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A Multi-Scale, Multi-Disciplinary Approach for Assessing the Technological, Economic, and Environmental Performance of Bio-Based Chemicals

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In recent years, bio-based chemicals have gained interest as a renewable alternative to petrochemicals. However, there is a significant need to assess the technological, biological, economic, and environmental feasibility of bio-based chemicals, particularly during the early research phase. Recently, the Multi-scale framework for Sustainable Industrial Chemicals (MuSIC) was introduced to address this issue by integrating modeling approaches at different scales ranging from the cellular to the ecological scales. This framework can be further extended by incorporating modeling of the petrochemical value chain and the de novo prediction of metabolic pathways by using generic biochemical reaction operators in conjunction with genome-scale models.