Supporting Information

Catalytic hydrogenolysis of Kraft lignin to monomers at high yield in alkaline water

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Table S1. Selectivity (S_i) of monomer products from KL and OKL-M.[a]

No.	*t*/min	Compound	KL-M	OKL-M
			S_i/%	S_i/%
1	28.0	Phenol	2.2	1.6
2	28.8	Guaiacol	40.8	33.4
3	32.4	2-Methoxy-4-methylphenol	5.1	7.2
4	35.3	2-Methoxy-4-ethylphenol	13.9	19.9
5	38.0	2-Methoxy-4-propylphenol	2.7	7.5
6	42.1	Vanillin	14.1	6.7
7	44.4	1-(4-Hydroxy-3-methoxyphenyl)ethanone	7.1	3.9
8	45.8	1-(4-Hydroxy-3-methoxyphenyl)propanone	5.4	7.2
9	49.2	2-(4-Hydroxy-3-methoxyphenyl)acetic acid	8.7	12.6

a, $S_i = \frac{The\ intergrated\ GC-MS\ area\ of\ product\ (i)}{The\ total\ intergrated\ area\ of\ all\ detected\ products\ in\ GC-MS} \times 100\%$

Table S2. Individual yields of the nine monomers in OKL-M.[a]

No.	Compound	wt%-KL	wt%-oil
1	Phenol	1.8	2.2
2	Guaiacol	38.0	45.6
3	2-Methoxy-4-methylphenol	3.7	4.4
4	2-Methoxy-4-ethylphenol	9.5	11.4
5	2-Methoxy-4-propylphenol	2.4	2.9
6	Vanillin	8.2	9.8
7	1-(4-Hydroxy-3-methoxyphenyl)ethanone	3.6	4.3
8	1-(4-Hydroxy-3-methoxyphenyl)propanone	2.2	2.6
9	2-(4-Hydroxy-3-methoxyphenyl)acetic acid	6.7	8.0
	Total	76.1	91.2

a, The yields were determined quantitatively by GC/MS

Table S3. FTIR bands assignment of KL, OKL, KL-R, and OKL-R.

No.	Assignment	Wavenumber (cm^{-1})			
		KL	OKL	HR	OHR
1	−OH stretching	3300	3290	3384	3380
2	C−H of $–CH_3$/$−CH_2−$ stretching	2940	2946	2936	2940
3	Non-conjugated C=O stretching	1700	1716	1711	1710
4	Conjugated C=O stretching	1600	1595	1612	1601
5	Aromatic ring stretching	1513	1520	1512	1515
6	Deformation of $–CH_3$/$−CH_2−$	1450	1452	1448	1463
7	Deformation of aromatic C−H	1427	1400	1419	1431
8	Aliphatic C−H and phenolic –OH stretching	1368	1361	1385	1368
9	Guaiacyl and C=O stretching	1268	1267	1268	1269
10	C−C, C−O, and C=O stretching	1222	1222	1222	1222
11	Guaiacyl C−C and C−O stretching, secondary alcohol C−O stretching, and aromatic C-H out-of-plain bending	1130	1117	1140	1143
12	In-plain bending of aromatic C−H	1030	1020	1027	1025
13	Aromatic *2,6*-C-H out-of-plain bending	840	870	858	858

