Biological Routes for Synthesizing the Industrial Platform Chemical, Propylene, from Deconstructed Lignin Waste and Captured Carbon Dioxide Produced during Lignin Valorization into Bio-oil

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Each year the chemical industry invests more energy than anywhere else to make ethylene and propylene chemicals for the manufacturing of plastics, textiles, solvents, building materials, and detergents that enable modern society. This energy burden is due to the large amounts of heat required to transform petroleum hydrocarbons into ethylene and propylene and subsequently purify them. Currently these demands are met through the combustion of fossil fuels, leading to significant greenhouse gas emissions, and thereby necessitating the development of alternate processes with low heat and energy consumption. Lignin, a major component of plant biomass is abundantly available but difficult to utilize to produce platform chemicals. Lignin can be transformed by modest heating through a process called Hydrothermal Liquefaction (HTL) to make renewable transportation biofuels. However, about 15% of the processed lignin ends up as aromatic compounds and 15% as gaseous carbon dioxide that are environmentally harmful waste byproducts of the nascent biofuel industry. In recent years, bacteria like *Rhodospeudomonas palustris* have been discovered that can utilize lignin monomers for growth and thus serve as promising chassis for upscaling lignin monomers and CO_2. In addition, *R. palustris* and related bacteria possess newly discovered enzymes distantly related to nitrogenase that can synthesize essential platform chemicals like ethylene, propylene, propanol and propylamine from ubiquitous organic sulfur compounds. Most notably, *R. palustris* performs these biological transformations anaerobically, allowing safe hydrocarbon production by avoiding oxygen combustion hazards. This project will design and implement in *R. palustris* biosynthetic pathways that convert lignin aromatic acids and CO_2 into volatile organic sulfur compounds that serve as substrates to produce propylene, propanol, and propylamine. Next bioinformatics and gene synthesis technologies will enable mining and screening for protein homologs in the engineered pathways that are highly active and increase product yields. Pathway design for optimal conversion of lignin aromatic acids and CO_2 into hydrocarbons will be guided by advanced physics-based thermo-kinetic modeling of *R. palustris* metabolism, which will provide predictive insights on needed enzyme activities, transcriptional regulation strategies, and elimination of pathway bottlenecks. Synergistically, this project will quantify and understand the mechanism and product distribution of the lignin HTL process to generate both bio-oil for transportation and aromatic acids and CO_2 for *R. palustris* to upscale into hydrocarbon platform chemicals. To address CO_2 capture from lignin HTL and delivery challenges to *R. palustris,* this project will develop and understand the fundamental physical principles of new carbon dioxide removal (CDR) technologies involving CO_2 absorbent-coated ceramic honeycomb microchannels and water-based CO_2 desorption in a manner that minimizes energy requirements. Ultimately, this project will generate new technologies that will 1) maximize plant biomass utilization for bio-oil production by the lignin HTL process, 2) minimize thermal energy inputs to produce ethylene and propylene platform chemicals for the growing bioindustry, and 3) contribute to next-generation CDR technologies for capture and biological conversion of CO_2 into biofuels and biochemicals.

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