CURRICULUM VITAE

Bojan Zagrovic, PhD

Professor of Molecular Biophysics
Department of Structural and Computational Biology
Max F. Perutz Laboratories & University of Vienna
Campus Vienna Biocenter 5, A-1030 Vienna, Austria
Email: bojan.zagrovic@univie.ac.at
Tel.: +43-1-4277-52271, Fax: +43-1-4277-9522

PERSONAL INFORMATION

Date of birth: November 8th 1974; Nationality: Croatian

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

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: 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: Eva J. Neer)

CURRENT POSITION

2017 – present **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, University Professor of Molecular Biophysics

PREVIOUS POSITIONS

2015 – 2017 **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, Associate Professor with tenure

2014 – 2015 **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, Assistant Professor

2010 – 2014 **University of Vienna**, Max F. Perutz Laboratories, Department of Structural and Computational Biology, junior group leader

2007 – 2010 **Mediterranean Institute for Life Sciences**, Split, Croatia, group leader

2004 – 2007 **ETH Zurich**, Switzerland, EMBO postdoctoral fellow in W. F. van Gunsteren's group

MAIN AREAS OF RESEARCH

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

- classical atomistic molecular dynamics simulations
- mechanism and thermodynamics of protein-protein and RNA-protein interactions
- conformational entropy in biomolecular interactions
- conformational averaging and its influence on biomolecular structure determination

PRINCIPAL RESEARCH ACCOMPLISHMENTS

- founding member of **Folding@Home**, a grid-computing project to study protein dynamics
- carried out and analyzed some of the first atomistic simulations of complete protein folding
- showed effects of conformational averaging in NMR, fiber diffraction and X-ray crystallography
- founded **Vienna PTM**, a resource for MD simulations of protein PTMs
- discovered and characterized cognate mRNA-protein compositional complementarity

SUPERVISION OF STUDENTS AND POSTDOCTORAL FELLOWS

- **Principal advisor** to 7 PhD theses (University of Vienna, 5 completed, 1 in progress), principal advisor to 7 master theses (University of Split & University of Vienna, 4 completed, 2 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.
- **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 – 2018 Computational Biophysics, course, University of Zagreb & University of Vienna
2009 – 2010 Protein Folding: Theory and Experiment, course, University of Split
2013 – 2018 Physical Chemistry for Molecular Biologists, course, University of Vienna
2013 – 2018 Practical Course in 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, 2012/2014/2016; Future Biotech Winter School, Zvenigorod, Russia, 2014).

PRINCIPAL ORGANISER OF SCIENTIFIC MEETINGS

- CECAM “Entropy in Biomolecular Systems” workshop, 2014, Vienna, Austria (56 participants)
- “Regional Biophysics Conference”, 2010, Primosten, Croatia (110 participants)
- "MedILS Summer School on Biomolecular Entropy”, 2008, Split, Croatia (30 participants)

- co-organizer of monthly seminars for molecular dynamics community in Vienna (2011-present)

ESTEEM FACTORS

- **Coordinator of PhD Student Selections**, MFPL Vienna, 2011-2014
- **Steering Committee member**, Unity through Knowledge Fund, Croatia, 2012-2014
- **Management Board member**, MedILS Institute, Split, Croatia, 2007-2010
- **Reviewer in scientific journals**: Journal of the American Chemical Society, PLOS Computational Biology, Biophysical Journal, Journal of Molecular Biology and 20+ other journals
- **Grant reviewer**: Wellcome Trust UK, UKF Fund Croatia, National Science Fund Croatia
- **Given more than 80 talks** 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
- **Published 58 original scientific articles** (2632 citations, h-index = 22, WoS, 20.07.2018).