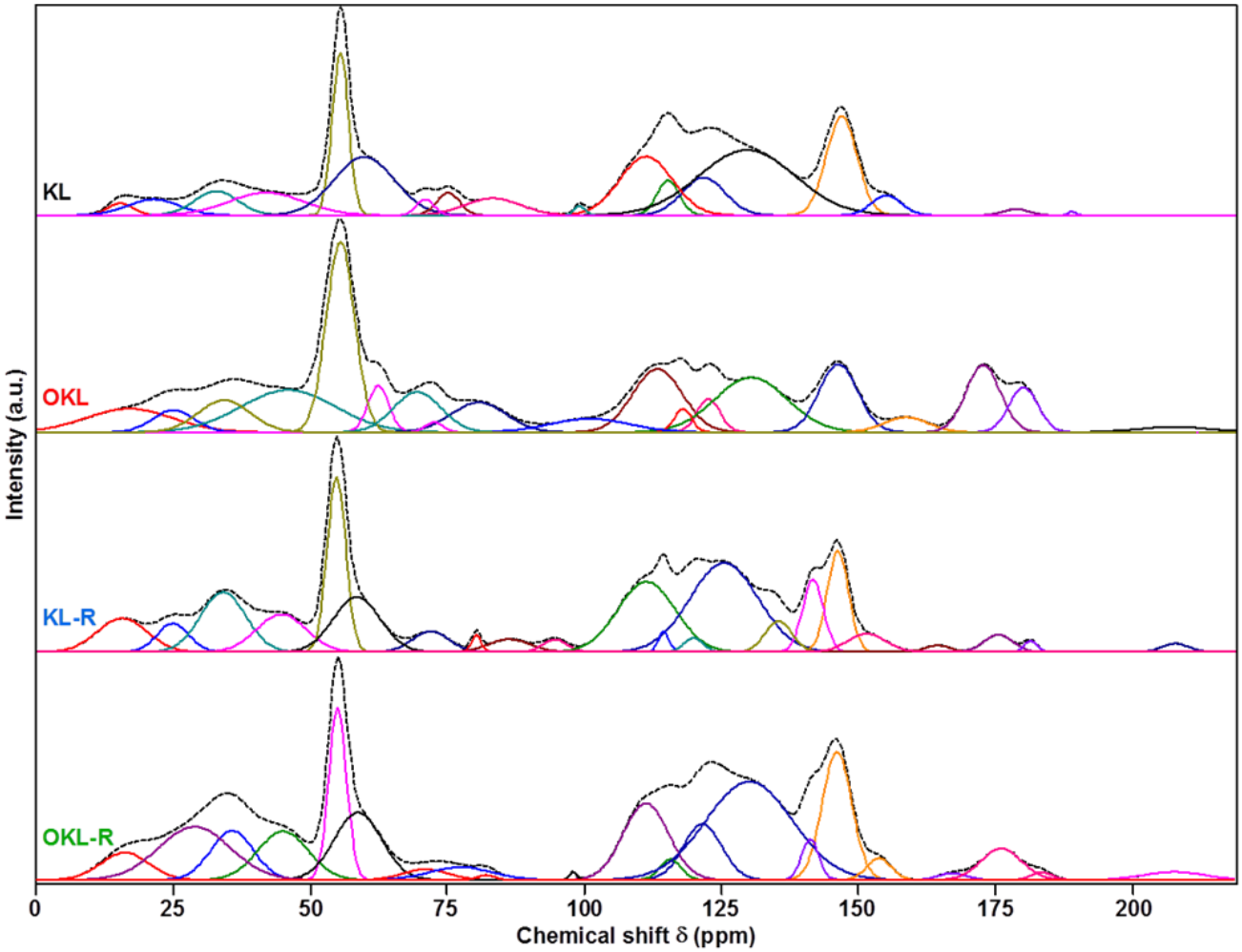
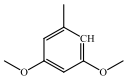
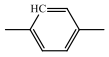
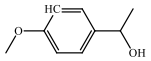
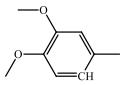


Fig. S1 Solid ^{13}C-NMR spectra of KL, OKL, KL-R, and OKL-R.

Table S4. ^{13}C-NMR bands assignment of KL, OKL, KL-R, and OKL-R.

Assignment	δ (ppm)			
	KL	**OKL**	**KL-R**	**OKL-R**
$–CH_3$	15.7	17.3	16.0	16.3
$–CH_2Me$	21.7	25.4	25.3	29.0
Tertiary carbon	33.2	34.6	34.4	35.9
$-CH_2Et$ or Tertiary carbon	42.3	46.3	45.0	45.2
$–O–CH_3$	55.8	55.8	55.1	55.2
$–CH_2–OH$	60.1	62.7	58.8	58.9
C_γ of *β*-*β*' pinoresinol	71.2	69.8	72.3	71.3
–CH(OH)–	75.4	72.8	80.6	77.7
C_α of *β*-*β*' pinoresinol	83.6	81.0	86.6	82.3
	99.4	101.2	94.9	98.2
	111.5	113.6	111.6	111.6
	115.5	118.2	114.7	116.1
	122.0	122.9	120.2	121.9
Ar (C) bonding with C_α in *β*-O-4	129.9	130.6	125.7	130.5
Ar (C)–(C) Ar	--	--	135.7	--
Ar (C)−O of dibenzodioxocin	--	--	142.0	141.6
Ar (C) bonding with O in *β*-O-4	147.2	146.6	146.5	146.5
Ar (C)–O–CH_3	155.4	158.9	151.8	154.2
–COO–	--	--	164.7	167.6
–COOH	179.0	173.0	175.7	176.6
–CO–	189.1	180.3	181.6	184.0
–CHO	--	207.8	208.0	208.2

Atomic Coordinates For the Molecules Involved In This Paper

(Please download the file of the atomic coordinates *via* the following link:)

https://www.dropbox.com/s/9f23bkb3xzvav0n/Atomic%20Coordinates%20For%20the%20Molecules.pdf?dl=0