

## **Postdoctoral position for the development of methodologies in the areas of in silico toxicology**

A postdoctoral position is available for a highly motivated researcher at the Pharmacoinformatics (PhI) group led by Manuel Pastor at the **Research Programme on Biomedical Informatics, GRIB (IMIM-UPF)** in Barcelona. The candidate will be given responsibilities in the development of methodologies in the areas of in silico toxicology. She/he will participate in the development and validation of computational methods supporting the assessment of the toxic properties of chemical compounds (drugs, consumer chemicals, cosmetics), including data visualization, read-across and quantitative structure-activity relationships (QSAR) modeling. The 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.
- Good programming skills on Python and/or R, including common libraries and packages as numpy, scipy, matplotlib, Bioconductor, etc.
- Experience in the application of chemometrics and machine learning methods (PCA, PLS, RF, SVM).
- Experience with chemical formats like SMILES, SDFfile, InChI. Manipulation of chemical structures using RDKit or similar toolkits 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.

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 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 will depend 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](mailto:manuel.pastor@upf.edu) before **30<sup>th</sup> of June**.