



Job ID: #JOB06/2016

Job Description

Job Title: Post-Doc in Computational Biophysics

Job Summary:

Applicant should have a PhD degree in biochemistry, biology, physics or equivalent. A successful candidate is expected to perform computer simulations of biomolecular systems with focus on protein aggregation associated with neurodegenerative diseases. Good knowledge of all-atom simulations, molecular docking, and molecular visualization programs are required. Programming skills, and familiarity with the linux operating system are advantageous.

Job Description:

A successful applicant will be involved in one of the following projects:

1. Aggregation of amyloid beta (A β) peptides is a hallmark of the Alzheimer's disease (AD) which is popular among the elderly. On the other hand, binding of metal ions like Cu(II) and Zn(II) to A β peptides in amyloid fibrils triggers the production of neurotoxic reactive oxygen species such as H₂O₂. Thus, study of the effect of metal ions on A β aggregation is important for understanding the etiology of AD. First, one has to develop the classical force field for interaction between Cu(II) with A β taking into account the torsion interactions which have been neglected so far. Then a newly developed force field, which is compatible with Amber, will be used to study the impact of Cu(II) on A β self-assembly at various Cu:A β stoichiometry.
2. A β deposits cause membrane disruption and increase permeability, leading to excessive leakage of ions, especially calcium ions. The imbalance in calcium homeostasis stimulates neuronal excitotoxicity. Therefore, we propose to consider the effect of A β systems with and without Cu(II) on the penetration of free ions Ca(II) through the lipid bilayer using all-atom molecular dynamics simulations.
3. Despite intense research during last decades no efficient medication has been found for AD. This is probably because FDA approved drugs are inhibitors of either Acetylcholinesterase (AChE) or N-methyl-D-aspartate (NMDA) but many other proteins are also involved in AD. Thus, we plan to employ the computer-aided drug design approach to screen out potential drugs that can target not only one but several proteins including A β oligomers. The full list of receptors will be obtained from molecular network and pathways associated with AD. Our goal will be achieved using the docking, pathways analysis and molecular dynamics simulations. The activity of multi-target top leads revealed by simulation will be further checked by in vitro experiment.

Main research field: Physics

Sub Research Field: Biophysics

Career Stage: Experienced researcher or 4-10 yrs (Post-Doc)

Research Profile ([details](#)): Recognised Researcher (R2)

Type of Contract: Temporary for 2 years

Status: Full-time

Salary: Depends on qualifications
From 2500 to 3300 PLN per month (before taxes).

Contact

More information can be obtained from
prof. Mai Suan Li (e-mail: masli@ifpan.edu.pl).

Application details

Application deadline: April 21 2016. Applications after deadline are not considered.

Required materials:

- Curriculum Vitae
- List of publications
- Names and contact informations of 2 references familiar with candidate research

All materials should be submitted in electronic form to the address: jobs@ifpan.edu.pl
with Job ID in the subject.