

BIO/CHEMO-INFORMATICS IN PREDICTIVE TOXICOLOGY

LORRAINE RESEARCH LABORATORY IN COMPUTER SCIENCE AND ITS APPLICATIONS (LORIA) IN PARTNERSHIP WITH HARMONIC PHARMA, NANCY, FRANCE

LORIA : www.loria.fr/en/ ; HARMONIC PHARMA : www.harmonicpharma.com

Position Description:

LORIA and Harmonic Pharma seek an engineer who wants to build their career in toxicological sciences to better understand how chemical compounds may impact our health and environment. This position will provide experience in both innovative computer science methodologies and applications to predictive toxicology. The mission is to improve coverage through data and knowledge development that are translatable, predictive, and timely.

Harmonic Pharma develops and applies innovative informatic solutions to produce fit-for-purpose predictions, including literature assessments and regulatory requirements, that provide timely support for clients. The main goal of this position is to develop QSAR and/or AI-based tools that analyze, aggregate, and visually represent the toxicological profile of chemical compounds.

Main activities of the candidate:

Bio/Chemo-informatics

- Manage and improve scripts
- Perform data extraction / categorization to support the project database
- Participate in QSAR/AI-based model generation and associated statistical analyses
- Participate in the development of new solutions
- Bring chemistry/biology expertise to the team

Data management

- Make regular updates of databases
- Participate in the retrieval of databases according to evolving needs as part of the "Safety by Design" offer, which relates to in silico predictive toxicology
- Make data backups
- Maintain documentation on scripts, methods and processes developed

Teamwork

- Interact with other team members on a regular basis
- Organize work according to priorities
- Assist in the writing of scientific publications and technical documents
- Report to the scientific director

Main scientific skills and knowledge:

- Applicants should have a background in biology and/or chemistry
- Informatics
 - Data mining methods
 - Machine learning / Artificial intelligence algorithms e.g. GLM, Random Forest, KNN, Decision Tree, Neural Network
 - Knowledge of sdf, smiles, mol2 formats
 - knowledge of ChemAxon and RDKit tools
 - Programming language (C/C++/java/perl/python)
 - Unix/linux system and bash language
 - Knowledge in php and sql

In addition to the appropriate scientific and technical skills, knowledge regarding regulatory requirements in toxicology will be appreciated.

Duration and Perspective:

18-month fixed-term contract with the prospect of a permanent contract at the end.

Eligibility:

To be eligible for this position, applicants should hold an engineer degree. or equivalent. All applicants receive consideration without regard to race, religion, color, national origin, gender, sex, sexual orientation, physical or mental disability, political affiliation, age (with statutory exceptions).

To apply:

Applications should be submitted as a **single email** including:

- *Curriculum Vitae*.
- A one-page cover letter describing your background.
- Names and contact information for professional references.

Please submit your application to **Dr. Sinan Karaboga** via email at karaboga@harmonicpharma.com.

This deadline for applications has been extended and will remain open until filled.

