ESR 8 position

Project title: Computational exploration of container-guest complexes

Location: Mind the Byte, Spain

Supervisor: Dr. Alfons Nonell

Objectives of the individual project:

The PhD student (ESR8) host by Mind the Byte will be focused on the computational exploration of container guest complexes.
The student will be in charge of developing a computational tool for virtual screening (structure based by means of docking and MD simulations) to identify potential guests for the new synthetic supramolecular containers designed by the consortium, that, in a second phase, will be extended to predict binding constants of the host/guest complex in different solvents (i.e. organic solvents and aqueous media) through QM calculations. Additionally, ESR8 will implement a simulation protocol that could allow the evaluation of the behaviour of the host/guest complex under different stimuli (e. g. pH or light by means of mainly MD and maybe QM calculations). Finally, it is expected also to create a database containing all the information obtained theoretically and experimentally of the analysed host-guest complexes as well as their potential indications in disease.

Planned secondment(s):

Academic Secondment: The work is based on Barcelona with an academic secondment in Strasbourg the last 9 months in order to actively work in synthetic chemistry.

Eligibility requirements

EU eligibility criteria for candidates: Candidates of any nationality, but in order to be eligible for the positions the following criteria applies to all applicants:

- The applicant shall at the time of recruitment be in the **first four years of his/her research career** and have **not been awarded a doctoral degree**.
- The applicant must not have resided or carried out his/her main activity **in Spain for more than 12 months in the 3 years immediately prior to the recruitment**.

Candidates profile:

- Bsc. in chemistry, biochemistry or closely related fields.

- Msc. in computational chemistry, medicinal chemistry, biochemistry, biophysics or closely related fields
- Strong skills and experience in biomolecular simulations (Molecular Dynamics, QM/MM and Docking).
- Experience using popular software tools for simulating biological systems (Gromacs, NAMD, Autodock Vina, AmberTools, Orca, Gamess, etc).
- Understanding of protein-ligand interactions
- Modelling experience is a plus
- Experience in scientific computing using python or similar. Knowledge of SQL and NoSQL databases (MongoDB) is a plus
- Experience in computer-aided drug design and code development is a plus
- Work independently and adapt to a changing environment
- Creative, motivated and communicative team player with strong presentation skills

- Excellent organizational, communication and interpersonal skills
- Excellent communication skills in English. High level in writing and speaking is a must. Other languages are a plus.

Questions regarding the recruitment can be sent to: noah@noah-itn.eu.

If you are interested, please apply now at www.noah-itn.eu sending a copy of the documents to hr@mindthebyte.com before May 31st.