# Phenolic Compounds: Production, Reaction Scheme, and Applications.

Group: 24

Members:

Shivam Kalambe 210107079

Shivaraj R Kolli 210107080

Siddhant Srivastava 210107081

# **Introduction to Phenolic Compounds:**

A broad class of chemical molecules with one or more phenol rings is known as phenolic compounds. They are found in large quantities in nature and are vital to many different biological processes. Because of their antioxidant qualities, these chemicals are useful in the food, pharmaceutical, and materials science industries. Lignin, a naturally occurring amorphous polymer obtained from lignocellulosic biomass, is one prominent phenolic chemical.

## Phenolic Compounds: Nature's Versatile Molecules:

Phenolic compounds are plentiful in nature and have a diverse spectrum of characteristics, making them adaptable and useful in a variety of applications. From basic compounds like phenol to intricate polymers like lignin, their structures can differ greatly. These substances are identified by the presence of one or more hydroxyl groups bonded to their aromatic rings.

# **Lignin: A Significant Component of Biomass:**

Lignin makes up between 15–35% of the weight of lignocellulosic biomass, making it a significant component. It is an amorphous polymer with three dimensions that is made up of derivatives and methoxylates of phenylpropane units. Because lignin is abundant in biomass sources, it has considerable potential as a renewable resource.

#### **Utilization of Lignin in Bio-Renovation Materials:**

Lignin is a naturally occurring amorphous polymer that has great promise for use as a building block in the creation of biorenovation materials. Lignin is produced in significant quantities each year by the pulp and paper industry, and the construction of biorefineries is anticipated to significantly boost this output. A sizable amount of the total energy in lignocellulosic biomass is provided by lignin, cellulose, and hemicellulose.

# 1. Production of Lignin:

A key component of lignocellulosic biomass, lignin is extracted from plant materials like wood using a variety of industrial techniques. In order to produce lignin, extraction techniques are used to separate the protein from the other main biomass components, cellulose and hemicellulose. The Kraft process, which includes the following phases, is one often employed technique in the pulp and paper industry:

- 1. Pulping: Under high temperatures and pressures, a combination of sodium hydroxide (NaOH) and sodium sulphide (Na<sub>2</sub>S) is used to pulp the wood chips or biomass feedstock. The lignocellulosic structure is broken down during this process, dissolving the lignin into a substance called "black liquor."
- Recovery: The pulp is recovered from the black liquor, which contains dissolved lignin and other byproducts. Recovering the lignin from the black liquor is the next step.
- 3. Precipitation: Sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) is used to acidify the black liquor, causing lignin to precipitate out of the solution as lignin salts.

# Lignin salts (from black liquor) + Sulfuric acid → Precipitated lignin + Sodium sulphate

(Na+)(Lignin) + H<sub>2</sub>SO<sub>4</sub> → Precipitated lignin + Na<sub>2</sub>SO<sub>4</sub>

- 1. Filtration: The precipitated lignin is then separated from the solution using filtration methods.
- 2. Washing: The separated lignin is washed to remove impurities and residual chemicals.
- 3. Drying: The washed lignin is dried to obtain the final product, which is lignin in solid form.

Precipitated Lignin → Washed Lignin

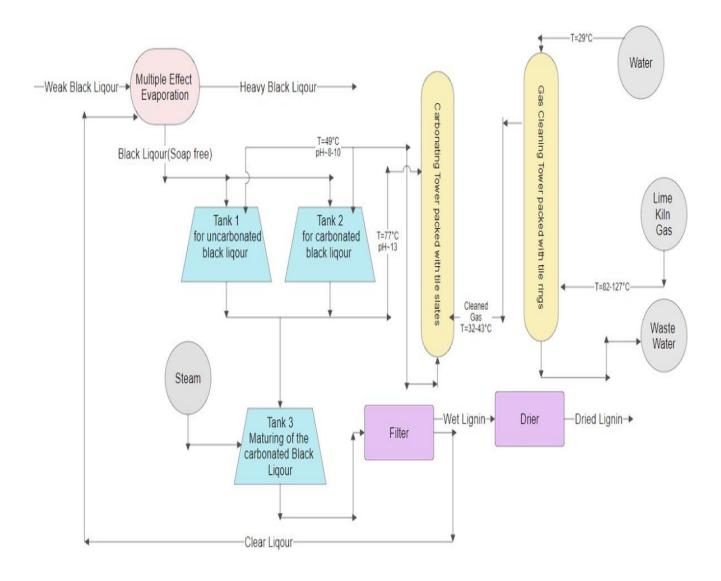
Washed Lignin → Dried Lignin

Lignin is produced as a result of this process, and it can be further processed and altered for a variety of industrial uses. Due to its primary composition of phenylpropane units and derivatives, lignin's chemical structure allows for potential alteration through chemical reactions. The addition of functional groups to the lignin molecule via the reaction with epichlorohydrin is a popular technique for modifying lignin.

