

Supplementary Information

Depolymerized Lignin as an Enabler for Superior Lignin–Acrylonitrile Copolymers for Sustainable Wet-spun Fibers

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Calculation of incorporation fractions

Assuming the nitrogen content in the lignin (LB and/or DLB) structure negligible, the mass fraction of acrylonitrile (AN) incorporated into the copolymer was determined by comparing the nitrogen content of the copolymer to that of the pure PAN homopolymer measured by Elemental Analysis (EA).

$$I_{AN} = \frac{N_{Copolymer}}{N_{PAN}} \cdot 100 \quad \text{Equation (S1)}$$

$$I_{lignin} = 100 - I_{AN} \quad \text{Equation (S2)}$$

I_{AN} = Incorporation fraction of AN into the copolymer (%)

I_{lignin} = Incorporation fraction of DLB (or LB) into the copolymer (%)

$N_{copolymer}$ = Nitrogen content in the purified copolymer measured by EA (%)

N_{PAN} = Nitrogen content in the pure PAN homopolymer measured by EA (%)

Calculation of conversions

The overall conversion of each monomer was calculated by mass balance, relating the mass of each component present in the final purified copolymer to its initial mass in the feed.

$$C_{AN} = \frac{m_{copolymer} \cdot (I_{AN}/100)}{m_{AN, initial}} \cdot 100 \quad \text{Equation (S3)}$$

$$C_{lignin} = \frac{m_{copolymer} \cdot (I_{lignin}/100)}{m_{lignin, initial}} \cdot 100 \quad \text{Equation (S4)}$$

C_{AN} = Conversion of AN (%)

C_{lignin} = Conversion of DLB (or LB) (%) $m_{copolymer}$ = Final mass of the purified copolymer (g)

$m_{AN, initial}$ = Initial mass of acrylonitrile added to the reaction (g)

$m_{lignin, initial}$ = Initial mass of DLB (or LB) added to the reaction (g)

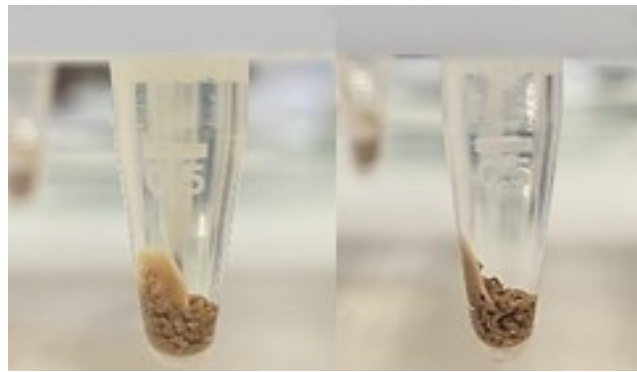


Figure SI.1- Purification of poly(AN-DLB)-3.4 copolymer with methanol.

