

## CURRICULUM VITAE

Bojan Zagrovic, PhD

Department of Structural and Computational Biology  
University of Vienna, Vienna, Austria

### PERSONAL INFORMATION

Family name, First name: **Zagrovic, Bojan**

Researcher unique identifier: ORCID ID 0000-0003-3814-3675

Date of birth: November 8<sup>th</sup> 1974

Nationality: Croatian

URL for web site: <http://www.mfpl.ac.at/groups/mfpl-group/group-info/zagrovic.html>

### EDUCATION

- 2004            **Stanford University**, USA, PhD in Biophysics  
Thesis: "Studying protein folding and dynamics using worldwide distributed computing"  
(advisor: prof. dr. Vijay S. Pande)
- 1997            **Harvard University**, USA, AB in Biochemical Sciences  
Thesis: "Coordination of G-protein subunit levels and the activity of adenylyl cyclase"  
(advisor: prof. dr. Eva J. Neer)

### CURRENT POSITION

2015 – present **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, associate professor with tenure

### PREVIOUS POSITIONS

- 2010 – 2015    **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, junior group leader & assistant professor
- 2007 – 2010    **Mediterranean Institute for Life Sciences**, MedILS, Split, Croatia, group leader
- 2007 – 2008    **Mediterranean Institute for Life Sciences**, MedILS, Split, Croatia, scientific director
- 2004 – 2007    **ETH Zurich**, Switzerland, EMBO postdoctoral fellow in Wilfred F. van Gunsteren's group

### MAIN AREAS OF RESEARCH

*Computational and experimental studies of biomolecular structure, dynamics and interactions including:*

- mechanism and thermodynamics of protein-protein and RNA-protein interactions
- classical atomistic molecular dynamics simulations
- conformational entropy in biomolecular interactions
- structure, dynamics and interactions of proteins in crowded environments
- conformational averaging and its influence on biomolecular structure determination
- evolution of the genetic code and RNA-protein interactions

### PRINCIPAL RESEARCH ACCOMPLISHMENTS

- pioneered the usage of worldwide distributed computing in biological research (**Folding@Home** project to study protein dynamics)
- carried out the **first-ever unbiased molecular dynamics simulations of complete protein folding** and elucidated the paramount role of the unfolded state residual structure in the process
- demonstrated the critical importance of **an ensemble view in biomolecular structure determination** using nuclear magnetic resonance, X-ray crystallography and fiber diffraction
- founded **Vienna PTM**, a leading resource for molecular dynamics simulations of protein post-translational modifications
- discovered and characterized **cognate mRNA-protein compositional complementarity**

## SUPERVISION OF STUDENTS AND POSTDOCTORAL FELLOWS

- **Principal advisor** to 7 PhD theses (University of Vienna, 4 completed, 3 in progress), co-advisor to 2 completed PhD theses (MedILS & ETH Zurich), principal advisor to 4 completed master theses (University of Split & University of Vienna, 3 completed, 1 in progress) and principal advisor to 5 completed bachelor theses (ETH Zurich, University of Split & University of Vienna). Directly supervised the work of 10 postdoctoral fellows.
- **External PhD Thesis Committee member:** 10 theses (ETH Zurich, BOKU Vienna, U of Vienna)
- **Recognition of associated students/postdocs:** Doc.Award by the City of Vienna for one of the 7 best PhD theses in 2013 at the University of Vienna to PhD student Anita Kuzmanic (2014); Academia Europaea prize for young Russian scientists to postdoc dr. Anton A. Polyansky (2015)

## TEACHING ACTIVITIES

2008 – 2016 Computational Biophysics, course, University of Zagreb & University of Vienna  
2009 – 2010 Protein Folding: Theory and Experiment, course, University of Split  
2013 – 2013 Noise in Biological Systems, seminar, University of Vienna  
2013 – 2016 Physical Chemistry for Molecular Biologists, course, University of Vienna  
2013 – 2016 Molecular Biophysics, practical course, University of Vienna

- **Lecturer at summer/winter schools of science** for high-school and university students: (S3 School, Visnjan, Croatia, 2005, 2006, 2009 & 2014; Computer Science Summer School, Pazin, Croatia, 2010; VBC Summer School, Vienna, Austria, 2012; Summer School of Biophysics, Primosten, Croatia, 2012, 2014; Future Biotech Winter School, Zvenigorod, Russia, 2014).

