

CHARLES UNIVERSITY

FACULTY OF PHARMACY IN HRADEC KRALOVE

Department: Dpt. of Pharmaceutical Chemistry and Pharmaceutical Analysis

Master's degree program in Pharmacy

Mentor's evaluation of Master's thesis

Student's name: Legae G. B. Kebakuile

Thesis mentor's name: PharmDr. Jan Zitko, Ph.D.

Year of the thesis defense: 2018

Title of the thesis:

Creation and analysis of in-house database of pyrazine derivatives with potential antimicrobial activity

The topic of the thesis was chosen from the list of topic in the department

Working with literature very good.

Language skills very good.

Student invention very good.

The student was working independently with mentor help.

Problems and issues were solved independently with mentor help.

Working in the lab was not available, literature review.

Interpretation of the results correct with small corrections.

Processing of the thesis was correct with mentor corrections.

Graphical processing of the thesis excellent.

I recommend Diploma thesis for the recognition as Rigorous thesis .

Mentor's comments both on the thesis and the student's approach:

Legae Kebakuile is a very enthusiastic student. Originally, he wanted to do experimental work in the lab, but due to time constrains we gave priority to a topic, which was crucially needed to be solved in our lab, that is, creation of an in-house database of our compounds, both published and unpublished. Mr. Kebakuile was working very precisely and with patience in the phase of extracting the data from published articles and other

sources, and managed to create a complete database of more than 600 compounds. My random check on the database revealed only very few errors.

The second part of work was the analysis of distribution of values of calculated descriptors among subsets of the database. Mr. Kebakuile was able to perform these analyses correctly and created very informative graphical representations of the results. Unfortunately, some analyses did not start sooner than two weeks before the submission deadline. Generally, if proper time was dedicated to this phase, the results and outcomes might have been significantly more comprehensive. The lack of time issue is visible also in the introduction part, where the text is not very organized and inaccuracies and errors are present.

To sum up, although the data analyses could/should have been significantly deeper, the main objective of the thesis was fulfilled. We are using the database almost on daily bases as an input for CADD studies.

Evaluation of Master's thesis: very good

Recommendations for the thesis defense: recommended

In Hradec Kralove 9. 9. 2018

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Mentor's signature