



Leiden / Amsterdam
Center for Drug Research

PHARMA-IT

www.PHARMA-IT.net

Student Research Project with the Pharma-IT Platform Suitable for Bachelor's and Master's level, for student with a chemical/biological/life science as well as a computer science / machine learning background

Leiden / Amsterdam Center for Drug Research (LACDR, www.lacdr.nl) and
Leiden Institute for Advanced Computer Science (LIACS, www.liacs.nl)

Proteochemometric modeling of hERG channel inhibitors

Human Ether-à-gogo Related Gene (hERG) is a gene that codes for a voltage gated potassium channel expressed in heart and nervous tissue. Suppression of its function due to adverse drug effects can lead to life-threatening arrhythmias. (Tseng 2001) Currently the information known about the channel is limited as the protein has not been crystallized yet. Proteochemometric modeling is a relative new technique (Lapinsh, Prusis et al. 2001), able to construct a quantitative structure-activity relationship (QSAR) based on both compound and target similarities in order to *predict* which compounds are likely to block this ion channel, and which ones are not.

The goal of the project is to apply proteochemometric modeling to a set of known hERG channel inhibitors. The project should produce a valid QSAR that enables the *in silico* screening of compounds for possible hERG channel interactions.

Requirements

We are looking for a master student with an interest in computational research/ bioinformatics. **No previous experience in the field is required and both a chemical/biological/life science or a computer science/machine learning background are suitable for this project.** We encourage students to publish their results together with the group if possible and the project results allow.

What can you learn?

Ligand and protein similarity measuring, QSAR modeling, using industry standard software Pipeline Pilot

For information: Gerard van Westen (gerard@chem.leidenuniv.nl)
Or have a look at: www.medchem.leidenuniv.nl or www.pharma-it.net

Contact:

For more information and to discuss details of the project contact Andreas Bender (Andreas.Bender@pharma-it.net) or Michael Emmerich (Michael.Emmerich@pharma-it.net). We are looking forward to hearing from you!

More information about the Pharma-IT Platform, currently ongoing research projects and people involved can be found on the Internet at www.pharma-it.net.

