IN-DEPTH LOOK INTO NATIVE LIGNIN SOLUBILITY AND SOLVATION

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Lignin is one of the principal organic polymers found in biomass, consisting of cross-linked phenolic monomers [1]. To date, lignin has been mostly considered as a by-product of papermaking and has been mainly used for energy purposes in paper mills. Recent environmental concerns have attracted profound interest in searching for alternatives for waste materials. Although lignin is chemically valuable, valorisation remains challenging [2]. Moreover, dissolution lignin is difficult due to the high variability of molecule mass of the polymer fragments.

Understanding solubility of complex molecules is predicated on understanding their solvation. Recent investigations into computer simulations of lignin solvation have laid a foundation for future research by generating useful tools for compiling lignin polymer topologies [3]. Building on the available research, our group has measured experimental solubilities in various solvent mixtures of a specific native lignin and managed to fractionate lignin polymer fragments by molecule mass. Additionally, we employed molecular dynamics simulations of specific lignin polymer fragments in same solvent mixtures to give a more in-depth look into the solvation and solubility of native lignin.

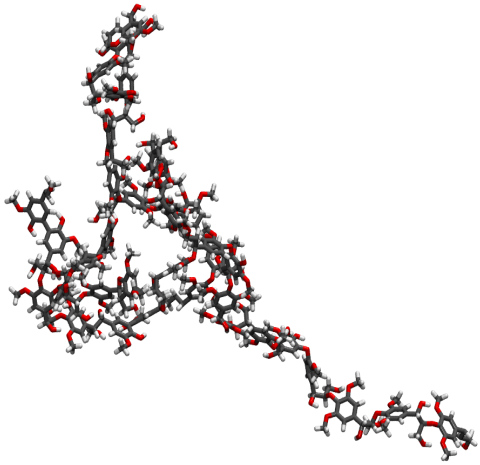

Fig 1. Visual representation of specific lignin simulated in the presented work.

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