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FACULTEIT GENEESKUNDE EN FARMACIE

Doctoraat in de Farmaceutische Wetenschappen
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UITNODIGING

Voor de openbare verdediging van het doctoraatsproefschrift van

Mohammad GOODARZI

Donderdag 24 mei 2012

U wordt vriendelijk uitgenodigd op de openbare verdediging van het proefschrift van

Mohammad GOODARZI

'Feature-selection techniques and modeling approaches in QSAR and QSPR'

Op **donderdag 24 mei 2012** om **17 uur** in **auditorium 5** van de Faculteit Geneeskunde & Farmacie Laarbeeklaan 103, 1090 Brussel

Situering van het proefschrift

A Quantitative Structure–Activity Relationship (QSAR) is a linear or nonlinear model, which relates variations in molecular descriptors (containing information about the structure) to variations in biological activity using a series of active and/or inactive compounds. It can either be used for prediction of the activity of untested drugs or to set up a priority plan of synthesis and experimental testing of new compounds. There are several steps which are important to build a QSAR/QSPR models. For instance, the feature selection and the modeling are two of them.

The selection of the relevant molecular descriptors from more than one thousand calculated descriptors is a crucial step in the development of QSAR models. In spite of the fact that many feature-selection methods already have been applied, it is still unclear which to use best to find a stable and reliable feature selection for a given type of data set.

The main aim of the thesis was to compare different feature-selection and modeling techniques in QSAR/QSPR studies.

Curriculum Vitae

Mohammad Goodarzi was born on May 10, 1982 in Borujerd, Iran. He obtained his degree in applied chemistry at the Islamic Azad University, Arak, Iran, on September 22nd 2006.

After his studies, his interest in the application of chemometric techniques to analyze data sets grew and he became a researcher at the Azad University.

After 5 years of research at the Islamic Azad University of Iran, in 2010 he started a Ph.D. in Pharmaceutical Sciences at the department of Analytical Chemistry and Pharmaceutical Technology (FABI) of the Vrije Universiteit Brussel (VUB) under the guidance of Prof. Y. Vander Heyden. In 2011, he had a stay at the Institute of Chemistry Timisoara of Romanian Academy, (Prof. S. Funar-Timofei), to study conformational analysis and docking studies, which are very important in drug design and drug development.

Since he started his Ph.D, Mohammad Goodarzi published 8 papers (of three he is first author) which some other papers, are still under review.