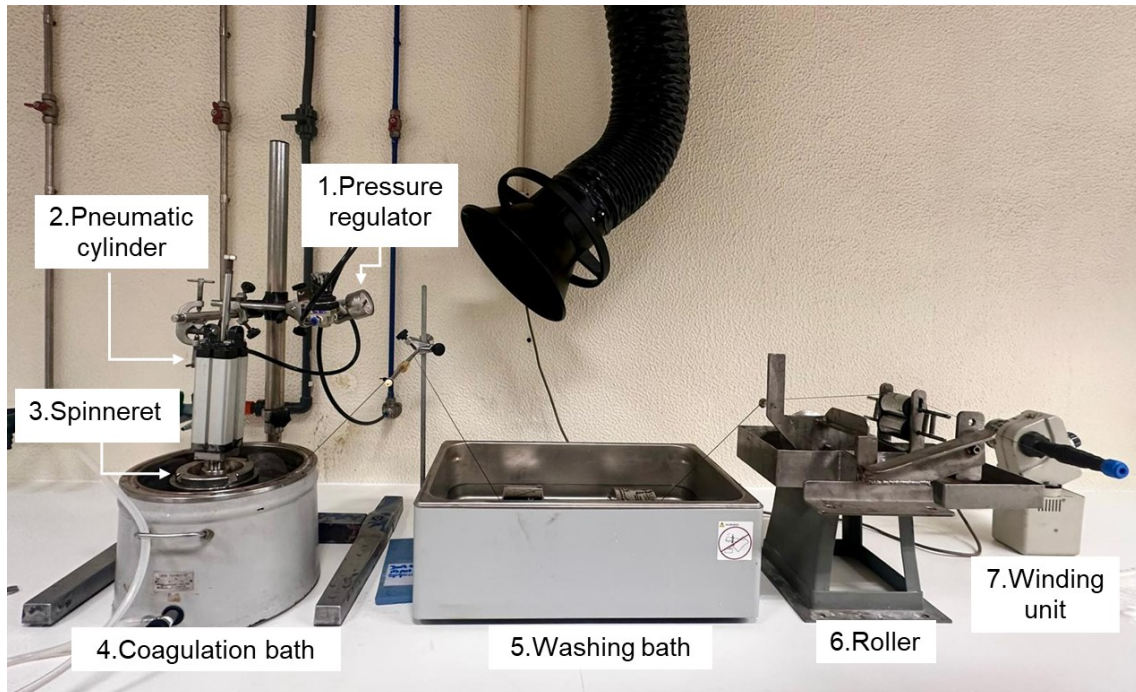


Figure SI.2- Laboratory wet-spinning line

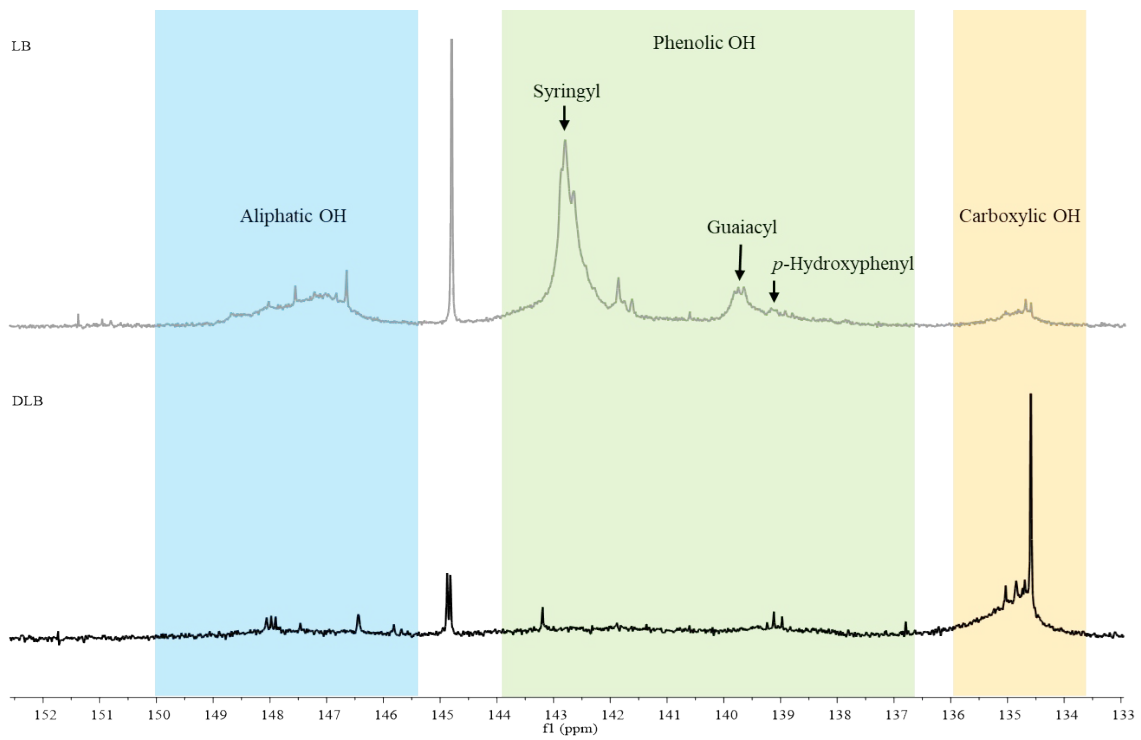


Figure SI.3 - ^{31}P NMR spectra of LB and DLB and quantification of OH groups.

