

Job description: a position is available for a **highly motivated database expert** 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, implementation and maintenance of databases supporting computational methods for the assessment of the toxic properties of chemical compounds. The candidate will participate in the design and programming of database exploitation tools in Linux environment and the connection of these databases with other components using web interfaces. The results of this work would allow the candidate to prepare a PhD thesis at the UPF PhD program in Biomedicine (optional). Our group participates in several large and ambitious European research projects. The research will be carried out in close collaboration with some of the best toxicity experts in Europe, multinational industries in the areas of pharmaceutical, cosmetic and consumer chemicals as well as representatives of regulatory bodies.

Required skills and expertise:

- University degree in Informatics, Bioinformatics or related areas.
- 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 and/or Scala and/or Java.
- Experience in web application development.
- Fluent in English, with good written and oral communication skills.

We will consider valuable assets:

- A master in Bioinformatics, Biomedicine or related areas will be considered a plus.
- Experience in virtual environments (e.g. VirtualBox, Docker)
- Experience with chemical formats like SMILES, SDFfile, InChI. Manipulation of chemical structures using RDKit or similar toolkits.
- Any previous experience with machine learning (numpy, scipy) and deep learning libraries and toolkits.
- Any formal training or research experience in Chemistry, Biomedicine or Toxicology.

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 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>.

We offer a full-time position for 12 months, to be renewed for a period open to discussion. To apply, please send a CV and a letter of interest by email to manuel.pastor@upf.edu.