Date of publication of the job offer: 30/05/ 2022

Job Offer : **PhD/technical position at the PharmacoInformatics group**

(development of a dashboard to support NAM-based IATAs)

The Pharmacoinformatics group (PhI) is integrated in the Research Programme on Biomedical Informatics (GRIB), a joint research programme of the Hospital del Mar Medical Research Institute (IMIM) and the Department of Experimental and Health Sciences of the Universitat Pompeu Fabra, located at the Barcelona Biomedical Research Park (PRBB) in Barcelona (Spain).

Research Outline of PhI group (http://phi.upf.edu)

The Pharmacoinformatics group lead by Manuel Pastor is a multidisciplinary team with strong experience in the development of novel computational methods and their application in the drug safety areas. Some relevant achievements in these areas include: i) the development of methods for robust applicability domain and reliability indexes in the prediction of toxicological endpoints, ii) development of Flame, 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, eTRANSAFE, TransQST and RiskHunt3R. A description of the group and the most recent publications can be accessed at http://phi.upf.edu

Job Description:

We are seeking for a research student, interested in obtaining the PhD in bioinformatics, with capacity to implement on-line web applications supporting the application of NAM-based IATAs, within the framework of EU project RiskHunt3R.

The successful candidate will be involved in the design, development and implementation of this web application, in collaboration with other members of the RiskHunt3R consortium (e.g., Edelweis Connect).

Summary: in most industrial and regulatory settings the safety assessment of chemicals is carried out using standardized approaches, called IATAs (Integrated Approaches to Testing and Assessment), that integrate and weigh different types of data. This data can be the

result of *in vivo* experimental testing, but recently the tendency is to apply the 3R principle and replace this testing by NAMs (New Approach Methods). NAMs include classical *in vitro* methods (functional analysis in cell cultures), but also the use of reporter genes, organoids, HTT (hight-throughput transcriptomics), etc. NAMs can also include purely *in silico* assessment, using knowledge-based methods (Machine Learning, and Deep Learning models), and structural-based methods (docking, virtual screening), among others.

In practice, the number of NAM method which could be applied is broad and very often the toxicologist is overwhelmed by the number of choices. For this reason, the use of well-designed IATAs and software supporting tools is essential to guide the experimental and in-silico work, as well as for integrating their results.

The integration of multiple results should be carried out a weight-of-evidence approach. Ideally, probabilistic principles should be applied to combine the results obtained from different sources of evidence to obtain a quantitative estimation of the uncertainty associated to the integrated result.

In this work, we aim to develop software supporting the following activities:

1. Identification of the best NAMs applicable in a particular chemical safety study
2. Offer alternatives to the initial IATA design when, for any reason, one of the suggested NAMs could not be applied
3. Collection of the experimental results
4. Estimation of the uncertainty of every data source (epistemic, aleatory) and of their mutual independence
5. Combination of the results and uncertainties, presenting an integrated result in suitable ways for supporting decision making, particularly in regulatory settings.

This software should be accessible as an on-line web service with a graphical interface specifically designed for supporting the aforementioned activities.

Project and Institution that finance the contract, PREUR02921 - EC-H2020-SC1-2020-RISK-HUNTER3R-M.PASTOR

Project: RISK assessment of chemicals integrating HUman centric Next generation Testing strategies promoting the 3Rs

Official number reference: PREUR02921 - EC-H2020-SC1-2020-RISK-HUNTER3R-M.PASTOR

Skills and Experience

Knowledge of structural bioinformatics techniques (docking, template-based homology modelling, sequence and structure alignment, etc.)

Oral and written communication skills. Fluent spoken and written English. Excellent programming/scripting skills in at least one of each of the following bullet points: Script/Programming languages: Python Specificities: BioPython, Numpy, SciPy, TkInter. Programming languages: C, C++, Java. Web programming knowledge on at least one of the following points: Angular JS, JavaScript, PHP. Django, Bottle. HTML5, CGI. Databases in: SQL, MySQL, SQLite, MongoDB Graduate/engineer in one of the following areas: biology, biomedical engineering or related fields. Master or equivalent in bioinformatics or computational biology, or in the process of obtaining it.
Benefits of the opening, We offer a part-time contract (20hrs week), for 6 months. Gross salary 18,800 eur
Information on the application process: Send CV and letter of interest, to manuel.pastor@upf.edu, Ref: RiskHuntr **Deadline to submit applications – June 10th, 2022**