Learning the Art of Chemical Synthesis with Deep Neural Networks and Discipline Scale Data

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Since E. J. Corey first proposed to use a computer to assist in traversing deep synthetic trees in the 1960s, chemists have tried to algorithmically discover the rules of chemistry. My research group recently demonstrated how well modern methods could perform when planning complex retrosynthetic routes. This accomplishment was built on top of two key technologies: firstly, we showed that single step reactions could be quickly predicted using a neural network. Secondly, the other key component was an algorithm known as Monte Carlo Tree Search (MCTS). We have also developed a novel method for reaction prediction and retrosynthesis based on link prediction. This means we are not limited to rules based approaches, so we can effectively discover brand new reactions that have no precedence in the literature.