Lignin + Epichlorohydrin ( $C_3H_5ClO$ )  $\rightarrow$  Modified lignin with functional groups

The production of carbon fibers, phenolic chemicals, oxidised products,

multifunctional hydrocarbons, and other materials can then be accomplished using this modified lignin. Through these extraction and modification methods, lignin is produced, demonstrating its potential as a renewable and adaptable resource for a range of sectors and assisting in the creation of sustainable materials and goods.



Overall process-flow diagram

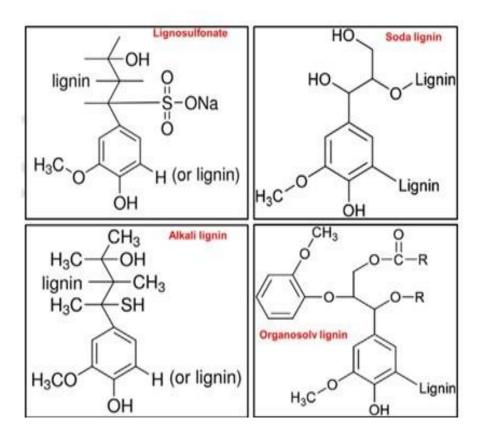
# 2. Lignin Isolation Process:

Several isolation approaches document the process of separating lignin from other polymers containing biomass. More than 90% of industrial lignin is produced via sulphate and sulphite procedures, which are the major isolation methods. During these procedures, kraft lignin and lignosulfonates are created as byproducts of the processing of wood. Under highly alkaline conditions, kraft lignin is isolated from the other ingredients by a sulphate process that breaks the lignin into smaller chains and makes it soluble in water and alkaline solutions. Lignin is made of sulphur compounds, such as sodium sulphide, which have hydrophobic aliphatic thiol groups. Lignosulfonate is produced by the same sulfite pulping method as Kraft lignin. Nevertheless, an acidic solution is used in place of the alkaline medium.

Although it is sulfonate-like (SO<sub>3</sub>-), the LS is sulphide-like.

Additional techniques are developed to separate organosolv lignin, soda 160 lignin, and ionic liquid lignin in pilot plants and lab settings. This is produced using liquid salts (ionic fluids), heavy alkaline conditions (soda lignin), and acidic or alcoholic solutions (organosolv lignin). The process of pulping non-wood items yields lignins. For example, organosolv and soda lignins are thought to be the purest lignins due to their low impurity levels and sulphur-free nature, making them the most natural of these lignin-structures. While organosolv lignin is being extensively researched to expand its application, neither soda lignin nor organosolv lignin have proven to be effective enough to be employed on a commercial basis. In terms of their uses, sulphur-free lignins and solid lines fold down to make LS the most researched lignin. For energy storage applications, these lignin types are more intriguing than others with LS antiflocculant qualities. Amphiphilic compounds are lingo sulfonates, which have both hydrophilic and hydrophobic components and a high water solubility.

For instance, in pluma-acid batteries, the hydrophilic SO<sub>3</sub>-anions are absorbed on the surface of the plum particles, increasing the repulsion potential and inhibiting particle sintering or coalescence.

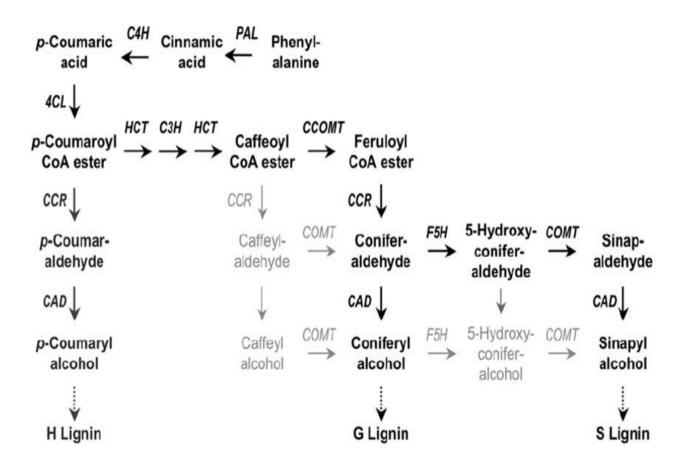


[Figure 1] The simplified chemical structure of sulfur-containing and sulfur-free lignin, Organosolv, and soda lignin

## 3. Reaction Scheme of Lignin:

Lignin biosynthesis and polymerization involve complex reactions that lead to the formation of the lignin polymer from monolignol precursors. The reaction scheme includes several key steps:

- Monolignol Biosynthesis: Monolignols are the building blocks of lignin and are synthesised from the amino acid phenylalanine. The biosynthesis of monolignols involves a series of enzymatic reactions that convert phenylalanine into the three primary monolignol precursors:
  - Coniferyl alcohol
  - Sinapyl alcohol
  - Coumaryl alcohol



