



Universitat
Pompeu Fabra
Barcelona

Departament
de Ciències Experimentals
i de la Salut



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Job Offer

Position is available for a highly motivated PhD with experience in Pharmaco/Chemoinformatics

Job Description

A position is available for a highly motivated PhD with experience in Pharmaco/Chemoinformatics at the Pharmacoinformatics (PhI) group led by Manuel Pastor at GRIB (IMIM-UPF) in Barcelona. The candidate will participate in the development and application of computational methodologies in the areas of biomedicine and computational toxicology.

General Description:

She/he will participate in the development and implementation of data collection and analysis, oriented to the safety assessment of drugs, drugs candidates and consumer chemicals. This will imply the development and maintenance of databases, programming of workflows and scripts supporting computational methods for the data collection, transformation and analysis. The candidate will lead the design and programming of diverse computational tools and their integration with other components using web interfaces. This position will require abilities to direct the work of a small group of programmers and data experts. Our group participates in several large and ambitious European research projects and the research will be carried out in close collaboration with some of the best data scientists and toxicity experts in Europe, multinational industries in the areas of pharmaceutical, cosmetic and consumer chemicals as well as representatives of regulatory bodies.

Project and Institution that finance the contract:

The work is supported by grant: PR02717 - H2020-JTI-IMI2-2016- eTRANSafe M.PASTOR

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Skills and Experience

- PhD in Informatics, Bioinformatics, Biology or related areas.
- Knowledge on Pharmacoinformatics or Chemoinformatics. At least, experience with chemical formats like SMILES, SDFfile, InChI. Manipulation of chemical structures using RDKit or similar toolkits.
- Strong, demonstrable skills to work in Linux environments as advanced user.
- Demonstrable experience in the development, installation and handling of relational databases (e.g. MySQL, PostgreSQL, Oracle). Familiarity with SQL.
- Good programming skills on Python.



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- Fluent in English, with good written and oral communication skills.

We will consider valuable assets:

- A PhD in related areas would be positively considered.
- Experience in the Pharmaceutical or Biomedical industry will be considered a plus.
- Any experience with virtual environments and microservices systems (e.g. VirtualBox, Docker, Kubernetes) would be useful.
- Any previous experience with machine learning (numpy, scipy) and deep learning libraries and toolkits.
- Any formal training or research experience in Chemistry or Toxicology.

In addition to these skills we will value the candidate creativity, leadership, commitment and ability to integrate in a highly multidisciplinary team.

The PhI group lead by Manuel Pastor is a multidisciplinary team with strong experience in the development of novel computational methods and its application in the drug safety areas. Some relevant achievements in these areas include: i) the development methods for robust applicability domain and reliability indexes in the prediction of toxicological endpoints, ii) development of eTOXlab, a flexible framework for the implementation of prediction systems, iii) development of multiscale prediction systems for drug-induced QT prolongation, iv) participation in the European projects Open PHACTS, iPiE and EU-ToxRisk. Leading of European IMI and IMI2 projects eTOX and eTRANSAFE. A description of the group and the most recent publications can be accessed at <http://phi.upf.edu>

Benefits of the opening; Initially a full-time position for 12 months will be offered, 37,5 hours/week, which can be renewed for a period open to discussion.

Information on the application process: Send CV and letter of interest, to carina.oliver@upf.edu (REF: MP_eT)

Contact: Carina Oliver, Management - Research Programme on Biomedical Informatics (GRIB, IMIM/UPF)