MOST IMPORTANT RESEARCH PROJECTS FUNDED

1. **ERC Proof of Concept Grant** (European Research Council, "Short, weakly interacting RNA ligands for the development of high-concentration monoclonal antibody therapeutics", € 150.000, Jul 2018 – Jan 2020)
2. **FWF Stand-alone Project** (Austrian Science Fund, "RNA-protein interactions in an unstructured context", € 323.450, Apr 2018 – Mar 2021)
3. **FWF Stand-alone Project** (Austrian Science Fund, "2' vs. 3' aminoacylation in biological translation", € 323.450, Aug 2017 – Jul 2020)
4. **ERC Starting Independent Grant** (European Research Council, "Towards a quantitative framework for understanding protein-protein interactions: from specific effects to protein ecology", € 1.495.790, Sept 2011 – March 2017)
5. **START Award** (FWF Austrian Science Fund, "Towards a quantitative framework for understanding protein-protein interactions: from specific effects to protein ecology", € 1.140.600, Aug 2010 – Aug 2016, discontinued in Aug 2011 in favor of the ERC grant)
6. **Unity Through Knowledge Fund 1A grant** (Ministry of Science of Croatia, "Worldwide distributed computing in molecular biology: from dynamic activation of enzymes to the problem of conformational averaging in structure determination", € 120.000, Dec 2007 – April 2010)
7. **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", € 125.000, Jan 2008 – April 2010)

5 SELECT FELLOWSHIPS AND AWARDS

2013. member of the Young Academy of Austrian Academy of Sciences; **2010.** START Prize, Austrian Science Fund; **2008.** Tomorrow's PI Award, Genome Technology magazine; **2005.** EMBO Postdoctoral Fellowship; **2003.** McGraw-Hill Award (best talk), European Protein Society Meeting, Florence, Italy

5 SELECT CONTRIBUTED* AND INVITED TALKS

2018. FEBS Congress, Prague, Czech Republic; **2016.** EMBO Workshop on RNA Structure and Function, Stockholm, Sweden*; **2015.** Computational Analysis of RNA Structure and Function, Benasque, Spain*; **2013.** CECAM workshop on Modeling Cellular Life, Lausanne, Switzerland**; **2011.** CECAM Workshop on Protein Folding, Lugano, Switzerland.

KEY RESEARCH PARTNERS (last 5 years)

John D. Sutherland, LMB Cambridge, UK; Gordan Zitkovic, University of Texas, USA; Ivo F. Sbalzarini, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany; Navraj S. Pannu, Leiden University, Netherlands; Sascha Martens, University of Vienna, Austria

PEER-REVIEWED ARTICLES OVER THE LAST FIVE YEARS (2013-2018)

25. Zagrovic B, Bartonek L & Polyansky AA (2018) "RNA-protein interactions in an unstructured context", **FEBS Letters**, DOI:10.1002/1873-3468.13116.

24. Fleck M, Polyansky AA & Zagrovic B (2018) "Self-Consistent Framework Connecting Experimental Proxies of Protein Dynamics with Configurational Entropy", **Journal of Chemical Theory and Computation**, 14(7), 3796-3810.

23. Kaufmann T, Grishkovskaya I, Polyansky AA, Kostrhon S, Kukolj E, Olek KM, Herbert S, Beltzung E, Mechtler K, Peterbauer T, Gotzmann J, Zhang L, Hartl M, Zagrovic B, Elsayad K, Djinovic-Carugo K & Slade D (2017) "A novel non-canonical PIP-box mediates PARG interaction with PCNA", **Nucleic Acids Research**, 45(16), 9741–9759.

22. de Ruiter A, Polyansky AA & Zagrovic B (2017) "Dependence of binding free energies between RNA nucleobases and protein side chains on local dielectric properties**", Journal of Chemical Theory and Computation**, 13(9), 4504-4513.

21. Bartonek L & Zagrovic B (2017) "mRNA/protein sequence complementarity and its determinants: The impact of affinity scales", **PLOS Computational Biology**, 13(7), e1005648.

