

# Passive membrane transport is sufficient for many lignin-related compounds

## Background

- The mechanism of membrane transport of lignin-related compounds in both plants and microbes remains mostly unknown
- Understanding the transport of lignin-related compounds is important for both lignin biosynthesis and microbial conversion of lignin

## Approach

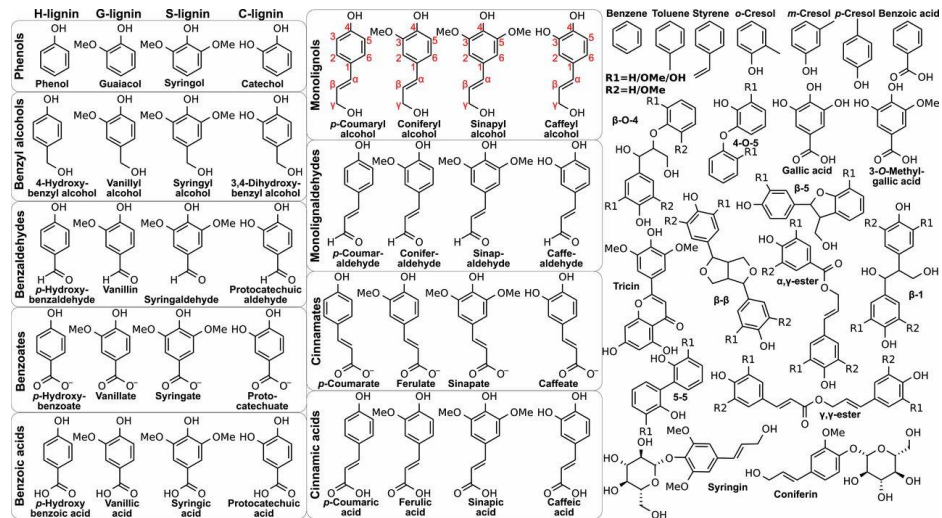
- Free energy simulations using biased molecular dynamics techniques were employed with ~70 lignin-related compounds that vary in chemistry and size to determine partitioning and diffusion into bilayer membranes.

## Outcome

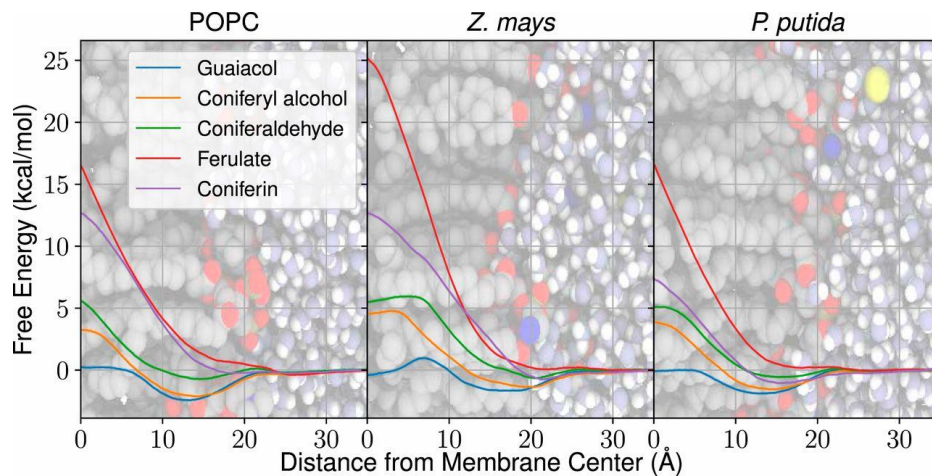
- Most compounds, including the monolignols, dimers, and flavonoids (e.g., triclin), likely diffuse passively across membranes
- Carboxylates and aromatic glucosides likely will require transporters

## Significance

- For lignin biosynthesis, it is likely that monolignol synthesis rates control the transport rates into the forming cell wall (to control lignin chemistry)
- For microbial lignin conversion, transporters for key aromatic acids (and aromatic glucosides) likely remain to be discovered and are critical to increase lignin bioutilization
- This work was jointly supported by CBI, GLBRC, NREL and BETO.



Lignin-related compounds, grouped by their chemistry, employed in molecular simulations for studying membrane transport.



Free energy profiles of selected lignin-related compounds as a function of distance from the membrane center across a model membrane (left), a model plant membrane (middle), and a model *P. putida* membrane (right).