



Date of publication of the job offer: May 3rd, 2018

Job title: Molecular Simulations Research Scientist

Job description

Our laboratory will provide a focal point for the development and sustainability of software tools and services which are capable of delivering high fidelity three and four dimensional (including time) modelling and simulation of all aspects of the human body, from the genomic level to the whole human and beyond, in health and disease. Computational models are becoming very powerful at different stages in drug discovery and development from molecule design to assessment of toxicity. Computational models can also be used for repositioning and targeting therapies for precision medicine, through rapid and accurate assessment of drug efficacy in specific disease cases. They can also provide added value to medical device measurement data, for example as acquired by various imaging modalities.

Research lines

Drug discovery using large distributed computational resources (GPUGRID.net) with thousands of GPUs for molecular dynamics simulations, binding prediction, binding kinetics, Markov state models, online sampling methods (ACEMD, HTMD). The approach is computationally driven but we like to collaborate with experimental laboratories and industries where we work by rationalizing experimental results.

Project and Institution that finance the contract

European Commission – H2020

Official number reference

PR08416 - H2020-CompBioMed-Gianni de Fabritiis

Information on the minimum requirements

Required

University degree in medicinal chemistry, chemistry, pharmaceuticals
Experience in drug design
Phd in molecular simulations
Familiarity with scripting languages (e.g. Python)



Demonstrated strong verbal and written communication skills
Good English communication skills
Excellent attention to detail and organization skills
Knowledge/expertise on molecular simulations

Benefits of the opening

The candidate will have a one month contract, 37.5 hours per week.

Information on the application process:

Send CV and letter of interest, to carina.oliver@upf.edu (REF: **Comp_GdF**)

Deadline to submit applications – May 28th, 2018

Contact: Carina Oliver / GRIB