

Supplementary Material

Catalytic Selective Oxidation of β -O-4 Bond in Phenethoxybenzene as a Lignin Model Using (TBA)₅[PMo₁₀V₂O₄₀] Nanocatalyst: Optimization of Operational Conditions

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Table S1. Analysis of variance (ANOVA) for experimental results of fractional factorial screening design to obtain the statistically significant variables in the conversion of phenethoxybenzene.

Source	Sum of squares	Df. **	Mean squares	F-value	P-value
Model	55.6	4	13.91	59.67	0.001*
Residual Error	0.93	4	0.23	-	-

Lack of fit	0.68	2	0.34	2.78	0.265
Pure Error	0.25	2	0.12	-	-
Total	56.53	8	-	-	-
$R^2 = 0.984$					
Adj. $R^2 = 0.967$					

* Significant at 95% confidence level; ** Degrees of freedom

Table S2. Analysis of variance (ANOVA) for the quadratic polynomial model.

Source	Sum of squares	Df. **	Mean squares	F-value	P-value
Model	236.1	9	26.2	10.16	0.010*
Residual Error	12.9	5	2.58	-	-
Lack of fit	8.98	3	2.99	1.524	0.420
Pure Error	3.93	2	1.96	-	-
Total	249.0	14	-	-	-
$R^2 = 0.948$					
Adj. $R^2 = 0.855$					

* Significant at 95% confidence level; ** Degrees of freedom.

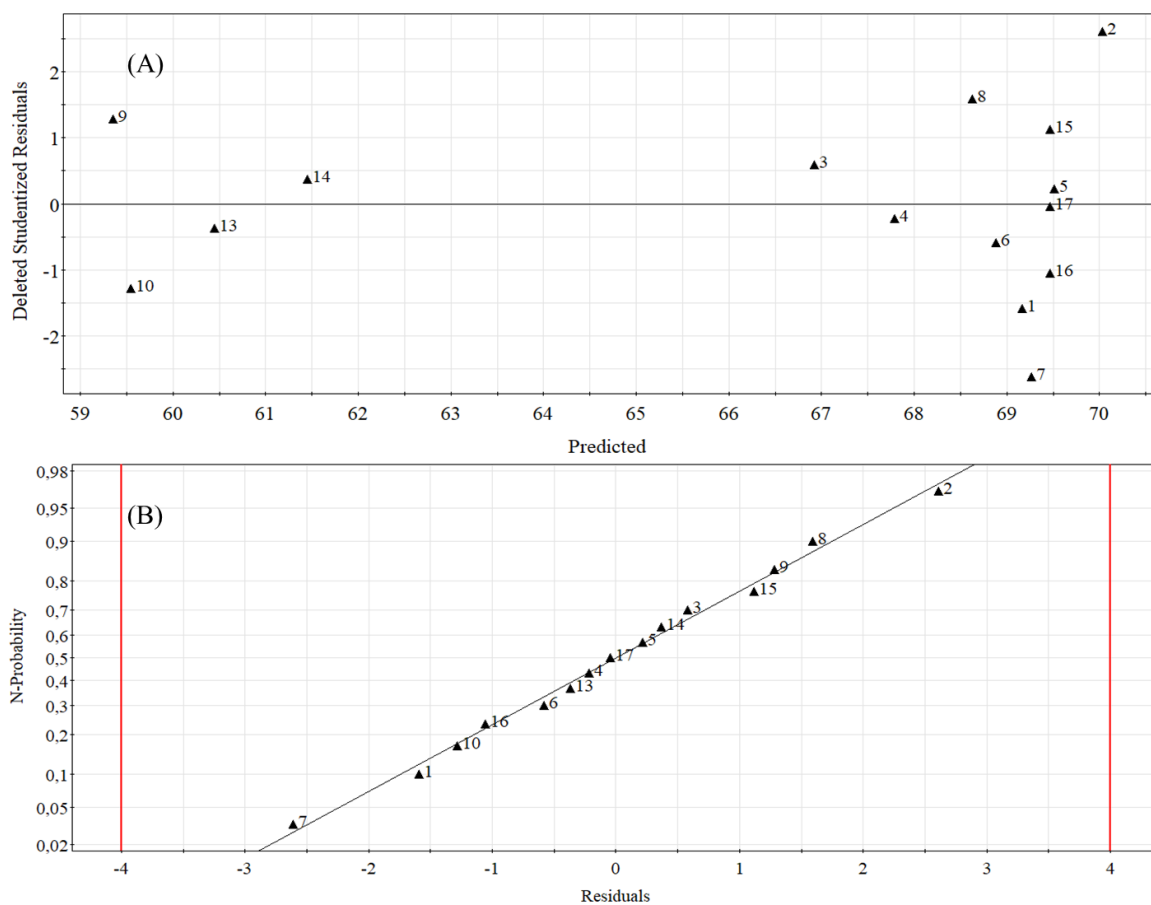
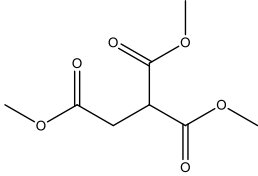
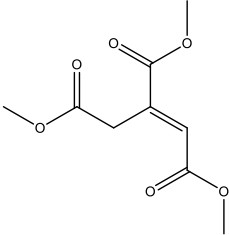
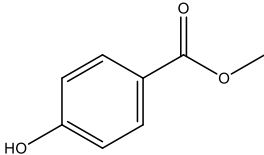
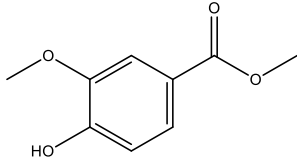
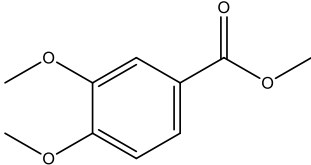
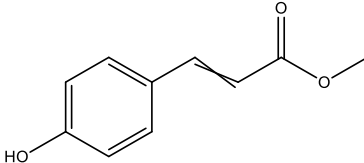
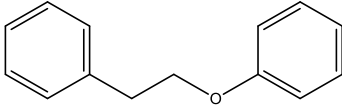
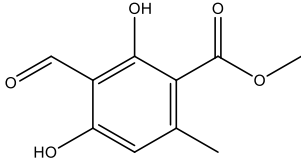


