Artificial Intelligence: The Future for Synthetic Chemistry?

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Rapid development of robotic platforms in drugs and materials design stimulates creation of efficient chemoinformatics tools able to plan and to guide synthesis of target molecules. These tools aim to suggest feasible synthetic roots linking target molecule with the available starting materials, to predict a major product of chemical reaction, its thermodynamic and kinetic characteristics and to propose optimal reaction conditions (solvent, catalyst, temperature, etc) leading to reasonable yield. Most of these tasks could be efficiently realized with the help of the Condensed Graph of Reaction (CGR) approach. CGR allows to represent a chemical reaction as a sole molecular graph (pseudomolecule). In this presentation we consider applications of CGR to large reaction database visualization and analysis, to modeling of reaction rate constants of different types of reactions, to theoretical assessment of tautomeric equilibrium constants and to prediction of optimal reaction conditions for different types of reactions. Particular attention will be paid to the application of the Artificial Intelligence methods to *de novo* design of novel chemical transformations and the *SynPlanner* tool for retrosynthetic analysis.