ANDREAS BENDER, PhD
Lecturer for Computational Drug Design, Unilever Centre for Molecular Science Informatics
Department of Chemistry, University of Cambridge, Lensfield Road
Fellow of The King's College of our Lady and Saint Nicholas in Cambridge

Lecturer for Cheminformatics and Pharmaceutical IT, Unilever Centre for Molecular Science Informatics, Department of Chemistry, University of Cambridge and Fellow of King's College Cambridge (5/2010 – 7 / 2013 unestablished lecturer; 1 / 2013 – today established lecturer)

- Established a premier centre for data mining and cheminformatics within the Unilever Centre, leading a group of currently ca. 20 members (12 PhD students as main supervisor, plus visitors, shared postdocs and project sutdents, as of October 2013)
- Recipient of an ERC Starting Grant 2013
- Received funding received from major pharmaceutical companies (Johnson&Johnson, Eli Lilly, BASF, AstraZeneca) for ongoing collaborative research projects
- Recipient of the European Chemical Industry Council (CEFIC) Long Range Initiative Award (EUR 100.000) for a proposal on integrated chemical and biological toxicity modelling
- Recipient of the 'Bayer Early Excellence in Science Award' (Chemistry Category)
- Published >30 peer-reviewed scientific publications, the majority as corresponding author
- Presented *ca.* 30 invited and plenary lectures internationally and nationally

Assistant Professor (tenure track) for Cheminformatics and Head of the Pharma-IT Platform, Leiden/Amsterdam Center for Drug Research, Leiden, The Netherlands (1/2008 – 4/2010)

- Established a cheminformatics research group in the context of the Leiden/Amsterdam Center for Drug Research, heading a group of 6 (1 Postdoc, 2 PhD and 3 MSc Students)
- Research concerned the analysis of toxicology data (specifically hERG blockage), chemogenomics data analysis, development of ligand bioactivity models
- Published >20 peer-reviewed scientific publications
- Recipient of EFMC Young Medicinal Chemist in Academia Award

Presidential Postdoctoral Fellow, Novartis Institutes for BioMedical Research and Broad Institute of Hardvard and MIT, **Cambridge/MA, USA** (1/2006 – 12/2007)

- Analysis of safety profiling and adverse drug reaction data using chemical and biological data integration, developing and applying data analysis methods on heterogeneous data
- Collaboration with molecular pathways team on the analysis of phenotypic (high-content screening) data led to a publication in *Nature Chemical Biology (Nature Chem. Biol.* **2008** (4) 59-68.)
- Invited speaker at EuroQSAR (the central conference in our scientific field)
- Published >20 peer-reviewed publications

PhD Candidate, University of Cambridge, UK (1/2003-12/2005)

- Developed two novel methods for describing the similarity of molecules for virtual screening; methods were validated thoroughly and are currently being applied at a number of academic and industrial research institutions
- Joint winner of the *McMaster High-Throughput Screening* Competition with the methods developed above (invited for publication in the *Journal of Biomolecular* Screening)
- Thesis title: *"New Approaches To Molecular Similarity"*, with Prof. Robert C. Glen
- Recipient of Gates Cambridge Scholarship (1% success rate)
- Published >20 peer-reviewed publications

M. Sc. Candidate, Johann Wolfgang Goethe University, Frankfurt, Germany (10/1997-12/2002)

- Analysed mitochondrial transit peptides of the malaria-causing organism *P. Falciparum*
- Work has found considerable resonance in *P. falciparum* research
- Recipient of German National Merit Foundation Scholarship
- Thesis title *"Analysis and Prediction of Transit Peptides of Plasmodium falciparum"*

Prizes, Awards and Other Honours

Prizes and Awards

2013 ERC Starting Grant
2012 European Chemical Industry Council (CEFIC) LRI Innovative Science Award
2011 Bayer Early Excellence in Science Award in Chemistry
2011 Silver Jubilee Prize of the Molecular Graphics and Modeling Society (MGMS)
2011 Prize for Innovation in Pharmaceutical and Medicinal Chemistry, by GDCh and DPhG
2010 EFMC Prize for Young Medicinal Chemist in Academia
2008 ThermoFisher 'Cellome' Award ("best publication using HCS", (*Nature Chem. Biol.* **2008** (4) 59 - 68.)
2004 Computational Chemistry Group Excellence Award

