Postdoc bioinformatics position, UIC, Barcelona, Spain

Objective

Applications are invited for the position of a Postdoc bioinformatics researcher, working under the supervision of Bernhard Knapp in the Department of Basic Sciences, Faculty of Medicine and Health Sciences, UIC University, Barcelona, Spain.

The work group of Bernhard Knapp (https://www.uic.es/bioinformatics) focuses on computational simulations of the (human) immune system. We provide novel insight in fundamental processes of the immune system by means of quantitative analysis and predictive models. More specifically the work focuses on how T-cell receptors (TCRs) recognise Major Histocompatibility Complex (MHC) bound peptides in different health and disease conditions as for example allergies, cancer, autoimmune diseases, or infections. Apart from TCR/peptide/MHC interactions also antibody/antigen interactions are a key research interest of the group.
We apply a wide range of bioinformatics methods but put the emphasis on structural techniques (e.g. protein structure modelling, Molecular Dynamics, Monte Carlo simulations) and machine learning (e.g. Genetic Algorithms, Artificial Neural Networks, Regressions, Classifications, Clustering).

Examples of work include: by far the largest dataset of T-cell receptor recognition processes (Knapp et al., 2014), comparison of the molecular design (Dunbar et al., 2014) and instability (Knapp et al., 2017) of antibodies with T-cell receptors, obtaining novel insights in peptide/MHC detachment processes (Knapp et al., 2016), giving accurate and reproducible predictions of peptide/MHC binding affinities (Wan et al., 2015), optimising binding affinities using Genetic Algorithms (Knapp et al., 2011), and investigating protein/protein interactions (Esmaielbeiki et al., 2016), and development of tools (Knapp et al., 2018). Highly parallel calculations are carried out on different supercomputers.

The purpose of this call is to hire a postdoctoral researcher to promote the internationalisation of research at UIC Barcelona.

Beneficiaries

Potential candidates must:

- Have earned a PhD degree in the ten years preceding the year of this call.
- Certify at least a minimum of one year postdoctoral stay in one or several research centre outside of Spain.

Essential requirements:

- Strong experience and fluency in several programming languages such as Python, Matlab, C++, Java, Perl, and/or R
- Strong statistics and data analysis skills
- Basic knowledge of UNIX-like operating systems and shell scripting

- Strong analytical skills, in addition to creativity, curiosity, enthusiasm, and ability to work in a team
- Excellent command of the English language
- Legal right to work full time in Spain

Ideal skills:

- Knowlegde of data science skills: Regression (e.g. ANN, Lasso, Ridge) , classification (e.g. SVM, KNN), clustering (e.g. k-means, hierarchical), heuristic optimisation (e.g. genetic algorithms, monte carlo simulations), parallel computing (e.g. MPI, pySpark, parallel computing toolbox, map/reduce), SQL, noSQL
- Knowledge of common bioinformatics techniques: Immunoinformatics, B- and T-cell epitope predictions, molecular dynamics simulations, free energy predictions, protein/ligand and protein/protein docking, virtual screening, protein structure prediction, sequence alignments, tree building
- Experience with the use of computing clusters
- Previous teaching experience

Characteristics of the fellowship

- The contract will be valid for two years from the date the researcher starts. The expected start date is 3 September 2018.
- The Postdoctoral "La Caixa" Foundation researcher's gross annual salary will be €37,000.
- The researcher will also have 6.500€ per year for expenses associated with the correct development of the research proposal. The expenses may include: consumables, travels, article reviews, congresses, etc.
- Under no circumstances does this postdoctoral research contract implies a commitment by the University to subsequently hire the beneficiary as a permanent member of the University's staff.

Application documents (as one pdf):

1) CV
2) Publication list (including journal impact factors and ranking of the journal within the respective category based on webofknowledge.com e.g. The journal "Bioinformatics" has an impact factor of 7.3 and is ranked 2nd of 57 (top 3%) in "mathematical & computational biology").
3) Letter of motivation (short, max 1 page)
4) One letter of recommendation (e.g. from the PhD or Postdoc supervisor)

Apply via email to: bknapp@uic.es

The deadline for submission is 30 April 2018.

Reference List

Dunbar,J., Knapp,B., Fuchs,A., Shi,J., and Deane,C.M. (2014). Examining Variable Domain Orientations in Antigen Receptors Gives Insight into TCR-Like Antibody Design. PLoS Comput Biol *10*, e1003852.

Esmaielbeiki,R., Krawczyk,K., Knapp,B., Nebel,J., and Deane,C.M. (2016). Progress and Challenges in Predicting Protein-Protein Interfaces. Brief Bioinform *17*, 117-31.

Knapp,B., Alcala,M., Zhang,H., West,C., van der Merwe,P.A., and Deane,C.M. (2018). pyHVis3D: Visualising Molecular Simulation deduced H-bond networks in 3D: Application to T-cell receptor interactions. Bioinformatics.

Knapp,B., Demharter,S., Deane,C.M., and Minary,P. (2016). Exploring peptide/MHC detachment processes using Hierarchical Natural Move Monte Carlo. Bioinformatics *32*, 181-186.

Knapp,B., Dunbar,J., Alcala,M., and Deane,C.M. (2017). Variable Regions of Antibodies and T-cell Receptors may not be Sufficient in Molecular Simulations Investigating Binding. J. Chem. Theory Comput. *accepted*.

Knapp,B., Dunbar,J., and Deane,C.M. (2014). Large Scale Characterization of the LC13 TCR and HLA-B8 Structural Landscape in Reaction to 172 Altered Peptide Ligands: A Molecular Dynamics Simulation Study. PLoS Comput Biol *10*, e1003748.

Knapp,B., Giczi,V., Ribarics,R., and Schreiner,W. (2011). PeptX: Using Genetic Algorithms to optimize peptides for MHC binding. BMC. Bioinformatics. *12*, 241.

Wan,S., Knapp,B., Wright,D., Deane,C., and Coveney,P.V. (2015). Rapid, Precise and Reproducible Prediction of Peptide-MHC Binding Affinities from Molecular Dynamics that Correlate Well with Experiment. J. Chem. Theory Comput. *11*, 3346-3356.