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Big Data and Machine Learning for Reaction Design

Reaction optimisation plays a fundamental role in the drug discovery process; for many this is at the reaction design stage[1]. This optimisation process is often expensive and time consuming, and generally follows one of two approaches, the first being the use of a chemist's intuition (this however relies on the chemist having knowledge of the reaction domain) with the alternative being a purely computational approach (this however has no understanding as to the underlying chemistry)[2]. We present a solution to this by capturing chemical intuition with a machine learning (ML) model trained on literature data to predict reaction outcomes, passing these predictions into the optimisation process to help guide it through its understanding of the chemical space. This capturing of chemical intuition in the reaction optimisation process can lead to experimental savings of up to 50% when trying to find the optimal reaction. With the approaches used not being limited to the reactions considered in this work, and the creation of a predictive model for reaction outcomes based on either in-house or publicly available data, this approach could be utilised to accelerate the optimisation process in general, reducing both the cost and time associated with it.

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