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**Opponent Review “Generating and Classifying Molecules”  
by Stefan Moser**

The thesis is concerned with the topic of training a generative model for molecules on a large public dataset of structures and subsequently predict their toxicity by a machine learning model. This framework could be used as a starting point in a drug discovery pipeline.

The thesis treats a relevant topic and the experimental execution is rigorous.

While the work is interesting and practically well executed, I think that the presentation could be improved. Some statements are rather vague and could be refined. Overall the thesis is not written too clearly and it could be hard to understand the motivations and goals for a reader unfamiliar with the topic.

There are also figures (e.g. 4.2 / 4.4 ) which could probably be omitted. Also I am not sure why the performance analysis of the classification algorithm has been presented in two different sections (3.2 / 4.2).

However, these few minor problems are not able to outweigh the positive aspects of this work. Given the hardships of getting LSTMs to work in practice, the extensive evaluation of the trained classifiers and the methodologically clean procedures I can recommend accepting this thesis.

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