

CBC SEMINAR ANNOUNCEMENT



Assistant Prof Connor W. Coley
Massachusetts Institute of Technology, Cambridge
AI-Assisted Chemical Synthesis

Drug discovery is an enormously complex multi-objective optimization problem. Machine learning and artificial intelligence techniques are increasingly used in the design of new compounds, yet the synthesis of those compounds continues to be a predominantly manual task. This talk will describe ongoing efforts to streamline the design, validation, and implementation of small molecule synthetic routes through a computational understanding of synthetic chemistry learned from the chemical literature. We have developed an open source software suite, ASKCOS, that is capable of proposing retrosynthetic routes to new molecules, proposing reaction conditions for each step, and assessing the likelihood of experimental success. A proof-of-concept demonstration shows how these tools, in combination with laboratory automation and robotics, can streamline chemical development.

Biography

Connor W. Coley is an Assistant Professor at MIT in the Department of Chemical Engineering. His work in computer assistance and automation for organic synthesis has included the development of a data-driven synthesis planning program and in silico strategies for predicting the outcomes of organic reactions. His continuing research interests are in how data science, statistical learning, and laboratory automation can be used to streamline discovery in the chemical sciences. Connor has been named one of C&EN's "Talented Twelve" and one of Forbes Magazine's "30 Under 30" for Healthcare. He received his B.S. and Ph.D. in Chemical Engineering from Caltech and MIT, respectively.

Date: 18th September 2020 (Friday)
Time: 09.00 am to 11.00 am
Venue: Zoom Platform
Host: Dr Lu Yunpeng

For Zoom registration:

