

Felix A Krüger | C V

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Summary

Combines an analytical mindset with curiosity and the will to make things happen. Considerate and engaging co-worker. Broad variety of technical and communicative skills and strong background in computational biology and biomedical research.

Academic

UCL

Research Associate in Genetic Epidemiology

Research with Aroon Hingorani and Juan-Pablo Casas

London

2014 – current

University of Cambridge

PhD in Computational Biology, degree awarded 17th May 2014

Predoctoral fellow at the EMBL European Bioinformatics Institute

Cambridge

2009 – 2014

University of Bonn

Diploma in Molecular Biomedicine, Degree grade 1.1

Diploma thesis in computational drug discovery under Dr. Jürgen Bajorath

Bonn

2004 – 2009

Experience

Projects

EMBL-EBI

Predoctoral fellow, Drug Discovery Informatics Group

Dr John P Overington, Developed analytic methods for bioinformatics databases including ChEMBL, Pfam, PDB. Programming skills in Python, R, SQL, rdkit, pymol and MODELLER.

Hinxton

Oct 2009 – current

Bonn-Aachen Center for Information Technology

Research student, Institute of Life Science Informatics

Dr Jürgen Bajorath, "Fragment formal concept analysis accurately classifies small molecules that target members of protein families". Developed a framework to classify small molecule bioactivity. Developed skills in Perl, Pipeline Pilot, MOE and SVL.

Bonn

Sep 2008 – Mar 2009

Weizmann Institute of Science

Intern, Department of Biological Chemistry

Dr. Yechiel Shai, "Antibiotic peptides" (DAAD travel grant). Solid phase peptide synthesis, HPLC, bacterial cell culture, electron microscopy.

Rehovot

Jul 2008 – Aug 2008

Science outreach

EMBL Science and Society program

Conference co-chair

Co-organised EMBL Science and Society symposium "Biodiversity and Endangered Species: Rethinking the Balance of Nature". Drafted and developed the conference program, liaised with speakers, venue booking, advertising.

Heidelberg/Cambridge

Jan 2011 – Jan 2012

Other.....

Hack 4 Health at Open Data Institute

Participant in 3-day hackathon

Part of a team developing an analysis platform for NHS public GP prescribing data.

London

Nov 2012

Conference presentations

- **InCoB 2012**, Bangkok, oral presentation: Mapping small molecule binding to protein domains. (APBioNet Travel grant)
- **ISMB 2012**, Long Beach, oral and poster presentation: Data integration illustrates evolutionary mechanisms of ligand selectivity between related protein targets. (ISMB 2012 Travel Fellowship)
- **ICCS 2011**, Nordwijkerhout, oral presentation: Global mapping of ligand and target binding spaces.
- **Young Modeler's Forum 2010**, London, poster presentation: Global mapping of small molecule binding affinities to homologous proteins.

PhD Thesis

Title: *Integration of small molecule bioactivity data and protein evolutionary relationships*

Supervisor: Dr John P Overington

Advisory Committee: Prof Tom Blundell, Prof Peer Bork, Dr Julio Saez-Rodriguez

Description: I explored approaches of integrating the ChEMBL database, a public repository of small molecule bioactivity measurements, with database resources describing protein evolutionary relationships. I then used the established links to analyse aspects of the molecular and evolutionary mechanisms that determine drug action.

Languages

German: Native proficiency

English: Full professional proficiency

French: Limited working proficiency

References

References are available upon request.

Publications

Louisa J Bellis, Ruth Akhtar, Bissan Al-Lazikani, Francis Atkinson, A Patricia Bento, Jon Chambers, Mark Davies, Anna Gaulton, Anne Hersey, Kazuyoshi Ikeda, Felix A Krüger, Yvonne Light, Shaun McGlinchey, Rita Santos, Benjamin Stauch, and John P Overington. Collation and data-mining of literature bioactivity data for drug discovery. *Biochemical Society transactions*, 39(5):1365–70, October 2011.

A Patrícia Bento, Anna Gaulton, Anne Hersey, Louisa J Bellis, Jon Chambers, Mark Davies, Felix a Krüger, Yvonne Light, Lora Mak, Shaun McGlinchey, Michal Nowotka, George Papadatos, Rita Santos, and John P Overington. The ChEMBL bioactivity database: an update. *Nucleic acids research*, 42(1):D1083–90, January 2014.

Felix Krüger, Eugen Lounkine, and Jürgen Bajorath. Fragment formal concept analysis accurately classifies compounds with closely related biological activities. *ChemMedChem*, 4(7):1174–81, July 2009.

Felix A Kruger and John P Overington. Global analysis of small molecule binding to related protein targets. *PLoS computational biology*, 8(1):e1002333, January 2012.

Felix A Kruger, Raghd Rostom, and John P Overington. Mapping small molecule binding data to structural domains. *BMC bioinformatics*, 13 Suppl 1(Suppl 17):S11, January 2012.