

Supporting Information

Table S1. Identified chemical shifts for HSQC spectra of GVL lignin, pyrolytic lignin, and hydrogenated pyrolytic lignin in DMSO-*d*₆ and pyridine-*d*₅ solvent mixture. Referenced to residual DMSO peaks at $\delta_{\text{H}}/\delta_{\text{C}}$ 2.49/39.5 ppm.

Peak	HSQC Identified Chemical Shifts (ppm)	
	¹ H	¹³ C
GVL Lignin		
B-β	5.56	87.17
B-β	5.70	88.10
S-2/6	6.93	103.69
S-2/6	6.77	103.92
S-2/6	6.67	103.29
S'-2/6	7.10	106.29
S'-2/6	7.25	106.80
S'-2/6	7.42	106.45
G'-2	7.62	111.57
G-2	7.09	111.02
G-2	6.98	110.13
G-5/6	6.83	115.23
G-5/6	7.02	115.31
G-5/6	6.94	114.89
G-5/6	6.82	118.67
G-5/6	6.99	119.48
Py	7.32	123.51
H-2/6	7.24	127.68
Py	7.72	135.75
Py	8.57	149.36
X3-α	9.82	190.99
B-β	3.54	53.30
C-β	3.08	53.68
OMe	3.71	55.57
A-γ	3.77	60.00
A-γ	3.45	60.00
A-α	5.03	72.09
C-γ2	4.20	71.23
C-γ1	3.84	71.28
A-Gβ	4.43	83.54
C-α	4.69	85.16
A-Sβ	4.24	86.24
A-Sβ	4.13	87.38
B-γ	3.82	62.48
GVL	1.22	20.48
GVL	1.65	28.98
GVL	2.19	28.93
GVL	2.46	28.54
DMSO	2.49	39.52
X2-γ	9.64	193.92
FA-2	7.37	110.85
FA-β	6.56	114.42
FA-6	7.14	123.20
FA-α	7.63	144.95
Fatty Acids	5.28	127.66
Fatty Acids	5.29	129.56

Pyrolytic Lignin	¹H	¹³C
S''	6.52	105.91
G-2	6.87	112.58
G-2	6.70	112.91
S-2/6	6.67	103.38
S-2/6	6.90	103.58
LGA-1	3.54	64.90
LGA-1'	3.95	64.95
LGA-6	3.41	72.03
LGA-4	3.32	71.91
LGA-5	3.56	73.79
LGA-7	4.42	76.59
LGA-3	5.29	102.54
G-5/6	6.82	115.45
G-5/6	6.74	115.21
G-5/6	6.62	119.13
X3-2/6	7.25	106.83
X2-2/6	7.10	106.52
X2-β	6.88	125.87
OMe	3.82	55.69
OMe	3.71	55.57
Hydrogenated Pyrolytic Lignin	¹H	¹³C
G''-2	6.75	112.18
S''	6.43	103.65
S''	6.44	105.29
S''	6.59	105.38
G''-5/6	6.74	115.18
G''-5/6	6.56	120.16
OMe	3.72	55.52
LGA-1	3.54	64.90
LGA-1'	3.95	64.95
LGA-6	3.41	72.03
LGA-4	3.32	71.91
LGA-5	3.56	73.79
LGA-7	4.42	76.59
LGA-3	5.29	102.54

Table S2. Chemical shifts for HSQC of cyclohexane, cyclohexanol, and *trans*-2-methoxy-cyclohexanol in DMSO-*d*6 and pyridine-*d*5 solvent mixture. Referenced to residual DMSO peaks at $\delta_{\text{H}}/\delta_{\text{C}}$ 2.49/39.5 ppm.

HSQC Identified Chemical Shifts (ppm)		
C-C Aliphatic Peaks	¹H	¹³C
Cyclohexane	1.31	25.95
Cyclohexanol	1.03	24.92
Cyclohexanol	1.14	23.51
Cyclohexanol	1.14	35.21
Cyclohexanol	1.38	25.15
Cyclohexanol	1.59	23.51
Cyclohexanol	1.73	35.21
<i>trans</i> -2-methoxy-cyclohexanol	1.06	28.27
<i>trans</i> -2-methoxy-cyclohexanol	1.09	22.89
<i>trans</i> -2-methoxy-cyclohexanol	1.19	32.48
<i>trans</i> -2-methoxy-cyclohexanol	1.51	22.89
<i>trans</i> -2-methoxy-cyclohexanol	1.75	32.48
<i>trans</i> -2-methoxy-cyclohexanol	1.88	28.04
C-O Aliphatic Peaks	¹H	¹³C
Cyclohexanol	3.41	67.96
<i>trans</i> -2-methoxy-cyclohexanol	2.86	83.25
<i>trans</i> -2-methoxy-cyclohexanol	3.28	55.88
<i>trans</i> -2-methoxy-cyclohexanol	3.32	71.32