

Job description: A **postdoctoral position** is available for a highly motivated researcher at the Pharmacoinformatics (PhI) group led by Manuel Pastor at GRIB (IMIM-UPF) in Barcelona. The candidate will be given responsibilities in the **development of predictive models and methodologies in the areas of in silico toxicology**.

General description: She/he will be responsible of the design and development of innovative computational methods with application in the prediction of the toxic properties of chemicals. The work involves the prototyping of novel methods for toxicity prediction and data visualization in languages as R or Python, as well as participate in its testing, validation and final implementation in production systems. Its research work will be funded by a large and ambitious European research project aiming to delineate how toxicological risk assessment will be carried out in the XXI century. The candidate will collaborate with multiple partners of an international consortium involving some of the best toxicity experts in Europe, multinational industries in the area of cosmetic, pharmaceutical and consumer chemicals as well as representatives of regulatory bodies.

Desired Skills and Expertise:

- University degree in Informatics, Biology, Biomedical sciences, Bioinformatics or related areas.
- A PhD on a topic related with the main subject or the methods of the proposed research.
- High interest in the biomedical application of computational methods.
- Fluent in English, with excellent written and oral communication skills.
- Excellent programming skills on Python and R, including common libraries and packages as numpy, scipy, matplotlib, Bioconductor, etc.
- Strong expertise in machine learning (PLS, RF, SVM). Solid background in statistics.
- Strong expertise in pharmacoinformatics or chemoinformatics. Experience with chemical formats like SMILES, SDFfile, InChI. Manipulation of chemical structures using RDKit or similar toolkits.
- Experience in data extraction from open data resources of drugs and chemicals, like ChEMBL, Open PHACTS, DrugBank, Unichem or similar.
- Experience in toxicology or drug development will be highly valued asset.

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

About the group

The PhI group (<http://phi.imim.es/phi>) led by Manuel Pastor (<http://grib.imim.es/about-us/manuel-pastor.html>) 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 this 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 elongation, iv) participation in the European projects eTOX, Open PHACTS, iPiE, EU-ToxRisk. A description of the group and the most recent publications can be accessed at <http://phi.imim.es>

Contract: Full-time position for 12 months with the possibility of extension. Salary depending of the experience of the candidate.

To apply: Please send a CV, the summary of the PhD thesis and a letter of interest by email to manuel.pastor@upf.edu