Computational Methods to Assess the Production Potential of Bio-Based Chemicals - DTU Orbit (30/10/2018)

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Elevated costs and long implementation times of bio-based processes for producing chemicals represent a bottleneck for moving to a bio-based economy. A prospective analysis able to elucidate economically and technically feasible product targets at early research phases is mandatory. Computational tools can be implemented to explore the biological and technical spectrum of feasibility, while constraining the operational space for desired chemicals. In this chapter, two different computational tools for assessing potential for bio-based production of chemicals from different perspectives are described in detail. The first tool is GEM-Path: an algorithm to compute all structurally possible pathways from one target molecule to the host metabolome. The second tool is a framework for Modeling Sustainable Industrial Chemicals production (MuSIC), which integrates modeling approaches for cellular metabolism, bioreactor design, upstream/downstream processes, and economic impact assessment. Integrating GEM-Path and MuSIC will play a vital role in supporting early phases of research efforts and guide the policy makers with decisions, as we progress toward planning a sustainable chemical industry.

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