

Mediterranean Institute for Life Sciences
Meštrovićevo šetalište bb
21000 Split, Croatia
Tel: 00385-21-555-602

Permanent address:
Borisa Papandopula 15
21000 Split
Croatia

Bojan Zagrovic, PhD

zagrovic@medils.hr

- born November 8th 1974
- citizen of the Republic of Croatia

Education

- 1997 - 2004 **Stanford University**, Stanford, CA, USA
PhD in Biophysics, 2004
Thesis: "Studying protein folding and dynamics using worldwide distributed computing" (advisor: Vijay S. Pande, 2000-2004)

Other projects: "X-ray crystallographic analysis of a voltage and calcium sensitive ion channel Mslo" (advisors: Richard W. Aldrich and William I. Weis, 1997-2000)
- 1995-1997 **Harvard University**, Cambridge, MA, USA
AB in Biochemical Sciences, *magna cum laude*, 1997
Thesis: "Analysis of the enzymatic activity of the brain adenylyl cyclase" (advisor: Eva J. Neer)
- 1993-1995 **La Roche College**, Pittsburgh, PA, USA
Chemistry and Biology major

Work experience

- 2007 - **Mediterranean Institute for Life Sciences**, Split, Croatia
group leader in computational biophysics
- 2007 - 2008 **Mediterranean Institute for Life Sciences**, Split, Croatia
group leader in computational biophysics; scientific director
- 2004 - 2007 **Swiss Federal Institute of Technology ETH**, Zurich, Switzerland: EMBO Postdoctoral Fellow, Chemistry Department, group of Wilfred F. van Gunsteren

Research Interests

Computational and theoretical studies of structure and dynamics of biomolecules including:

- atomistic simulations of protein folding
- worldwide distributed computation
- unfolded state of proteins
- conformational averaging and its influence on what we know about biomolecular structure
- principles of protein structure determination by NMR and X-ray
- dynamic activation and entropy in enzyme function
- representation of protein structure and dynamics
- small angle X-ray scattering
- free energy calculations
- intrinsically unstructured proteins

Research Accomplishments

- member of the team of scientists who designed and used a super-cluster of more than 250,000 volunteer computer processors to address fundamental challenges in biomolecular simulations (Folding@Home project)
- simulated multiple complete folding events for several small proteins in atomistic detail at room temperature: first-ever complete atomistic simulations of protein folding events
- gave evidence that the topology of small single-domain proteins can be native-like on average (formulated in “the mean structure hypothesis”)
- used folding rate comparison as first-ever rigorous and absolute tests of the existing atomistic force fields in studying protein folding kinetics
- demonstrated close structural correspondence between the α -helix and the average random-flight chain with persistence length of 1 amino acid, suggesting how unfolded proteins can have native-like properties
- showed experimentally (SAXS) that alanine based α -helical peptides are more compact than usually thought, suggesting that they might adopt broken-rod configuration, even for very short sequences. Using the same technique demonstrated that an unfolded protein rarely or never adopts an extended polyproline type II configuration (ppII), despite the fact that individual residues likely do sample the ppII configuration to a high degree
- demonstrated the advantages of computational parallelization in single-step perturbation calculations of relative binding free energies
- showed that, under certain conditions, cylindrically averaged fiber diffraction patterns of random walks on lattices with fixed angles exhibit signature motifs of helical diffraction

Honors and grants

Tomorrow's PI – voted one of 30 up-and-coming young researchers in molecular biology worldwide by Genome Technology, 2008

EMBO YIP Installation Grant 2008 (NZZ Croatia)

Unity Through Knowledge Fund 1A Grant 2008 (MZOS Croatia)

EMBO Postdoctoral Fellowship, 2005-2007

McGraw-Hill Italia Award from the Protein Society for the best young scientist talk at the European Protein Society Meeting, Florence, Italy, 2003

Sun Microsystems Award for the best scientific talk at the BCATS Symposium, Stanford, CA, USA, 2002