## ORGANISATION OF SCIENTIFIC MEETINGS

- principal organizer of the CECAM “Entropy in Biomolecular Systems” workshop, 2014, Vienna, Austria, with participation of more than 50 scientists from more than 10 countries
- principal organizer of the “Regional Biophysics Conference”, 2010, Primosten, Croatia, with participation of more than 100 scientists from more than 10 countries
- principal organizer of the “MedILS Summer School on Entropy in Biomolecular Systems”, 2008, Split, Croatia, with participation of 30 scientists from more than 10 countries
- principal organizer of the “1st Split Meeting on Development and Applications of Novel Methods and Models in Computational Biophysics and Structural Bioinformatics”, 2007, Split, Croatia
- co-organizer of monthly seminars for molecular dynamics community in Vienna (2011-present)
- advisory committee member for the “International Summer School of Biophysics”, Primosten, Croatia (2011-present) and the “From Solid-state to Biophysics” conference, Cavtat, Croatia (2012)

## ESTEEM FACTORS

- **Coordinator of PhD Student Selections**, MFPL Vienna, 2011-2014
- **Curriculum Committee member**, Computational Science MS, University of Vienna, 2011-2013
- **Steering Committee member**, Unity through Knowledge Fund, Croatia, 2012-2014
- **Management Board member**, MedILS Institute, Split, Croatia, 2007-2010
- **Reviewer in scientific journals:** PLOS Computational Biology, Journal of the American Chemical Society, Biophysical Journal, Biochemistry, Journal of Physical Chemistry, BMC Structural Biology, Bioinformatics, European Physical Journal E, Journal of Molecular Biology, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Physica, Croatica Chemica Acta, Proteomics, PLOS One, Journal of Structural Biology, Journal of Molecular Graphics and Modeling, Journal of Physical Chemistry Letters, Proteins, Journal of Chemical Information and Modeling
- **Editorial Board member:** Biology Direct
- **Grant reviewer:** Wellcome Trust UK, UKF Fund Croatia, National Science Fund Croatia

- **Given more than 75 lectures** at international scientific conferences (see below for details) and universities and institutes including ETH Zurich, University of Cambridge, EPFL Lausanne, NTU Singapore, Washington University, CRG Barcelona and Max Planck Institutes.
- **Directly carried out research at 7 different scientific institutes and universities** and collaborated in published research with groups at more than 10 different academic institutions all around the world, including Harvard University, Stanford University, Princeton University, ETH Zurich, University of Chicago, University of Queensland, Leiden University, BOKU Vienna and UC Santa Barbara.
- **Published 54 original scientific articles** (3085 citations, h-index = 22, Google Scholar, 16.03.2017).

#### **MOST IMPORTANT RESEARCH PROJECTS FUNDED**

1. **ERC Starting Independent Grant** (European Research Council, "Towards a quantitative framework for understanding protein-protein interactions: from specific effects to protein ecology", EUR 1 495 790, September 2011 – March 2017)
2. **START Award** (FWF Austrian Science Fund, "Towards a quantitative framework for understanding protein-protein interactions: from specific effects to protein ecology", EUR 1 140 600, August 2010 – August 2016 – discontinued in August 2011 in favor of the ERC grant)
3. **Unity Through Knowledge Fund 1A grant** (Ministry of Science, Education and Sports of the Republic of Croatia, "Worldwide distributed computing in molecular biology: from dynamic activation of enzymes to the problem of conformational averaging in structure determination", EUR 120 000, December 2007 – April 2010)
4. **NZZ/EMBO Installation Grant** (National Science Foundation of the Republic of Croatia and administrated through EMBO, "Using distributed computing techniques to study structure and dynamics of biomolecules", EUR 125 000, January 2008 – April 2010)

#### **SELECT FELLOWSHIPS AND AWARDS**

- 2013. member of the Young Academy of the Austrian Academy of Sciences
- 2010. START Prize, FWF Austrian Science Fund
- 2008-2010. NZZ/EMBO YIP Installation Fellow
- 2008. Tomorrow's PI Award, Genome Technology magazine
- 2005-2007. EMBO Postdoctoral Fellowship
- 2003. McGraw-Hill Award (best talk), European Protein Society Meeting, Florence, Italy
- 2002. Sun Microsystems Award, BCATS Symposium (best talk)
- 1998-2003. Howard Hughes Medical Institute Predoctoral Fellowship
- 1997-2000. Stanford Graduate Fellowship (Lucille P. Markey Fellow)
- 1995-1997. John Harvard Scholarship, Harvard University
- 1993-1995. Dean's List, La Roche College
- 1993-1995. Pacem In Terris Fellowship, La Roche College and Pacem in Terris Institute
- 1993. National Junior Champion in Fencing, Croatia
- 1991. 3rd Prize in the National Competition in Mathematics, Croatia

#### **SELECT TALKS AT CONFERENCES**

- 2016. EMBO Meeting "RNA Structure Meets Function", Stockholm Archipelago, Sweden
- 2014. CECAM Workshop on Modeling Cellular Life, Lausanne, Switzerland
- 2013. Frontiers in Dynamics Simulations of Biological Molecules, workshop, IRB Barcelona, Spain
- 2011. CECAM Workshop on Protein Folding, Lugano, Switzerland
- 2010. Prague Protein Spring Workshop, Prague, Czech Republic

#### **KEY RESEARCH PARTNERS (last 5 years)**

Chris Oostenbrink, BOKU Vienna, Austria  
John D. Sutherland, LMB Cambridge, UK  
Alwin Koehler, University of Vienna, Austria  
Navraj S. Pannu, Leiden University, Netherlands  
Kristina Djinojic, University of Vienna, Austria