Enhanced artificial intelligence for retrosynthesis planning

In this PhD project, we will develop innovative enhancements of Monte Carlo tree search (MCTS) algorithm for the problem of retrosynthesis. Retrosynthesis is the process of repeatedly breaking down a 'target' molecule using valid chemical reactions to attain a series of more simple start molecules and several reaction routes which lead to the initial target molecule. The MCTS is an efficient search algorithm, most notably known for its use in Google Deepmind's AlphaGo. The algorithms developed in the project will be implemented in our ai4green electronic lab notebook, which is available as a web-based application: http://ai4green.app and which is the focus of a major ongoing project supported by the Royal Academy of Engineering.

The application of AI to chemistry is a rapidly growing field. Interest in computer-aided synthesis planning has reignited with the advent of more sophisticated algorithms such as MCTS. Chemistry presents an extremely large search space and MCTS can be used to efficiently search this space for optimal chemical routes. There are many ways that one can enhance an MCTS to improve performance in a specified domain. Thus, the AI content will focus on algorithm development, implementation in a user-friendly web-based platform and validation.

The project is a collaboration between the Schools of Chemistry and Computer Science, and will be supervised by Jonathan Hirst and co-supervised by Kristian Spoerer. The two supervisors have been collaborating for over a year, and a substantial amount of preliminary work has been accomplished through a 4th year Computer Science MSci project.