SUMMARY
Identifying Performance Advantaged Biobased Chemicals Utilizing Bioprivileged Molecules

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The project will integrate the chemistry of biomass conversion, reaction network analysis and data science to create a systematic process for identifying novel bioproducts that create enhanced performance properties in their end use application. To develop the identification process, the initial performance end use applications targeted will be ***organic corrosion inhibitors*** **and** ***flame retardant polymers***. Previous identification of bioproducts with enhanced performance properties has been largely serendipitous with no defining systematic process that can be replicated to other bioproducts for the same application or alternative applications. Given the enormous number of molecules that can be generated in biological systems, it has been difficult to conceptualize such a systematic process. Fortunately, a great deal of performance screening has been performed on plant-derived natural products, which has led to isolated demonstration of positive performance attributes for specific "identified molecules" in the literature. We will create a computational framework to leverage this information to identify promising novel bioproducts for the target applications. This computational framework will be developed in such a manner as to enable a systematic process that can also be extended to other end use applications.

The process to be developed will aggregate natural product performance screening results through a data mining approach. Using machine learning tools, identified natural products will be organized by structure and function and then a reaction network generation algorithm will be used to find potential biochemical/chemical pathways leading to the product. From the reaction network generation computational platform, key intermediate molecules (i.e., bioprivileged molecules) common across multiple pathways will be established. These bioprivileged molecules will then be used as the starting compounds to synthesize the literature identified molecular structures. Importantly, the bioprivileged molecules will not only be leveraged for the synthesis of the "identified molecule" but also to provide the starting compound for synthesizing a library of compounds with similar chemical structure to that of the "identified molecule." The molecular libraries will then be subjected to corrosion inhibition or polymer flame retardancy testing to find performance advantaged products.

The project will advance two technological areas; a) novel molecules with improved performance in the specific end use application of organic corrosion inhibitors and flame retardant polymers and b) development of a systematic process for identifying biomass-derived molecules with improved performance in end use applications. The two end use applications, while technologically important in their own right, are ideal test cases for aiding the construction of a broader systematic process for novel molecule identification. Project deliverables will include ≥ 5 identified novel bioproducts with enhanced performance properties ***and*** an identification process that can be extended to bioproducts in additional application areas.