הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

Monday, November 30th, 2026 at 13:30
Room 6

Toward Automated Generation of Predictive Biochemical Kinetic Models: Fatty Acid Synthesis as a Case Study

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MSc Seminar

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Researchers across biology, chemistry and medicine study biochemical systems, networks of interacting biological components, for a range of applications, from uncovering new mechanisms to harnessing cells for producing valuable chemicals and designing new therapies and drug delivery methods. Kinetic models in this domain use mathematical frameworks to describe how concentrations and rates change over time, letting us explore a system before testing it in the lab: which step limits production, which products to expect or what happens if one component is changed? Yet, in many cases, these models have far more parameters than data to determine them, so fitting them to the very data they should explain admits many sets of reactions and parameters that match well but are physically wrong, and the models struggle to predict new, untested conditions.

In this seminar, I will present BEES, a framework that automatically turns starting species, enzymes and reaction conditions into a full kinetic mechanism in a single loop. Adapting the flux-based algorithm from reaction mechanism generation, BEES discovers reactions from curated biochemical knowledge and adds species only when their rates cross a user-set threshold, so the model grows only where needed. Missing kinetic and thermodynamic parameters are estimated with machine learning and classical statistical optimization, while built-in biochemical rules keep the predictions consistent with general and system-specific biochemical knowledge that the estimators alone cannot supply.

As a case study, BEES reconstructed fatty acid synthesis, a pathway central to biomanufacturing and diseases such as cancer and obesity. Built mostly from predicted constants, the model reproduced the shape and order of magnitude of production measured *in vitro* while sensitivity analysis showed that control is concentrated in the early steps, where building blocks are supplied and the fatty acid chain begins to grow, and deviations at later times point to missing feedback inhibition. The seminar will also discuss where the method still falls short and the insights it offers. This work highlights the potential of predictive kinetic modeling to accelerate cell factory design and suggests a practical framework for exploring biochemical systems.