Plant-Microbe Interfaces: Characterizing the perception of lipochitooligosaccharides signaling in fungi

Tomás Allen Rush[1*] (rushta@ornl.gov), Erica Teixeira Prates.[1] Omar N. Demerdash,[1] Chris Ellis,[1] Manesh Shah,[1] Joanna Tannous,[1] Daniel Jacobson,[1] Jessy Labbé,[1] and **Mitchel J. Doktycz[1]**

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

http://pmiweb.ornl.gov/

Project Goals: The goal of the PMI SFA is to characterize and interpret the physical, molecular, and chemical interfaces between plants and microbes and determine their functional roles in biological and environmental systems. *Populus* and its associated microbial community serve as the experimental system for understanding the dynamic exchange of energy, information, and materials across this interface and its expression as functional properties at diverse spatial and temporal scales. To achieve this goal, we focus on 1) defining the bidirectional progression of molecular and cellular events involved in selecting and maintaining specific, mutualistic *Populus*-microbe interfaces, 2) defining the chemical environment and molecular signals that influence community structure and function, and 3) understanding the dynamic relationship and extrinsic stressors that shape microbiome composition and affect host performance.

Lipochitooligosaccharides (LCOs) are signaling molecules with various moieties that were thought to be uniquely produced by symbiont microbes (rhizobia bacteria and mycorrhizal fungi) to communicate and colonize their hosts (Liang et al., 2014). A paradigm shift in this understanding was recently initiated with the discovery that LCOs are produced across the whole Fungi kingdom and are responsible for several changes in fungal growth patterns (Rush et al., 2020). However, the alternate roles of LCOs and how fungi perceive them remain largely unknown. Focusing on the *Populus* ectomycorrhizal associate *Laccaria bicolor* and the soilborne and opportunistic human fungal pathogen, *Aspergillus fumigatus,* as pilot fungal systems, we use a known mechanism of LCO recognition in plants to identify similarities in LysM domain receptors. We apply a computational workflow of extensive molecular dynamics simulations and machine-learning methods for binding affinity prediction of LysM-LCO complexes to investigate the molecular basis of the specificity towards different LCO molecules. Candidate binding sites were identified based on common structural features assembled for the optimum binding of the hydrophobic acyl chain and the carbohydrate moieties (and substituents) that constitute the LCOs. In addition, we provide a bioinformatic network map to highlight the commonality of LysM receptors across multiple kingdoms. The selected LysM candidates are being validated by genetic editing of mutants deficient in those LysM receptors. This pioneering work contributes to the understanding of the cross-talk and their signals between microbes, their host, and how this structures communities.

References/Publications

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