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Prof. Dr. Debby Mangelings, supervisor

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PhD in Pharmaceutical Sciences
2022-2023

INVITATION to the Public defence of

Yasmine GROOTEN

To obtain the academic degree of

'DOCTOR OF PHARMACEUTICAL SCIENCES'

**Evaluation of liquid and supercritical fluid chromatographic
systems in modelling the skin permeability of pharmaceutical
and cosmetic compounds**

The public defence will take place on

Wednesday, 8 February 2023 at 5 p.m.

In Auditorium R. Vanden Driessche

Faculty of Medicine and Pharmacy, Laarbeeklaan 103, 1090 Brussel

and can be followed online, accessible through the following link:

https://qf.vub.ac.be/redirects/PhD_defense_Yasmine_Grooten.php

Summary of the dissertation

Transdermal administration offers a good alternative for the disadvantages entailed by oral administration. Therefore, an increased interest is seen in the industry for skin permeability tests. Quantitative structure-activity relationship (QSAR) models, including chromatographic retention as a molecular descriptor, could provide alternatives for the current in-vivo and in-vitro methods to predict the skin permeability coefficient. In this PhD project, a fast and equally predictive chromatographic method was searched for as an alternative for the methods that are currently used to predict skin permeability of aspirant pharmaceutical or cosmetic compounds.

As a first step, skin permeability models were built containing only theoretical descriptors. In this way, the contribution of the chromatographic descriptor could be evaluated for each analytical method considered. In high-performance liquid chromatography (HPLC), a classical octadecyl silica, an immobilized artificial membrane (IAM) and a cholesterol-bonded column were tested. Furthermore, micellar liquid chromatographic conditions were examined on both a particle-based and a monolithic column (the latter offering the advantage of faster analyses). Besides HPLC, ultra-high-performance liquid chromatography (UHPLC) was applied to obtain an alternative high-throughput method. Lastly, supercritical fluid chromatography was implemented to model skin permeability, testing nine dissimilar stationary phases. Multiple modelling approaches were each time applied, after which the obtained models were compared to select the most suitable to model the skin permeability.

Curriculum Vitae

Yasmine Grooten was born on 13th August 1993 in Dilsen-Stokkem, Belgium. She completed secondary school in the field of Latin-Mathematical-Sciences in 2011, after which she started her academic career in Pharmaceutical Sciences at the Vrije Universiteit Brussel. She spent three months at the La Sapienza University of Rome in the context of her Master thesis. In 2016, she graduated as pharmacist and Master in Drug Development. Afterwards, she started a PhD at the research group Analytical Chemistry, Applied Chemometrics and Molecular Modelling, under the supervision of Prof. dr. Yvan Vander Heyden and Prof. dr. Debby Mangelings. Her research focused on the development of different analytical methods to model skin permeability, for which she obtained a fellowship from the Research Foundation Flanders (FWO).

Yasmine has published four peer-reviewed first-author papers and another first-author article is submitted. Her research results were presented at various national and international conferences. In addition to research, she assisted in different practical courses of Bachelor and Master students in the Pharmacy programme, and she was co-promotor of five Master theses. Since November 2021, Yasmine started a new adventure as platform manager of the chromatography laboratory at the Association of Pharmacists Belgium (APB), focussing on the quality control of (compounded) medicines on the Belgian market.