

## **Bioinformatics researcher with possible follow-up as PhD student, Barcelona, UIC**

Applications are invited for the position of a 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 newly established work group [1] of Bernhard Knapp 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).

Examples of recent work include the first peptide/MHC detachment simulations (Knapp et al., 2016), the by far largest simulation of TCR/peptide/MHC interaction (Knapp et al., 2014; Knapp et al., 2015b), and structural characterisation of protein helices (Hischenhuber et al., 2013; Wilman et al., 2014).

Successful interdisciplinary collaboration plays an essential role in our research (Knapp et al., 2015a). Examples include macrophage polarisation (Haschemi et al., 2012), cancer (Paulitschke et al., 2015), viral infection (Schwaiger et al., 2014), and (Zhang et al., 2016).

[1] <http://uic.es/es/salud/investigacion/bioinformatics-research-group>

### **Requirements**

Candidates must have a bachelor and master degree in a quantitative field (e.g. computer science, applied mathematics/statistics, (bio)physics, bioinformatics) with a strong interest in biological and immunological challenges. Prior knowledge of molecular biology, genetics, and immunology is an advantage.

#### **Essential requirements:**

- Strong experience and fluency in several programming languages such as Python, Matlab, C++, Java, Perl, and/or R.
- 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
- The average of all marks of the bachelor and master must be better than 0.75 (on a normalised scale of 0 (worst) to 1 (best)). This is a formal requirement by the UIC. Please state your average mark for your bachelor and master in your letter of motivation (and show supporting documents as an attachment). Applications not containing this information or marks averages below 0.75 cannot be considered. Also applicants without a master degree (or who already hold a PhD) can formally not be considered.

**Optional skills:**

- Knowledge of common bioinformatics techniques (e.g. molecular docking, clustering, sequence alignment) and tools (Autodock, Gromacs, Blast, etc)
- Experience with the use of computing clusters
- Teaching experience and/or ability in Spanish/Catalan is a plus

**Offer**

The successful candidate will work in an exciting project in the field of computational simulations of the immune system and assist the experimentalists of the department with their data analysis.

Access to high performance computers is available.

The position will be about 1200 EUR / month for 10 months. During the final months of this time a PhD student position funded for up to 4 years will be advertised for which the candidate is encouraged to apply.

Please note that Spanish living costs are considerably lower than in most central/northern European countries.

The successful candidate can start immediately.

For more information and to submit your application please email Bernhard Knapp (bknapp@uic.es). Application documents are a CV, a letter of motivation (short, max 2 page, containing marks average of the bachelor and master degree), and a publication list (if existing) including journal impact factors.

Application deadline: 15 January 2017

Haschemi,A., Kosma,P., Gille,L., Evans,C.R., Burant,C.F., Starkl,P., Knapp,B., Haas,R., Schmid,J.A., Jandl,C., Amir,S., Lubec,G., Park,J., Esterbauer,H., Bilban,M., Brizuela,L., Pospisilik,J.A., Otterbein,L.E., and Wagner,O. (2012). The sedoheptulose kinase CARKL directs macrophage polarization through control of glucose metabolism. *Cell Metab* 15, 813-826.

Hischenhuber,B., Havlicek,H., Todoric,J., Hollrigl-Binder,S., Schreiner,W., and Knapp,B. (2013). Differential geometric analysis of alterations in MH alpha-helices. *J. Comput. Chem.* 34, 1862-1879.

Knapp,B., Bardenet,R., Bernabeu,M.O., Bordas,R., Bruna,M., Calderhead,B., Cooper,J., Fletcher,A.G., Groen,D., Kijuper,B., Lewis,J., McNerny,G.J., Minssen,T., Osborne,J., Paulitschke,P., Pitt-Francis,J., Todoric,J., Yates,C.A., Gavaghan,D.J., and Deane,C.M. (2015a). Ten simple rules for a successful cross-disciplinary collaboration. *PLoS Comput Biol* accepted.

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., Demharter,S., Esmailbeiki,R., and Deane,C.M. (2015b). Current Status and Future Challenges in T-cell receptor / peptide / MHC Molecular Dynamics Simulations. *Brief Bioinform* 16, 1035-1044.

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.

Paulitschke,V., Berger,W., Paulitschke,P., Hofstaetter,E., Knapp,B., Dingelmaier-Hovorka,R., Fodinger,D., Jager,W., Szekeres,T., Meshcheryakova,A., Bileck,A., Pirker,C., Pehamberger,H., Gerner,C., and Kunstfeld,R. (2015). Vemurafenib resistance signature by proteome analysis offers new strategies and rational therapeutic concepts. *Mol. Cancer Ther.*

Schwaiger,J., Aberle,J.H., Stiasny,K., Knapp,B., Schreiner,W., Fae,I., Fischer,G., Scheinost,O., Chmelik,V., and Heinz,F.X. (2014). Specificities of Human CD4+ T cell Responses to an Inactivated Flavivirus Vaccine and Infection: Correlation with Structure and Epitope Prediction. *accepted Journal of Virology.*

Wilman,H.R., Ebejer,J.P., Shi,J., Deane,C.M., and Knapp,B. (2014). Crowdsourcing yields a new standard for kinks in protein helices. *J. Chem. Inf. Model.* 54, 2585-2593.

Zhang, H., Lim, H., Knapp, B, Deane, C. M., Aleksic, M. and van der Merwe, P. A. The contribution of major histocompatibility complex contacts to the affinity and kinetics of T cell receptor binding. *Scientific Report*, accepted, 2016.