20. Weichselbaum D, Zagrovic B & Polyansky AA (2017) "*Fuento*: Functional enrichment for bioinformatics", **Bioinformatics**, 16, 2604–2606.

19. Fracchiolla D, Sawa-Makarska J, Zens B, de Ruiter A, Zaffagnini G, Brezovich A, Romanov J, Runggatscher K, Kraft C, Zagrovic B & Martens S (2016) "Mechanism of cargo-directed Atg8 conjugation during selective autophagy", **eLIFE**, 5, e18544.

18. Gallego LD, Steger MG, Polyansky AA, Schuber T, Zagrovic B, Zheng N, Clausen T, Herzog F & Kohler A (2016) "Structural mechanism for the recognition and ubiquitination of a single nucleosome residue by Rad6-Bre1", **Proceedings of the National Academy of Sciences USA**, 113, 10553-10558.

17. Hajnic M, de Ruiter A, Polyansky AA & Zagrovic B (2016) "Inosine nucleobase acts as guanine in interactions with protein side chains", **Journal of the American Chemical Society**, 138, 5519−5522.

16. Fleck M, Polyansky AA & Zagrovic B (2016) "PARENT: A Parallel Software Suite for the Calculation of Configurational Entropy in Biomolecular Systems", **Journal of Chemical Theory and Computation**, 2(4), 2055-65.

15. Petrov D, Daura X & Zagrovic B (2016) "Effect of Oxidative Damage on the Stability and Dimerization of Superoxide Dismutase 1", **Biophysical Journal**, 110(7), 1499-1509.

14. Hajnic M, Osorio JI & Zagrovic B (2015) "Interaction preferences between nucleobase mimetics and amino acids in aqueous solutions", **Physical Chemistry Chemical Physics**, 17(33), 21414-21422.

13. Hlevnjak M & Zagrovic B (2015) "Malleable nature of mRNA-protein compositional complementarity and its functional significance", **Nucleic Acids Research**, 43(6), 3012-3021.

12. de Ruiter A & Zagrovic B (2015) "Absolute binding-free energies between standard RNA/DNA nucleobases and amino-acid sidechain analogs in different environments", **Nucleic Acids Research**, 43(2), 708–718.

11. Beier A, Zagrovic B & Polyansky AA (2014) "On the Contribution of Protein Spatial Organization to the Physicochemical Interconnection between Proteins and Their Cognate mRNAs", **Life**, 4(4), 788-799.

10. Hajnic M, Osorio JI & Zagrovic B (2014) “Computational analysis of amino acids and their sidechain analogs in crowded solutions of RNA nucleobases with implications for the mRNA–protein complementarity hypothesis”, **Nucleic Acids Research**, 42(21), 12984-12994.

9. de Almeida Ribeiro E, Pinotsis N, Ghisleni A, Salmazo A, Konarev PV, Kostan J, Sjoeblom B, Schreiner C, Polyansky AA, Gkougkoulia EA, Holt MR, Aachmann FL, Zagrovic B, Bordignon E, Pirker KF, Svergun DI, Gautel M and Djinovic-Carugo K (2014) “The structure of human muscle α-actinin: Insight into the intramolecular regulation of ligand binding and Z-disk assembly”, **Cell**, 159, 1447–1460.

8. Petrov D & Zagrovic B (2014) “Are current atomistic force fields accurate enough to study proteins in crowded environments?, **PLOS Computational Biology**, 10(5), e1003638.

7. Kuzmanic A, Pannu NS & Zagrovic B (2014) “X-ray refinement significantly underestimates the level of microscopic heterogeneity in biomolecular crystals”, **Nature Communications**, 5, 3220, 1-10.

6. Kuzmanic A & Zagrovic B (2014) “Dependence of Protein Crystal Stability on Residue Charge States and Ion Content of Crystal Solvent”, **Biophysical Journal**, 106(3), 677-686.

