Electronic Supplement Information (ESI)

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

Michel Bergs, Xuan Tung Do, Jessica Rumpf, Peter Kusch, Yulia Monakhova, Christopher Konow, Georg Völkering, Ralf Pude and Margit Schulze*





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	0-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-CH ₃	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.