

Reaction pathway prediction using neural sequence-to-sequence model

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Neural sequence-to-sequence (seq2seq) model, which commonly used in neural machine translation field, is implemented to predict the reaction income from the reaction outcome. The structure of the chemical species are expressed in SMILES so that they have the form of sequences and be able to be used as income and outcome of the seq2seq model. Some of researches have implemented the model in the field, but some difficulties have remained. Especially, predicting the reaction in the reverse direction is more complex than doing it in the forward direction. In this study, some modifications have been applied to the existing seq2seq model to overcome the difficulties in the problem such as having multiple outcomes from one income.