5. Polyansky AA & Zagrovic B (2013) “Evidence of direct complementary interactions between messenger RNAs and their cognate proteins”, **Nucleic Acids Research**, 41(18), 8434-8443.

4. Polyansky AA, Hlevnjak M & Zagrovic B (2013) “Analog encoding of physicochemical properties of proteins in their cognate messenger RNAs”, **Nature Communications,** 4, 2784, 1-11.

3. Polyansky AA, Hlevnjak M & Zagrovic B (2013) “Proteome-wide analysis reveals clues of complementary interactions between mRNAs and their cognate proteins as the physicochemical foundation of the genetic code”, RNA **Biology**, 10(8), 1248-1254.

2. Petrov D, Margreitter C, Grandits M, Oostenbrink C & Zagrovic B (2013) “A systematic framework for molecular dynamics simulations of protein post-translational modifications”, **PLOS Computational Biology**, 9(7), e1003154.

1. Margreitter C, Petrov D & Zagrovic B (2013) “Vienna-PTM: a toolkit for MD simulations of post-translational modifications of proteins”, **Nucleic Acids Research**, 41(Web Server issue), W422-6 (Featured Article).

OTHER SCHOLARLY CONTRIBUTIONS

3. Martinez J & Zagrovic B (2016), "A code within a code : how codons influence mRNA stability", **EMBO Journal**, 35, 2064-2065 (perspective article).

2. Zagrovic B (2014) "Life is translation", RNA **Biology**, 11, 1-3 (perspective article).

1. Zagrovic B (2014) "Of RNA-binding proteins and their targets: interaction determines expression", **Genome Biology**, 15(1), 102-104. (perspective article)

TOP 10 PEER-REVIEWED ARTICLES

10. Hajnic M, de Ruiter A, Polyansky AA & Zagrovic B (2016) "Inosine nucleobase acts as guanine in interactions with protein side chains", **Journal of the American Chemical Society**, 138, 5519−5522.

9. de Ruiter A & Zagrovic B (2015) "Absolute binding-free energies between standard RNA/DNA nucleobases and amino-acid sidechain analogs in different environments", **Nucleic Acids Research**, 43(2), 708–718.

8. Kuzmanic A, Pannu NS & Zagrovic B (2014) "X-ray refinement significantly underestimates the level of microscopic heterogeneity in biomolecular crystals", **Nature Communications**, 5, 3220, 1-10.

7. Polyansky AA & Zagrovic B (2013) "Evidence of direct complementary interactions between messenger RNAs and their cognate proteins", **Nucleic Acids Research**, 41(18), 8434-8443.

6. Polyansky AA, Hlevnjak M & Zagrovic B (2013) "Analog encoding of physicochemical properties of proteins in their cognate messenger RNAs", **Nature Communications,** 4, 2784, 1-11.

5. Hlevnjak M, Polyansky AA & Zagrovic B (2012) "Sequence signatures of direct complementarity between mRNAs and cognate proteins on multiple levels", **Nucleic Acids Research**, 40(18): 8874-8882 (Featured Article).

4. Wlodarski T & Zagrovic B (2009) "Conformational selection and induced fit mechanism underlie specificity in non-covalent interactions with ubiquitin", **Proceedings of the National Academy of Sciences USA**, 106(46), 19346-19351.

3. Zagrovic B, Lipfert J, Sorin EJ, Millet IS, van Gunsteren WF, Doniach S & Pande, VS (2005) “Unusual compactness of a polyproline type II structure”, **Proceedings of the National Academy of Sciences USA**, 102(33), 11698-11703.

2. Zagrovic B & Pande VS (2003) “Structural correspondence between the alpha-helix and the random-flight chain resolves how unfolded proteins can have native-like properties”, **Nature Structural Biology**, 10(11), 955-961.

1. Zagrovic B, Sorin EJ & Pande, VS (2001) “β-hairpin folding simulations in atomistic detail using an implicit solvent model”, **Journal of Molecular Biology**, 313(1), 151-169.