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Vrije Universiteit Brussel

Faculteit Geneeskunde & Farmacie

Doctoraat
Farmaceutische Wetenschappen
Academic year 2006-2007



INVITATION

To the public defence of the PhD thesis of

Sónia Caetano

14 September 2007

You are kindly invited to the public defence of the thesis of

Sónia Caetano

Chemometrics:

From pharmaceutical analysis to food traceability

On the 14th September 2007 at 18h
in auditorium P. Brouwer of the Faculteit
Geneeskunde & Farmacie,
Laarbeeklaan 103, 1090 Brussels

Context of the thesis

Chemometrics is a discipline with applications in many areas, like food industry, engineering, in particular in process control, pharmacy and drug design, agriculture, environmental sciences and medicine. This thesis has two different parts and is the result of the application of chemometrics to the fields of pharmaceutical and food analysis.

The part dedicated to the pharmaceutical analysis is mainly focused on the development of models capable of predicting enantioselectivity. Having models that, for a certain chiral stationary phase, under specific HPLC conditions, can determine whether the separation of two enantiomers is possible is very important, as the choice of stationary phase is a time consuming and expensive task. The second part of this thesis is the result of the work developed since 2005 for the *TRACE* European Project. It focuses on the development of a toolbox that can be used to analyse different types of data (e.g. analytical or spectroscopic data), in order to find a relation between the data and the origin of the analysed product.

This thesis shows that chemometrics are not limited to the analysis of chemical data. Its applications are much broader and can touch fields that at first glance have nothing in common. Independently of the problem treated the goal was always to derive models and/or rules that people can really use and that can help them in their work. Whether it is in pharmaceutical analysis, by trying to determine simple and interpretable models to predict the outcome of an enantioseparation, or in food traceability, with the development of specifications to prevent food fraud, chemometrics can be used to provide solutions and insight to problems.

Curriculum Vitae

Sónia Caetano was born in Lisbon, Portugal on the 2nd February 1979. She obtained a master degree in chemical engineering from Instituto Superior Técnico (IST), Lisbon, in September 2003.

She started her PhD on the 1st December 2003 in the department of analytical chemistry and pharmaceutical technology (FABI) under the supervision of Prof. Dr. Y. Vander Heyden. During her PhD she focused in the application of chemometrical techniques to the fields of pharmaceutical analysis, mainly dedicated to the prediction of enantioselectivity, and food traceability and authenticity, which was developed in the framework of the *TRACE* European Project. During this European project, she also had the opportunity to develop a toolbox that permits the determination of new specifications from multivariate analytical data, allowing the verification of the origin of a food product (authentication) and therefore tracing and controlling food (traceability).

She is the first author of five scientific publications which have been published in international scientific reviews.