**Artificial Intelligence Expert for the Experimental Therapeutics Programme**

**Description:**

The CNIO Experimental Therapeutics Programme (ETP) is a group constituted by biologists and medicinal-chemists dedicated to the discovery and development of new anti-tumoral drugs. We account with a very professional computational chemistry platform and we aim to expand it by adding Artificial Intelligence (AI) tools into the ETP's workflow. The application of AI and machine learning methods has the potential to revolutionize the drug discovery process, making it faster, cheaper and more efficient. These applications encompass a range of activities, including drug screening and design, polypharmacology prediction and drug repurposing, among others. We are currently seeking for an AI Expert with experience in the fields of computational chemistry, chemoinformatics and/or bioinformatics. The selected candidate will perform a diverse number of activities working in this environment:

1. She/he will carry out chemoinformatic analyses and data mining processes of chemical libraries and chemical-biology databases and computational related approaches for application in drug discovery.
2. She/he will generate and validate Machine Learning models for the prediction of pharmacokinetics, ADME and toxicity properties.
3. She/he will perform virtual screening, docking and molecular dynamics calculations of collections of small molecules and different target proteins of interest studied at ETP.

**We require:**

- BSc, MSc, Engineer, or PhD degree in biosciences or with experience in the fields of computational chemistry, chemoinformatics, bioinformatics and/or computing science.
- Knowledge in the application of computational chemistry, chemoinformatics and/or bioinformatics methods in drug discovery will be highly valued.
- Knowledge in Python and Machine Learning libraries (such as Scikit-learn, Pandas, and NumPy, and the chemoinformatic tool RDKit); and in the development of prediction models and analysis of high-dimensional data will be valued.
- Experience with Schrödinger's *Maestro* software and *AMBER* molecular dynamics software package will be valued.
- Comfortable with Unix based OS in a High Performance Computing Cluster (HPCC).
- Excellent written and verbal communication and presentation skills.
- High level of English, both written and spoken.
- Capacity for teamwork and motivation.
- Applications must include a detailed CV, synopsis of work experience and at least two reference letters.

**We offer:**

- The opportunity to be part of one of the few European Cancer Research Centres of excellence.
- An excellent working, multidisciplinary environment.
- Competitive salary and a 4-year contract.