

UNIVERZITA KARLOVA
Farmaceutická fakulta v Hradci Králové

Zápis o části státní závěrečné zkoušky
Obhajoba závěrečné práce

Akademický rok: 2017/2018

Jméno a příjmení studenta: Legae Kebakuile
Datum narození: 14.01.1993
Identifikační číslo studenta: 99989632

Typ studijního programu: magisterský
Studijní program: Farmacie
Studijní obor: Farmacie
Identifikační číslo studia: 456224

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

Pracoviště práce: Katedra farmaceutické chemie a farmaceutické analýzy
Jazyk práce: angličtina
Jazyk obhajoby: angličtina
Vedoucí: PharmDr. Jan Zitko, Ph.D.
Oponent(i): PharmDr. Marta Kučerová, Ph.D.

Datum obhajoby : 13.09.2018 **Místo obhajoby :** Hradec Králové

Průběh obhajoby: In the beginning, Legae Kebakuile used a PowerPoint presentation to illustrate the main concept and results of his work. He talked about molecular descriptors, lead-likeness and drug-likeness, and the usage of chemical databases in the context of drug design process. Then he demonstrated the data extraction and manipulation processes that were used to create and analyse the database. In the results part, he showed the statistical analysis of calculated descriptor values and their comparison among different subsets of the database (actives, inactives, all). Based on the properties of and average (median) molecule, he presented recommendation focused on what properties could be improved in compounds that will be designed and synthesized in the future.

Mentor Dr. Zitko in his evaluation of the thesis acknowledged the hard, time-consuming and precise work in the phase of data extraction from published and unpublished sources. The mentor was critical about the rather short time the student dedicated to the analysis and write-up. The mentor supported the defence based on the fact the main result of the thesis, the database, is very useful and already in use in the lab. Then the Reviewer's evaluation of Dr. Kučerová was read. The review was generally positive, although it demonstrated some errors in typography and definitions. The student responded to the questions raised by the reviewer in a sufficient way. The questions from the committee and audience followed. Doc. Miletín asked whether structural descriptors (based on the presence of functional groups) were considered in the evaluation of structure-activity relationship. Prof. Zimčík asked for the comparison of relative importance of individual physico-chemical properties (descriptors). Prof. Kučera asked about the supposed molecular target of active compounds in the database and asked about the

specifications of the CSV file format. The student was able to respond correctly to all the raised questions. At the very end, the student demonstrated the practical form and usage of the database. The committee agreed that the thesis was successfully defended.

Výsledek obhajoby:

výborně

Předseda komise:

doc. PharmDr. Radim Kučera, Ph.D.

Členové komise:

prof. PharmDr. Milan Nobilis, CSc.

doc. PharmDr. Miroslav Miletín, Ph.D.

doc. PharmDr. Petr Zimčík, Ph.D.