OFFER:

DOCTORAL CONTRACT (4 YEARS)
[51.807,13 € / year]

PROJECT:

Machine Learning for the Acceleration and Optimization of Pharmacophores for the Design of New Medicines by STD NMR Spectroscopy

Call "Momentum CSIC: Desarrolla tu Talento Digital"
Project Code: MMT24-IIQ-01
PI: Dr Jesús Angulo (IIQ-CSIC, Seville)
Co-PI: Dr Gonzalo Jiménez Osés (CIC bioGUNE, Bilbao)

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).

Requirements:

1. PhD in Chemistry
2. Experience in NMR and molecular modelling techniques.
3. Experience in NMR spectroscopy for molecular interactions.
4. Training/experience in Python programming, data analysis, and supervised/unsupervised machine learning algorithms.

Valuable:

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 at the IIQ-CSIC in Seville 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**.

CONTACT: please contact (INFORMAL QUERIES), **BEFORE 7th AUGUST**, the PI, Jesús Angulo at:
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