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Thermodynamic Analysis of Phenylpropanoid Pathway in *Arabidopsis Thanliana*

Patrick J Ioerger, Rohit Jaini, and Dr. John A. Morgan
Department of Chemical Engineering, Purdue University

ABSTRACT

Biofuels represent a renewable alternative to traditional fossil fuels. As dependence on fossil fuels rise so does the importance of improving the production of alternative fuels. Lignin poses one obstacle in the development of such alternative fuels. Its presence strengthens cell walls and hinders degradation of polysaccharides into monosaccharides, increasing cost and time while decreasing efficiency of the process. Lignin is composed of three monolignols, each of which is produced through the Phenylpropanoid pathway; a series of chemical reactions. This work aims to determine which reactions in the pathway are least thermodynamically favorable and thus most limiting. From metabolic mapping techniques on the Phenylpropanoid pathway in *Arabidopsis Thanliana* and thermodynamic data on the Gibbs free energy of formation for the biochemical compounds, the change in Gibbs free energy of the reaction at intracellular conditions is calculated. For compounds which data is unavailable, Group Contribution methods are used to determine the Gibbs free energy of formation. Reactions involving Cinnamoyl-CoA reductase, shikimate O-hydroxycinnamoyltransferase, and 4-coumarate-CoA ligase yielded positive Gibbs free energy values in the pathway. Since reactions involving these enzymes have positive Gibbs free energy values, these reactions require the greatest concentration of enzyme in order to facilitate production of the three monolignols. Knocking out these enzymes should result in a decrease in monolignol and lignin production.

KEYWORDS

Thermodynamic, Arabidopsis, Group Contribution, Phenylpropanoid, Phenylalanine, Limiting, Pathway