

Postdoctoral position: Ligand-based virtual screening and machine learning for drug discovery

2019 in Lille, France

University of Lille – Pasteur Institute Lille – Inserm U1177

Project Title: Ligand-based virtual screening and machine learning for drug discovery

Description

A postdoctoral research opportunity in ligand-based virtual screening is available starting March 2019. One final goal, beside the methodological developments, is to implement different in silico ligand-based strategies to assist the design of better/novel drugs and drug candidates and/or to optimize existing bioactive molecules.

Research will be performed in the University of Lille – Pasteur Institute Lille – Inserm U1177.

This project aims to develop new cheminformatics protocols to analyze and annotate screening compound collections that are used on the lab's HTS platform. The annotation could involve the prediction of putative targets and of selected ADME-Tox properties... Experimental validation of the developed statistical models will be carried out. The developed in silico protocols will also be used to assist the experimental screening of some selected targets and disease pathways.

The participant will collaborate with a highly skilled multidisciplinary research team that integrates different approaches including biochemistry, molecular biology, medicinal chemistry, experimental ADME-Tox, biophysics, applied data sciences... The research activities involve: (1) combining different ligand-based virtual screening strategies; (2) development of statistical models for selected endpoints; (3) applications on selected disease pathways.

Research findings will be disseminated and communicated through web-based dashboards, peer-reviewed publications, and meetings of professional societies.

The appointment is full time for **18 months**. The scientist in charge of this project is Bruno Villoutreix (Bruno.villoutreix@gmail.com) (DR Inserm). The desired start date is March 2019.

Qualifications - Skills

PhD degree or equivalent

Skills: ligand-based screening, machine learning, knowledge in python programming, shell scripting, basic Unix/Linux administration, databases, information retrieval, and Web search. The applicant should have experience in these areas and should know how to write the first draft of a research article.

How To Apply

A current resume/CV, including academic history, employment history, relevant experiences, and a publication list (PDF to send by email to BV).

Two educational or professional references. The referees should send directly their recommendation by email to BV.