

## PhD-Fellowship in Bioinformatics, Barcelona, UIC

Applications are invited for an PhD Studentship, 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 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), or viral infection (Schwaiger et al., 2014).

The research group aims to bring together the best of computer science, math, statistics, immunology, and (bio)medicine.

### **Requirements**

The PhD project will be in the field of computational simulations of the immune system. Candidates must have a master degree (ideally in bioinformatics, computational science, applied mathematics/statistics, or similar fields of study).

The (ECTS weighted) average of all marks must be better than 0.75 on a scale of 0 (worst possible mark) to 1 (best possible mark).

She/he should have strong analytical skills, in addition to creativity, curiosity, enthusiasm, and ability to work in a team.

### **Offer**

The fellowship will be about 1150 EUR / month for 3+1 years of funding. Please note that Spanish living costs are considerably lower than in most central/northern European countries.

The successful candidate can start in January 2017.

For more information and to submit your application (latest by the 30th of Sept) please email Bernhard Knapp (bknapp@uic.es). Application documents are a CV (including marks average (with and without ECTS weighting)), a letter of motivation (short, max 1 page), and a publication list (if existing).

- 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., McInerny,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.