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Supervisor Review of the Bachelor Thesis of Stefan Moser

The Bachelor Thesis of Stefan Moser „Generating and Classifying Molecules“ investigates the use of deep neural networks for generation and assessment of small molecules. The basis of this thesis are two publications: „Generating focused molecule libraries for drug discovery with recurrent neural networks.“ (Segler, 2018) and „DeepTox: Toxicity prediction using Deep Learning“ (Mayr, 2016). In this works, compound generation and toxicity prediction were separated from each other.

Mr. Moser has trained a long short-term memory recurrent network (LSTM) on publicly available compounds to obtain a generative model for molecules. In addition, he has obtained a predictive model for toxicity by training a deep multi-layer perceptron on the famous Tox21 data set. In the end, he was able to generate a new compound library using the LSTM model and to remove all predicted toxic compounds from it. The remaining library could be a starting point for drug discovery projects. Mr. Moser has worked relatively independently and needed little input for his practical work.

He was able to extract relevant information either directly from scientific publications or also from conversation with his supervisor. From the methodological point of view, there are a few minor problems or open question, that were not explored sufficiently enough, for example, the adjustment of thresholds towards a desired trade-off between sensitivity and specificity. In his thesis, Mr. Moser showed that he can cite appropriate references, write consistent lines of thoughts, and explain his approach clearly. He demonstrated also his capabilities at re-implementing and adapting algorithms.

We can confidently state that Mr. Moser is worthy of obtaining a Bachelor of Science title, given the work performed in this thesis.


Günter Klambauer