

Importance of Organic Synthesis: Essential for life sciences, particularly in pharmaceuticals and chemical biology. Quantum Mechanics (QM) Descriptors: Commonly used for predictions, including electrostatic and steric characterizations, but require a deep understanding of mechanisms and can be challenging to generalize. Early Approaches: Models like CAMEO and SOPHIA aimed to define mechanistic reactions but struggled with predicting novel chemistry. Prediction Challenges: Chemists face difficulties in predicting reaction outcomes and retro-synthesis routes due to sensitivity to small changes in reaction conditions.