Lignin Data Bank: A Key to Clarifying Aromatic Structure–Performance Relationships

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Lignin, a subject of extensive study in academies and industries, is known for its natural abundance, biodegradability, and potential to be transformed into biochemicals and biomaterials. However, the original biomass and extraction treatments, such as kraft pulping and the organosolv process, significantly influence its chemical structure, leading to variations in reactivity. Unfortunately, many scientific publications fail to provide comprehensive lignin property descriptions, which hampers experiment reproducibility and literature comparison. This, in turn, hinders fundamental studies and scientific advancements. This editorial aims to address this issue by advocating for including lignin characteristics in scientific papers when possible.

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Lignin Nomenclature: Limitations and Considerations

Lignin is a highly branched hetero-biopolymer composed of monolignols, phenyl propane units, linked by ether and carbon-carbon bonds. Lignin is the most abundant renewable source of aromatics on Earth, and it is present in woody and herbaceous biomass bonded with polysaccharides (cellulose and hemicellulose). This biopolymer (lignin) has attracted significant attention from academic and industrial research centers because it can be transformed into biochemicals and biomaterials such as aromatics platform chemicals, biodiesel, adhesives, binders and biocomposites. Moreover, its valorization is not just a scientific pursuit but a crucial step towards developing the circular economy. At the industrial level, lignin is a secondary stream of pulp and paper mills, making its valorization a significant economic and environmental opportunity. Therefore, this aromatic biopolymer is typically available at low prices. However, lignin shows a complex polymeric network composed of covalent intermolecular and intramolecular bonds, which is affected by the original biomass (*i.e.* softwood, hardwood, and herbaceous plants) and extraction processes. Several extraction processes were developed over the years, such as kraft pulping, sulfite pulping, soda pulping, organosolv process, ionoSolv process, steam explosion and acid hydrolysis, which operate in different process conditions in terms of solvents, chemicals, pressure temperature, and time. Moreover, several variants were developed inside the same class of extraction processes. Consequently, the chemical structure of lignin available on the market is not the same.

This editorial wants to point out a problem related to the abovementioned aspect: the limited reproducibility of the experiments described in the literature and the difficulties in comparing the results from different publications. Sometimes, the type of lignin studied is not entirely represented in scientific manuscripts. It is possible to read that "a lignin" was used, the original biomass is not reported, or the extraction process is not fully described. These omissions are several times reasonable considering the possible confidentiality agreements signed with the suppliers or the fact that the scientist is not a lignin expert and is using this biopolymer as "a part" of his research, for example, in the use of lignin as a carbon source for electronics. Despite the reasonability, the lack of information affects the comparison between scientific publications and the reproducibility of the experiments. Consequently, fundamental research for understanding the chemical properties of lignin and correlating it with its performance and applications is strongly reduced and limited.

This editorial does not pretend to be a guideline for writing lignin-related scientific articles but exposes the problem of experiment reproducibility and literature comparison in this research field and tries to suggest possible approaches to support fundamental research advances and progress. A second scope is to provide an overview of the main characteristics of interest of the lignin for the non-lignin experts using this biopolymer for their experiments.

Below, the main characteristics of lignin that could be reported in a scientific publication to help the readers reproduce the experiments are described and discussed.

Lignin Characteristics

Supplier, biomass, and extraction process: This information is important for identifying the lignin for the above reasons. Moreover, the kraft and sulfite pulping processes affect the lignin by adding sulfur to its chemical structure, influencing several properties such as water solubility. These data are generally available in scientific articles where the lignin is extracted and valorized by the manuscript authors. However, this information is not always written when the lignin is obtained by a chemical supplier or producer, such as a paper mill. For example, if the company has a confidential agreement with the authors, it could allow publication without specifying the type of lignin. Due to the high interest in lignin, it is understandable not to include the supplier when necessary. At the same time, reporting the type of biomass (softwood, hardwood, and grass) and the class of extraction process (*i.e.* kraft, organosolv…) would allow the scientist to determine if a type of lignin is more suitable or not for specific applications, for example as a coating agent for construction or electronics, without going into details.

Chemical structure: Characterizing lignin's chemical structure is a key descriptor for determining its properties and reactivity. For example, the content of hydroxyl groups influences the possible modification and functionalisation reactions. The main instruments used are NMR and GC-MS. In these cases, standard protocols for the analysis were developed, for example, the derivatization procedure for the lignin analysis using quantitative 31P-NMR to quantify hydroxyl and carboxylic functional groups. Therefore, reporting the lignin characterization using one of these analyses would benefit the fundamental understanding of lignin reactivity. Sometimes, certain lignin cannot be characterized under specific protocols due to their properties, for example, limited solubilization in certain solvents such as chloroform and dimethyl sulfoxide (DMSO). In this case, reporting this limitation in the manuscript would be beneficial.

Molecular weight (Mw): It is known that the Mw influences the applications of lignin. For example, high Mw lignin fractions are generally studied for flame retardancy applications; instead, low Mw fractions are studied as building blocks for synthesizing renewable polymers. The primary technique used to determine the Mw is the size-exclusion chromatography (SEC). However, the different solubility of lignins in the standard solvents (tetrahydrofuran, DMSO, and aqueous solutions), the type of standard used and the various chromatographic columns available in the market do not allow the development of standard protocols. Therefore, describing the procedure used to determine the Mw in scientific papers becomes critical.

Purity and contaminants: Apart from the presence of sulfur described above, lignin purity is an important parameter because residual organic matter, such as polysaccharides and inorganic compounds (ashes), influences the properties and possible applications. For example, a high cellulose content reduces the lignin solubility in DMSO. Also, the presence of ashes can exclude using target lignin for pharmaceutical applications. For these reasons, reporting the lignin purity with a general description of the type of contaminants, qualitatively or quantitatively, would help the quality of the manuscript and the fundamental studies of the lignin.

In conclusion, in our opinion, scientists interested in working on lignin should be aware that the description of the type of lignin studied is a crucial aspect to help the fundamental chemical understanding and scientific development.