[Figure 2]

- Lignin Polymerization: The monolignols undergo oxidative coupling reactions catalysed by enzymes such as peroxidases and laccases. These reactions result in the formation of lignin polymers through the creation of carbon-carbon and carbon-oxygen bonds. The polymerization process involves the formation of various linkages, including:
  - β-O-4 linkage (most common)
  - $\beta$ -5,  $\beta$ - $\beta$ , and 5-5 linkage

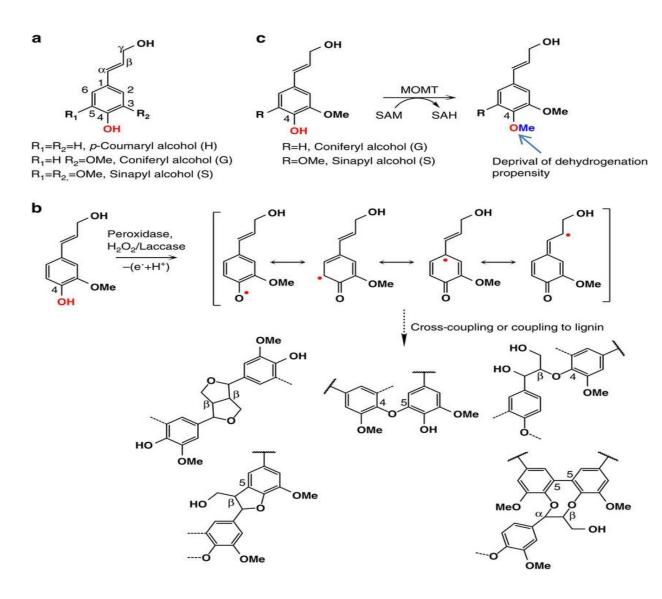


Figure 3

- Lignin Modification Reactions: Lignin is a highly complex polymer that can undergo various chemical modifications, leading to a diverse range of lignin derivatives. These modification reactions include:
  - Esterification: Addition of acetyl or other ester groups.
  - Etherification: Introduction of alkyl groups through reactions with alcohols.
  - Sulfonation: Addition of sulfonate groups, often used in lignin-based products.
  - Oxidation: Introduction of carbonyl or carboxyl groups.

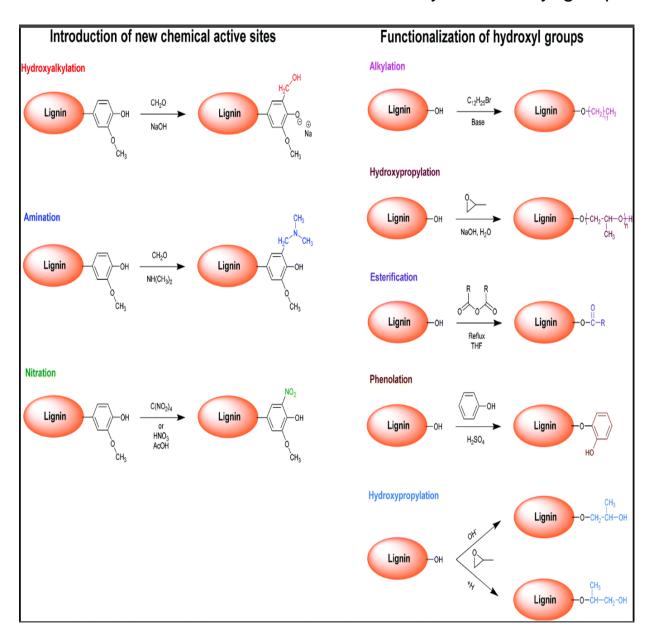


Figure 4

# 4. Applications of Lignin (Phenolic Compound):

Lignin, as a phenolic compound, exhibits a wide range of applications across various industries due to its unique properties:

- Adsorption of Heavy Metal Ions in Water:
  - Lignin has good adsorption characteristics for heavy metal ions in water due to its complicated chemical structure and presence of functional groups such as phenolic and carboxylic groups. Because of these functional groups, lignin is able to bind to and efficiently extract heavy metal ions from aqueous solutions.
- Nanoparticle Synthesis:
  - Lignin's polyphenolic structure and reducing agent properties make it a useful precursor for the creation of nanoparticles. Lignin can be transformed into nanoparticles with precise sizes and shapes using a variety of techniques, including chemical and biological ones. Because of these lignin nanoparticles' special qualities and biocompatibility, they have shown potential in industries like medicine delivery, imaging, and catalysis.
- Supercapacitor Electrodes:
  - Supercapacitor electrodes are energy storage devices with a high power density and quick charge/discharge capabilities. Carbon compounds produced from lignin have a high surface area, porosity, and strong electrical conductivity, which makes them good candidates for use in supercapacitors. The lignin-based electrodes' effective energy storage and release capabilities aid in the creation of long-term energy storage solutions.