Figure S1. (A) Residuals *versus* predicted values y (B) Normal probability of the residuals.

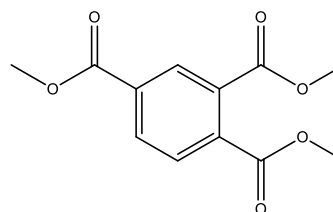
Table S3. Identification of catalytic Kraft lignin depolymerization products by GC-MS.

Peak number	Compound name	Retention time [min]	Structure
1	1,1,3-Trimethoxypropane	5.8	
2	Dimethyl malonate	6.3	
3	2-Butenedioic acid (Z)-, dimethyl ester	7.6	
4	2-Butanedioic acid dimethyl ester	7.7	
5	Benzoic acid, methyl ester	8.5	
6	2-Isopropoxypropanol	8.9	
7	Butanedioic acid, methoxy-, dimethyl ester	9.1	
8	Tributylamine	9.8	

9	Trimethyl ethane-1,1,2-tricarboxylate	10.8	
10	(1E)-1-propene-1,2,3-tricarboxylic acid 1,2,3-trimethyl ester	12.9	
11	<i>p</i> -hydroxybenzoic acid methyl ester	13.3	
12	Methyl 4-hydroxy-3-methoxybenzoate	14.9	
13	Methyl 3,4-dimethoxybenzoate	16.3	
14	2-Propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester	16.7	
15	Phenethoxybenzene	17.7	
16	Methyl 3-formyl-2,4-dihydroxy-6-methylbenzoate	18.6	

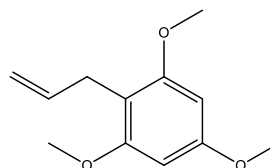
17 Trimethyl 1,2,4-
benzenetricarboxylate

19.5



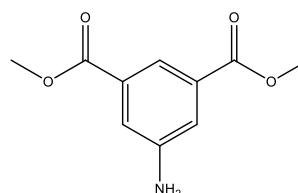
18 1-(2,4,6-
trimethoxyphenyl)-2-
propene

19.9



19 Dimethyl 5-aminobenzene-
1,3-dicarboxylate

20.1



20 4H-Benzo[def]naphtho[2,3-
b]carbazole

23.6

