

PhD project “Pathway-Based drug discovery of novel analgesics”

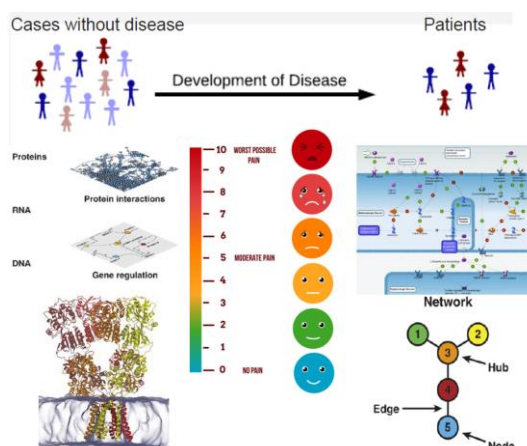
The Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) provides an interdisciplinary environment for educating the next generation of data scientists in close contact to domain-specific knowledge and research. All three domains – life & medical sciences, earth sciences, and energy systems/materials – are characterized by the generation of huge heterogeneously structured data sets, which have to be evaluated in order to obtain a holistic understanding of very complex systems. Visit HDS-LEE at: www.hds-lee.de

Project overview

We are currently searching students interested in combining data-science approaches with physics-based techniques for the identification of novel candidate modulators of pain. Pathway-based drug discovery approaches and in silico pharmacology will be applied. The project is in collaboration with Grünenthal Pharma Industry.

Agenda / Work plan:

- 1st year: knowledge organization and representation
- 2nd year: machine learning of classifiers, regressors, and pathway abstractions
- 3rd year: simulation, screening



Your Job:

- Use of NLP/text mining approaches to extract relevant interactions that can be assembled into more complex pathways building an adjacency matrix
- Biological pathway analysis using Metacore starting from lists of genes
- Extract pathway information in mathematical form, e.g. network node relations
- Compare and analyze with graph theoretical models using available programs e.g. R-packages (iGraph)
- Extend existing graph theoretical packages to merge and compare biological pathways
- Export pathway information into a format suitable to work with tensorflow/keras
- Prioritize and rank identified pathways by descriptors and probabilistic methods
- Use unsupervised learning to generate abstract representations of pathways (e.g. autoencoder)
- Build and optimize supervised classifiers
- Molecular simulation on identified pathway entities, disease specific
- Virtual screening and identification of potential therapeutic interventions
- Validate results by pathway-based repurposing of drugs and in vitro/in vivo tests

Your Profile

- University degree in either physics, chemistry, applied mathematics or computer science
- Experience with UNIX-like operating systems
- Mathematical and programming skills (R, Python, Keras, Tensorflow)
- Ideal prior knowledge on pathway/Systems biology or MD simulations
- Excellent knowledge of written and oral English: TOEFL or equivalent evidence of English-speaking skills
- Interactive person with good communication skills
- Used to work in international teams
- A high level of scholarship as indicated, for example, by bachelor and master study transcripts and two reference letters

Our Offer

This HDS-LEE PhD position will be located at the Institute for Advanced Simulations at the Forschungszentrum Jülich. The candidate will be supervised by Jun-Prof. Dr. Giulia Rossetti

- Outstanding scientific and technical infrastructure – ideal conditions for successfully completing a doctoral degree
- Unique HDS-LEE graduate school program
- A highly motivated group as well as an international and interdisciplinary working environment at one of Europe's largest research establishments
- Chance of participating in (international) conferences
- Continuous scientific mentoring by your scientific advisor
- Further development of your personal strengths, e.g. via a comprehensive further training program
- Pay in line with 100 % of pay group 13 of the Collective Agreement for the Public Service (TVöD-Bund)
- A contract for the duration of 3 years

Forschungszentrum Jülich aims to employ more women in this area and therefore particularly welcomes applications from women.

We also welcome applications from disabled persons.

Become a part of HDS-LEE and apply at https://www.fz-juelich.de/SharedDocs/Stellenangebote/_common/dna/2019D-136-EN-INM-9.html?nn=722008

Apply until: 30th June 2019

Starting date: 1st August 2019