

Determination of hydroxyl groups in biorefinery feeds via quantitative ^{31}P NMR spectroscopy

Background

- Hydroxyl groups are among critical functionalities that affect the physical/chemical properties and overall reactivity of lignin, playing an important role in lignin valorization and biorefinery process.
- ^{31}P NMR spectroscopy has its unique characterization capability and broad potential applicability for analysis of hydroxyl groups.

Approach

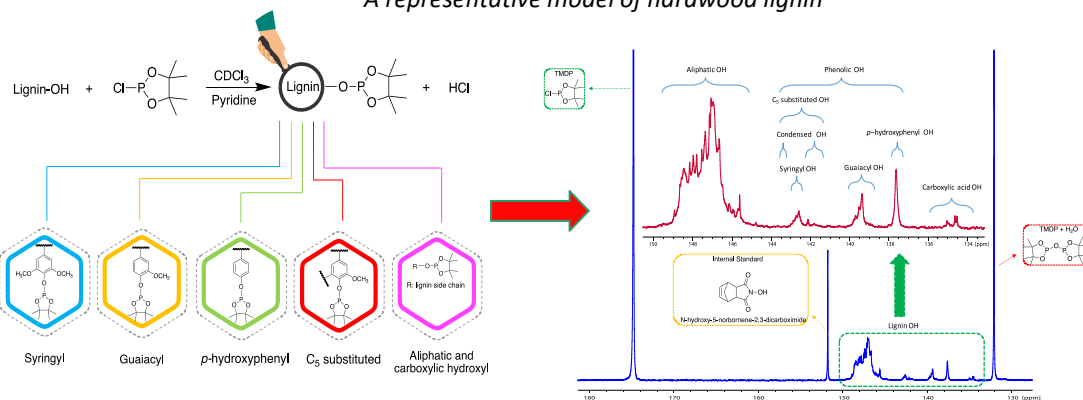
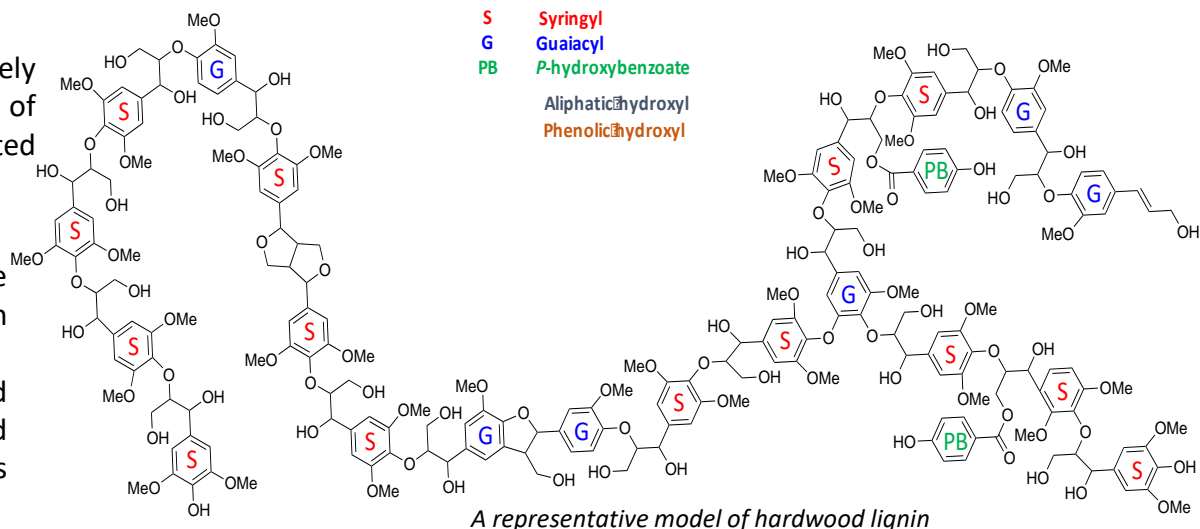
- A standardized ^{31}P NMR procedure to precisely measure the content of different types of hydroxyl groups in bio-aromatics and related compounds.

Outcomes

- The ^{31}P NMR technique provides complete quantitative information of hydroxyl groups in lignin, pyrolysis bio-oil, or tannin.
- Aliphatic hydroxyls (-OH), carboxylic -OH, and various types of phenolic -OH groups attached to syringyl, guaiacyl, and p-hydroxyphenyl units are readily measured.
- ^{31}P NMR offers unique advantages in measuring hydroxyl groups in a single spectrum with great signal resolution, small amounts of sample requirement, and in a short experimental time.

Significance

- A well-defined protocol was introduced to help maintain the accuracy and uniform application of this valuable methodology as widely used by both academia and industry.
- This method can improve our understanding of lignin conversion



Scheme of lignin derivatization and a quantitative ^{31}P NMR spectrum of a hardwood poplar lignin.

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