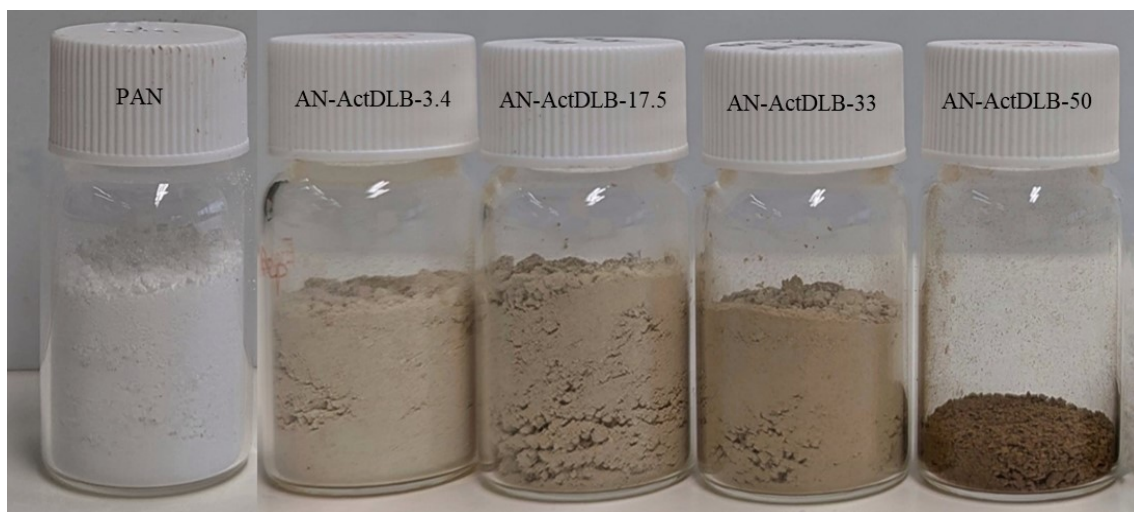


Figure SI.4- PAN and poly(AN-DLB) copolymers.

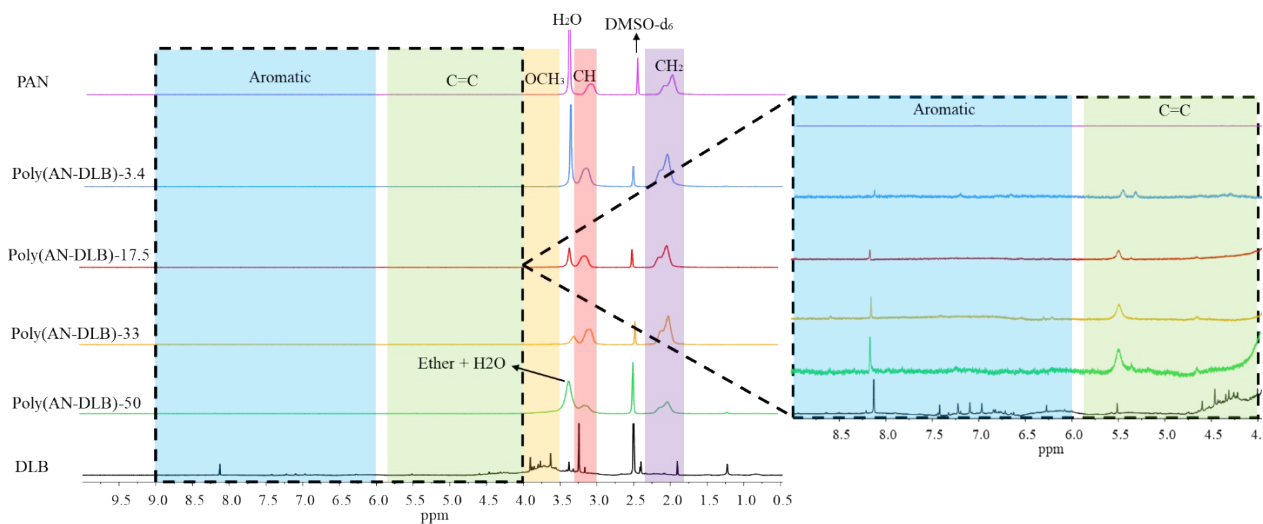


Figure SI.5 – ^1H NMR spectra of spectra of PAN, copolymers, and DLB.

