Position Offered: POSTDOCTORAL RESEARCHER
Project: *Machine Learning for the Acceleration and Optimization of Pharmacophores for the Design of New Medicines by STD NMR Spectroscopy*

Technological and scientific fields: Design of New Medicines, Artificial Intelligence

Location: Seville, Andalucia, Spain, Institute for Chemical Research, www.iiq.us-csic.es

Research Group/PI: Biomolecular Interactions and Structural Glycobiology, Jesús Angulo, http://angulolab.iiq.us-csic.es

PROJECT SUMMARY

AI, STD NMR spectroscopy and computational chemistry techniques are combined to accelerate fragment based drug design. The low affinity of the fragments in the chemical libraries used for screening poses a major challenge to obtaining 3D structures, making NMR the preferred technique for their characterisation. NMR data are interpreted using 3D models, which requires an accurate assessment of the degree of agreement between the model and the experimental data (model validation), and it is here that this project will develop AI and computational chemistry protocols to provide better solutions. Recent contributions of our research group in the field of digital methods for the analysis of weak interactions by NMR include Anal. Chem, 2024, 96, 615, and J. Med. Chem, 2024, in press. Both papers have developed new digital tools to speed up the characterisation of weak interactions: RedMat (http://redmat.iiq.us-csic.es) y RedDat (https://stdrdweb.streamlit.app/).

PROFESSIONAL PROFILE

Minimum requirements:

1. PhD in Chemistry, preferably awarded "cum laude"
2. Pre- and/or postdoctoral experience in NMR and molecular modelling techniques such as docking calculations and molecular dynamics (MD) simulations.
3. Specialised experience in saturation transfer difference NMR spectroscopy (STD NMR), preferably demonstrating methodological contributions in this field.
4. Training/experience in Python programming, data analysis, and supervised/unsupervised machine learning algorithms.

Merits to be considered:

1. Experience in advanced MD techniques (funnel metadynamics).
2. Experience in STD NMR matrix analysis (CORCEMA-ST, RedMat).
3. Postdoctoral stay/s abroad.
4. Advanced level of English (C1 or higher).

WHAT IS OFFERED

The candidate will work in a research group that is internationally recognised for its contribution to the study of weak protein-ligand interactions using STD NMR techniques, and that has a solid track record in the development of hybrid NMR/computational methods for biomolecular studies. The candidate will receive training equivalent to 270 ECTS, including training in machine learning, 3 research training periods at the CIC bioGUNE (Bilbao, Spain) and the University of La Rioja (Logroño, Spain), as well as participation in a series of advanced training schools in computational chemistry and NMR spectroscopy.

Contract conditions:

Indefinite contract for a Postdoctoral Researcher associated to the Momentum Project of 4 years' duration according to Spanish science law. Gross annual salary (41.000 € - 52.000 €).

Start of contract: before 31 December 2024

PRINCIPAL INVESTIGATOR CONTACT

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