# • LLDPE/Lignin Films:

Films with better tensile strength, flexibility, and barrier qualities are created when lignin and linear low-density polyethylene (LLDPE) are blended. These films are used in coatings, agricultural films, and packaging materials. Lignin's incorporation lessens the packaging industry's reliance on polymers derived from fossil fuels, promoting sustainability.

# • Biochemicals Derived from Kraft Lignin:

Through a variety of chemical processes, kraft lignin—a byproduct of the pulp and paper industry—can be further processed to yield valuable biochemicals. These biochemicals are used to make adhesives, resins, tastes, and scents. They also comprise aromatic and phenolic compounds. Kraft lignin's transformation into biochemicals enhances the value of this plentiful supply of lignin and advances the development of biorefinery techniques.

# • Lignin-Based Hydrogels

Lignin-based hydrogels have numerous uses in the environmental and medicinal sciences. Lignin is a good material for creating hydrogels with adjustable properties because of its hydrophilic nature and capacity to create crosslinked networks. These hydrogels made of lignin have applications in water purification, wound dressing, tissue engineering scaffolds, and medication delivery. They offer a biocompatible and eco-friendly substitute for hydrogels that are manufactured.

Application	Lignin modified compound	Reference
Photovoltaic	Nano-ZnO	16
Reusable catalyst	Ru/SiC	20
Cured epoxy resins	DMSO	27
Nanoparticle synthesis	N.A	46
Water flocculation (cationic polyacrylamide)	polyacrylamide (cationic)	85
UV aging resistance	TiO <sub>2</sub>	86
Application in epoxy asphalt	oil	89
Adsorption of heavy metal ions in water	-NH <sub>2</sub> groups	100
Application of renewable energy	N.A	101
Application of super capacitor electrode	mudstone	102
Application of lignin-stabilized silty soil in highway subgrade	stabilized soils	103
Application of lignin-derived polycarboxylic acids	NaOCl solution	104
Electro-fenton process for azo dye removal	Polypyrrole	105
Gaicling the preparation of lignin- colored lignin in micromorphology	lotion	106
Application in lignin-based hydrogels	N.A	107
Application in 3D printing		108
electrodes	MnO <sub>2</sub>	109
Application of nanoparticle modification	Cr(VI)	110
Filter	MgO	111
polyurethane foam for oil adsorption	Polyurethane	112
Application in effluent treatment from the textile industry	N <sub>s</sub> A	113
Hydrogel synthesis based on lignin use for agriculture	alginate	114
Microstructure analysis	N.A	115
High performance sustainable polymeric materials	N.A	116
membrane via air plasma for energy storage	Oxygen, nitrogen with carbon nano fiber	117
Alternative use for petroleum based polymers	N.A	118
Application of lignosulfonates and sulfonatedlignin	Sulfuric acid	119
Antioxidant activity for biomedical application	lactide	120
n paper making	N.A	121
in polyimine thermosets	Levulinic acid	122
High performance super- capacitors	Activated carbon	123

[Table 1] Other Applications And Lignin modified compounds

#### **Conclusion:**

To sum up, lignin, a phenolic molecule, is essential to several sectors of the economy, including materials science, agriculture, and energy. Harvesting biomass, pretreatment, extraction, and purification are steps in its production process. Polymerization, modification processes, and monolignol biosynthesis are all part of the intricate chemical system of lignin. Applications for lignin are numerous and include soil conditioners, carbon materials, polymer additives, biocomposites, and chemical feedstock. By supporting the circular economy and lowering reliance on fossil fuels, its use promotes eco-friendly and sustainable behaviours. Lignin's importance as a valuable phenolic molecule is anticipated to increase with further study and technological developments, providing creative solutions for a more environmentally friendly future.

#### References:

Text:

- 1) Dryden's Outlines Of Chemical Technology
- 2) <a href="https://www.jchemrev.com/article\_160707.html">https://www.jchemrev.com/article\_160707.html</a>

#### Figure 1:

https://www.jchemrev.com/article\_160707.html

#### Figure 2:

https://www.researchgate.net/figure/Simplified-scheme-for-monolignol-synthesis-The-main-pathway-in-dicotyledonous-plants-is\_fig1\_23792168

#### Figure 3:

https://www.researchgate.net/figure/Illustration-of-MOMT4-medidated-depression-on-lignin-polymerization-a-The-conventional\_fig1\_304568063

#### Figure 4:

https://pubs.rsc.org/image/article/2016/GC/c5gc02616d/c5gc02616d-f3\_hi-res.gif

#### Table 1:

https://www.jchemrev.com/article\_160707.html