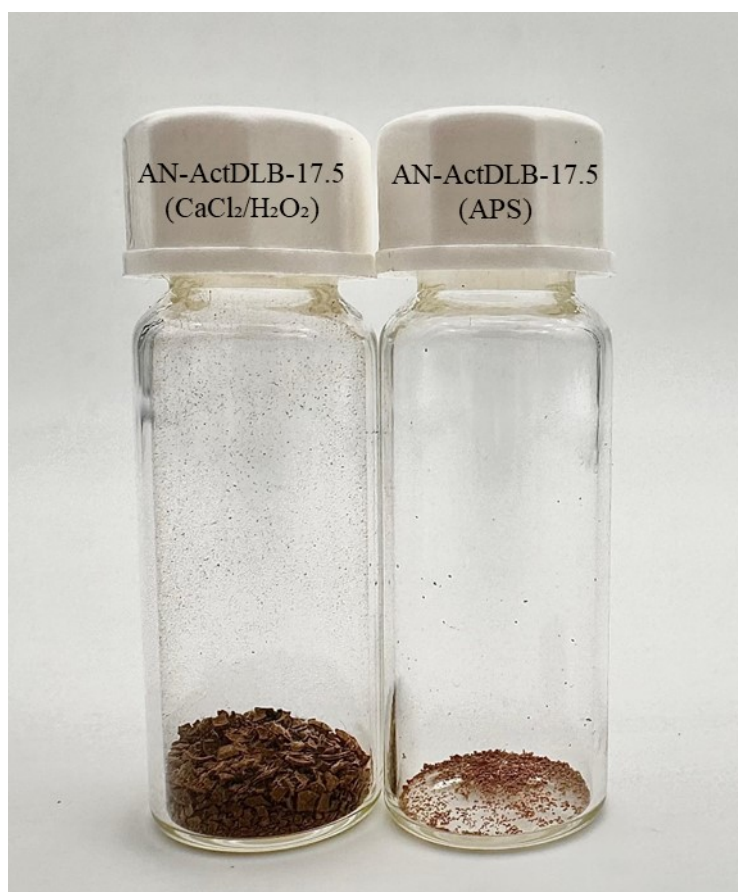


Figure SI.6 – Poly(AN-DLB)-17.5(APS) and poly(AN-DLB)-17.5($\text{CaCl}_2/\text{H}_2\text{O}_2$) copolymers.

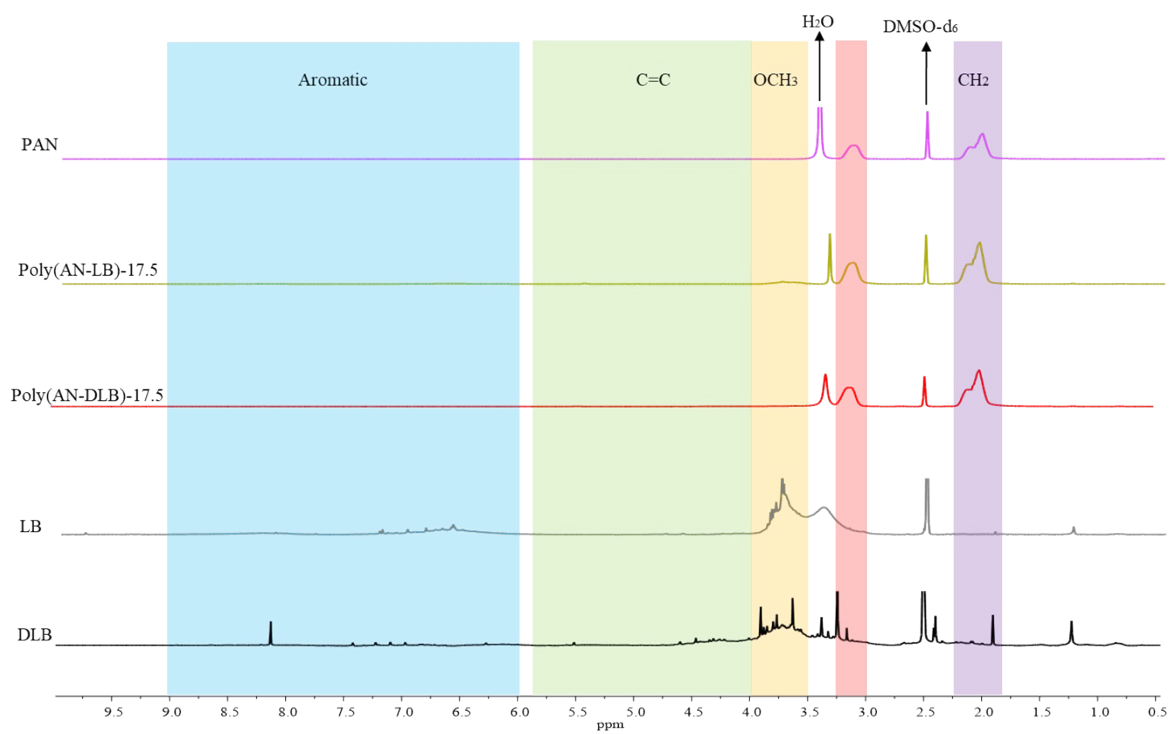


Figure SI.7- ¹H NMR of PAN, poly(AN-DLB)-17.5, poly(AN-DLB)-17.5, and DLB and quantification of functional groups.