | 6.99 | 115.55 | 114.74 | Lignin. aromatic | Guaiacyl |
| ROI.7 | 6.92 | 6.83 | 115.50 | 114.37 | Lignin. aromatic | Guaiacyl |
| ROI.8 | 6.82 | 6.76 | 115.66 | 114.34 | Lignin. aromatic | Guaiacyl |
| ROI.9 | 6.98 | 6.90 | 105.94 | 103.05 | Lignin. aromatic | Syringyl |
| ROI.10 | 6.89 | 6.79 | 105.69 | 103.22 | Lignin. aromatic | Syringyl |
| ROI.11 | 7.38 | 7.22 | 128.88 | 127.64 | Lignin. aromatic | *p*-Hydroxyphenyl |
| ROI.12 | 4.31 | 4.21 | 62.47 | 61.27 | Lignin. aromatic | Cinnamyl alcohol end group |
| ROI.13 | 7.27 | 7.18 | 124.29 | 122.87 | Lignin. aromatic | Ferulate |
| ROI.14 | 7.49 | 7.36 | 112.30 | 110.91 | Lignin. aromatic | Ferulate |
| ROI.15 | 3.96 | 3.88 | 56.95 | 55.30 | Others | Methoxyl |
| ROI.16 | 3.88 | 3.66 | 56.82 | 55.14 | Others | Methoxyl |
| ROI.17 | 5.18 | 5.04 | 83.88 | 82.45 | Lignin. aliphatic | 5-5/4-*O*-β |
| ROI.18 | 3.67 | 3.57 | 88.27 | 87.15 | Lignin. aliphatic | 5-5/4-*O*-β |
| ROI.19 | 5.19 | 5.13 | 73.57 | 72.39 | Lignin. aliphatic | β-*O*-4 |
| ROI.20 | 5.15 | 5.08 | 72.97 | 71.49 | Lignin. aliphatic | β-*O*-4 |
| ROI.21 | 5.07 | 5.00 | 72.86 | 71.68 | Lignin. aliphatic | β-*O*-4 |
| ROI.22 | 3.50 | 3.38 | 61.41 | 60.22 | Lignin. aliphatic | β-*O*-4-H/G |
| ROI.23 | 5.01 | 4.92 | 71.68 | 70.81 | Lignin. aliphatic | β-*O*-4-H/G |
| ROI.24 | 5.01 | 4.92 | 72.42 | 71.69 | Lignin. aliphatic | β-O-4-H/G |
| ROI.25 | 4.29 | 4.21 | 87.29 | 86.12 | Lignin. aliphatic | β-*O*-4-S |
| ROI.26 | 3.85 | 3.61 | 53.35 | 50.98 | Lignin. aliphatic | β-5 |