Comparing Chemical Composition and Lignin Structure of *Miscanthus x giganteus* and *Miscanthus nagara* Harvested in Autumn and Spring and Separated into Stem and Leaves

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**Figure S1.** FT-IR spectrum of stem-derived lignin obtained from *M. x giganteus* (Gig35S), harvested in April with numbered signals listed in Table A2.

**Tab. S1** FTIR signals and corresponding assignment for lignins isolated from *M. x giganteus* (Gig35, stem and leaf) and *M. nagara* (NagG10, stem and leaf). See Fig. S1 for signal numbering.

| Signal Number | Wave Number (cm⁻¹) | Functional Group | Type of Vibration                                      |
|---------------|--------------------|------------------|-------------------------------------------------------|
| 1             | 3428±60            | O-H-             | Stretch                                               |
| 2             | 2926±11            | C-H-             | Stretch                                               |
| 3             | 2850±6             | C-H-             | Stretch                                               |
| 4             | 1708±11            | C=O-             | Stretch                                               |
| 5             | 1655±4             | C=O-             | Stretch                                               |
| 6             | 1605±12            | Aromatic Ring    | Symmetric Stretch                                     |
| 7             | 1514±6             | Aromatic Ring    | Antisymmetric Stretch                                 |
| 8             | 1460±4             | C-H-             | Antisymmetric Deformation                             |
| 9             | 1424±4             | C-H in O-CH₃     | Antisymmetric Deformation (S-Mode)                    |
| 10            | 1398±4             | C-H              | Bending                                              |
| 11            | 1371±15            | Aromatic frame   | C-H in-plane Deformation                             |
| 12            | 1331±9             | Aromatic frame; C-O | Skeletal; Stretch (S-Mode)                  |
| 13            | 1267±2             | Aromatic frame; C-O | Skeletal; Stretch (G-Mode)                  |
| 14            | 1225±12            | C-C; C-O; C=O    | Stretch (G-Mode)                                     |
| 15            | 1166±10            | C-H in G-Ring    | Stretch                                              |
| 16            | 1124±2             | Aromatic C-H     | In-plane Deformation                                 |
| 17            | 1033±2             | Aromatic C-H     | In-plane Deformation                                 |
| 18            | 834±4              | Aromatic C-H     | Out-of-plane Deformation (S-Mode)                    |
Tab. S2 SEC results (detected via refractive index (RI) and ultraviolet (UV) detectors) including the number average (Mn) and weight average (Mw) molecular weight and polydispersity (PDI) of lignin obtained from *M. x giganteus* and *M. nagara*, resp., separated into leaves (Gig35L, NagG10L) and stems (Gig35S, NagG10S).

| Sample   | Harvesting | Detector | $M_n$ (g mol$^{-1}$) | $M_w$ (g mol$^{-1}$) | PDI |
|----------|------------|----------|----------------------|----------------------|-----|
| Gig35L   | September  | RI       | 910.01               | 1746.8               | 1.92|
|          |            | UV       | 882.6                | 1747.1               | 1.98|
|          | December   | RI       | 884.95               | 1720.6               | 1.94|
|          |            | UV       | 876.93               | 1678.8               | 1.91|
|          | April      | RI       | 994.95               | 1796.6               | 1.81|
|          |            | UV       | 960.46               | 1757.4               | 1.83|
| NagG10L  | September  | RI       | 915.59               | 1895.8               | 2.07|
|          |            | UV       | 900.93               | 1922.3               | 2.13|
|          | December   | RI       | 832.81               | 1637.3               | 1.97|
|          |            | UV       | 863.79               | 1630.5               | 1.89|
|          | April      | RI       | 961.66               | 1782.3               | 1.85|
|          |            | UV       | 951.22               | 1766.9               | 1.86|
| Gig35S   | September  | RI       | 1178.7               | 2143.1               | 1.82|
|          |            | UV       | 1089.4               | 2047.6               | 1.88|
|          | December   | RI       | 1229.4               | 2207.2               | 1.8  |
|          |            | UV       | 1125.9               | 2103.1               | 1.87|
|          | April      | RI       | 1298.2               | 2312                 | 1.78|
|          |            | UV       | 1197.5               | 2241.6               | 1.87|
| NagG10S  | September  | RI       | 1093.5               | 1915.7               | 1.75|
|          |            | UV       | 980.61               | 1821                 | 1.86|
|          | December   | RI       | 1180                 | 2063                 | 1.75|
|          |            | UV       | 1055.6               | 1937.2               | 1.84|
|          | April      | RI       | 1251.6               | 2127.5               | 1.7  |
|          |            | UV       | 1115.8               | 2053.3               | 1.84|

Figure S2. UV/Vis curves for lignins obtained from leaf-derived *M. nagara* (NagG10L) harvested in September, December and April.
Figure S3. UV/Vis curves for lignins obtained from stem-derived *M. nagara* (NagG10S) harvested in September, December and April.

Figure S4. UV/Vis curves for lignins obtained from leaf-derived *M. x giganteus* (Gig35L) harvested in September, December and April.

Figure S5. UV/Vis curves for lignins obtained from stem-derived *M. x giganteus* (Gig35S) harvested in September, December and April.
Figure S6. Non-Aromatic HSQC region of a lignin obtained from *M. x giganteus* (Gig35, stem, April harvest). Numbers are listed and assigned in the main text, Table 5.

Figure S7. Non-Aromatic HSQC region of a lignin obtained from *M. x giganteus* (Gig35, stem, April harvest). Numbers are listed and assigned in the main text, Table 5.