



Houk-Jung Organic Colloquium

Combinatorial Explosion: From Atom-Bond Arrangements to Exotic Diseases

Abstract: Chemical synthesis and data science are two fields that operate in synergy. Molecules and the routes to synthesize them are easily represented as graphs while automated chemical synthesis strategies allow more and more synthesis data to be captured, for instance to feed machine learning algorithms. This talk will detail our work in this area focused on a new class of amine-acid cross coupling reactions, and the computer-assisted synthesis of drugs and natural products. We have been exploring the breadth of all reactions that could exist, navigating combinatorial explosions of virtual and plausible reaction methods, routes to complex molecules, and the interconnectedness of reaction conditions, transformations, and biological functions. Our agnostic view of reactions and their mechanisms has recently extended to diseases, with a focus on One Health.

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Thursday, April 25, 2024 | 4:00 PM
Mani L. Bhaumik Collaboratory - YH 4222
Dongwon Yoo Seminar & Conference Hall

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