Learning patterns of chemical reactivity from experimental data

Connor COLEY

Department of Chemical Engineering, Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology, Cambridge, USA

The abundance of chemical reaction data in tabulated databases has enabled new data-driven approaches in reaction informatics. In particular, data-driven programs for Computer-Aided Synthesis Planning have rapidly matured and can now propose plausible synthetic pathways for many druglike compounds. We will discuss cheminformatic and machine learning-based approaches for learning patterns of chemical reactivity to perform the core tasks of synthesis planning: retrosynthesis, reaction condition recommendation, and reaction outcome prediction.