



2022-2023 POCC Lecture Series

April 27, 2023, 7:30 PM

Prof. Timothy Newhouse

Yale University

Computationally Augmented Total Synthesis

IN PERSON @:

Carolyn Hoff Lynch Lecture Hall Chemistry Building,
University of Pennsylvania

6:30 Reception in the Nobel Hall

Food and drinks to be provided!

SPECIAL NOTE: POCC POSTER SESSION!

*POCC Graduate Student Poster Session starts at 5 pm
in Nobel Hall, please try to attend and show your support!*

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Abstract: Efficient syntheses of complex small molecules often involve speculative experimental approaches. The central challenge of such plans is that experimental evaluation of high-risk strategies is resource intensive, as it entails iterative attempts at unsuccessful strategies. This presentation describes a complementary strategy that combines creative human-generated synthetic plans with robust computational prediction of synthetic feasibility (computational modeling density functional theory, and machine learning). This work defines how machine learning models can drive complex molecule synthesis.

Bio: Timothy R. Newhouse was born in New Hampshire and received his B.A. in Chemistry from Colby College (2005) in Waterville, ME, where he was mentored by Prof. Dasan M. Thamattoor. After moving to La Jolla, CA, he completed his Ph.D. at The Scripps Research Institute with Prof. Phil S. Baran (2010). During his time at Scripps, he also worked in the laboratories of Prof. Donna G. Blackmond. He then returned to the east coast for postdoctoral studies with Prof. E.J. Corey at Harvard University. He started at Yale University in 2013, and is a Professor in the Chemistry Department and Interdepartmental Neuroscience Program.

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