Other Appointments and Affiliations

Editor in Chief: *Expert Opinion on Drug Discovery*
Editorial Board Member: *Expert Opinion on Drug Discovery, Journal of Chemical Information and Modeling, Combinatorial Chemistry & High-Throughput Screening*
Research Referee: Genopole (France), National Science Foundation Small Business Innovation Research (SBIR) Program, United States
Journal Referee: Accounts of Chemical Research, Bioinformatics, Bioorganic and Medicinal Chemistry, BMC Bioinformatics, BMC Genomics, ChemMedChem, Chemical Biology and Drug Design, ChimicaOggi / ChemistryToday, Combinatorial Chemistry & High-Throughput Screening, Drug Discovery Today, Expert Opinion on Drug Discovery, Future Medicinal Chemistry, Journal of the American Chemical Society, Journal of Chemical Information and Modeling, Journal of Cheminformatics, Journal of Chemometrics, Journal of Heterocyclic Chemistry, Journal of Molecular Graphics and Modeling, Journal of Molecular Modeling, Journal of Pharmaceutical Sciences, Medicinal Chemistry Communications, Molecular Diversity,Molecular Pharmaceutics, Nature Biotechnology, Nature Chemical Biology, PLoS One, QSAR and Combinatorial Science, Statistical Analysis and Data Mining

Other Academic Appointments

Visiting Professor with the Faculty of Pharmacy, Universiti Teknologi MARA (UiTM), Puncak Alam, Malaysia
Astrazeneca Research Foundation of India Visiting Fellow at Institute of Bioinformatics and Applied Biotechnology (IBAB), Bangalore, India

Conference Organizer (Selected)

2013 Co-Organizer of Dagstuhl Seminar 'Computational Methods Aiding Early-Stage Drug Design', Dagstuhl, Germany
2009 Co-Organizer of Lorentz-Center Workshop on 'Optimizing Drug Design', Leiden, The Netherlands
2009 Program Committee Member, ISoLA BIO 2009, June 2009, Potsdam, Germany
2008 Program Committee Member, ECML Workshop 'Stat. Learning in Bioinformatics', Sep. 2008, Antwerp, Belgium
2008 Advisory Board Member, Compound Library Design, December 2008, Prague, Czech Republic
2006 Advisory Board Member, 'First International Conference on Chemoinformatics', Pune, India
2006 Co-Organizer, 'Modelling the Properties and Behaviour of Molecules', London, UK
2006 Publicity Chair, 'CompLife'06' (Computational Life Sciences 2006), Cambridge, UK

Lattest scientific papers and book chapters (out of 113)

Biofragments: an approach towards predicting protein function using biologically-related fragments, and its application to Mycobacterium tuberculosis CYP126.
Sean A. Hudson, et al., ChemBioChem. 2014 (in press).

How Diverse Are Diversity Assessment Methods? A Comparative Analysis and Benchmarking of Molecular Descriptor Space.
Alexios Koutsoukas, et al., J. Chem. Inf. Model. 2014 (in press).

Synthesis and biological evaluation of tetrahydropyridinepyrazoles ('PFPs') as inhibitors of STAT3 phosphorylation.
Revanna C. N., et al., MedChemComm 2014 (5) 32 - 40.

Predicting Toxic Effects of Metabolites.
Andreas Bender, In: Drug Metabolism Prediction. Johannes Kirchmair (Ed.), Wiley, New York 2014.

Are phylogenetic trees suitable for chemogenomics analyses of bioactivity data sets: the importance of shared active compounds and choosing a suitable data embedding method, as exemplified on Kinases.
Shardul Paricharak, et al., J. Cheminf. 2013 (5) 49.

Evaluation of antioxidant and antimicrobial activities of the phenolic composition of Algerian Arbutus unedo L. Roots.
Nassim Djabou, et al., Pharmacognosy J. 2013 (5) 275 - 280.

Experimental Confirmation of New Drug-Target Interactions Predicted by Drug Profile Matching.
Laszlo Vegner, et al., J. Med. Chem. 2013 (56) 8377 - 8388.

Design, Synthesis, and Biological Evaluation of an Allosteric Inhibitor of HSET that Targets Cancer Cells with Supernumerary Centrosomes.
Ciorsdaidh A. Watts, et al., Chem. Biol. 2013 (20) 1399 - 1410.

Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets.
Gerard J. P. van Westen, et al., J. Cheminf. 2013 (5) 42.

Benchmarking of protein descriptor sets in proteochemometric modeling (part 1): comparative study of 13 amino acid descriptor sets.
Gerard J. P. van Westen, et al., J. Cheminf. 2013 (5) 41.

Extensions to In Silico Bioactivity Predictions Using Pathway Annotations and Differential Pharmacology Analysis: Application to Xenopus laevis Phenotypic Readouts.
Sonia Liggi, et al., Mol. Inf. 2013 (11-12) 1009 - 1024.

In silico target predictions: defining a benchmarking dataset and comparison of performance of the multiclass Naïve Bayes and Parzen-Rosenblatt Window.
Alexios Koutsoukas, et al., J. Chem. Inf. Model. 2013 (53) 1957 - 1966.

Diversity selection of compounds based on 'Protein Affinity Fingerprints' improves sampling of bioactive chemical space.
Ha P. Nguyen, et al., Chem. Biol. Drug Des. 2013 (82) 252 - 266.

Significantly Improved HIV Inhibitor Efficacy Prediction Employing Proteochemometric Models Generated From Antivirogram Data.
Gerard J. P. van Westen, et al., PLoS Comp. Biol. 2013 (9) e1002899.