

OBAVEŠTENJE

**U četvrtak 9. maja 2024. godine u Sali za sednice, Hemijskog fakulteta
sa početkom u 12:00 časova
profesor Timothy R. Newhouse (Yale University) održaće predavanje:**

Computationally Augmented Total Synthesis

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.