

# Felix A Krüger | C V

• <http://fak.github.io/fakruger/> •  fak •  mo\_sander

## Academic

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### 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 17<sup>th</sup> 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

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### Projects.....

#### EMBL-EBI

*Predocutorial 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

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- **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

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**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

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**German:** Native proficiency

**English:** Full professional proficiency

**French:** Limited working proficiency

## References

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References are available upon request.

## Publications

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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.