Howard Hughes Medical Institute Predoctoral Fellowship, 1998-2003

Stanford Graduate Fellowship (Lucille P. Markey Fellow), 1997-2000

John Harvard Scholarship, Harvard University, 1995-1997

Ford Summer Research Fellowship, Harvard University, 1996

Dean's List, La Roche College, 1993-1995

Pacem In Terris Fellowship, La Roche College and Pacem in Terris Institute, 1993-1995

National Junior Champion in Fencing, Croatia, 1993

3rd Prize in the National Competition in Mathematics, Croatia, 1991

Studentships supervised

Tomek Wlodarski, FESB Summer Research Grant, July-September 2008

Publications and Contributions

Non-scientific

1. Let's Go Europe Travel Guide 1998 (chapters on Croatia, Slovenia and Hungary) Let's Go Publications, Inc., Cambridge, MA 02138, USA

Original research articles

21. Zagrovic B, Gattin Z, Lau JK, Huber M & van Gunsteren WF (2008) "Structure and dynamics of two beta-peptides in solution from molecular dynamics simulations validated against experiment", European Biophysics Journal, 37(6):903-912.

20. Schwab F, van Gunsteren WF & Zagrovic B (2008) "Computational study of the mechanism and the relative free energies of binding of anticholesteremic inhibitors to squalene-hopene cyclase", *Biochemistry*, 47(9), 2945-51.
19. Schmid N, Zagrovic B & van Gunsteren WF (2007) "Folding-unfolding equilibrium of a methylidene-substituted beta-peptide", *Helvetica Chimica Acta*, 90 (10), 1966-1979.
18. Zagrovic B (2007) "Helical signature motif in the fiber diffraction patterns of random walk chains", *Molecular Physics*, 105 (10), 1299-1306.
17. Schmid N, Zagrovic B & van Gunsteren WF (2007) "Thermodynamics and mechanism of binding of polypyrimidine tract binding protein to RNA", *Biochemistry*, 46(22):6500-6512.
16. Zagrovic B & van Gunsteren WF (2006) "Computational analysis of the mechanism and thermodynamics of inhibition of phosphodiesterase 5A by synthetic ligands", *Journal of Chemical Theory and Computation*, 3, 301-311.
15. Zagrovic B & Pande VS (2006) "Simulated unfolded-state ensemble and the experimental NMR structures of villin headpiece yield similar wide-angle solution X-ray scattering profiles", *Journal of the American Chemical Society*, 128 (36), 11742-11743.
14. Zagrovic B & van Gunsteren WF (2006) "Comparing atomistic simulation data with the NMR experiment: how much can NOEs actually tell us?", *Proteins*, 63 (1), 210-218.
13. 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.
12. Zagrovic B, Jayachandran G, Millet IS, Doniach S & Pande, VS (2005) "How large is an α -helix? Studies of the radii of gyration of helical peptides by small-angle X-ray scattering and molecular dynamics", *Journal of Molecular Biology*, 353 (2), 232-241.
11. Zagrovic B & Pande VS (2004) "How does averaging affect protein structure comparison on the ensemble level?", *Biophysical Journal*, 87, 2240-2246.
10. Kohn J, Millett IS, Jacob J, Zagrovic B, Dillon TM, Cingel N, Dothager RS, Seifert S, Thiyagarajan P, Sosnick TR, Hasan ZM, Pande VS, Ruczinski I, Doniach S & Plaxco KW (2004) "Do the dimensions of chemically unfolded proteins differ significantly from the expectations of a random-coil model?", *Proceedings of the National Academy of Sciences USA*, 101 (34), 12491-12496.
9. Lenz P, Zagrovic B, Shapiro J & Pande VS (2004) "Folding probabilities: a novel approach to folding transitions and the two-dimensional Ising model", *Journal of Chemical Physics*, 120 (14), 6769-6778.
8. 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.

7. Zagrovic B, Snow CD, Khaliq S, Shirts MR & Pande VS (2002) "Simulation of folding of a small alpha-helical protein using worldwide distributed computation", *Journal of Molecular Biology*, 323 (5), 927-937.
6. Zagrovic B & Pande VS (2003) "Solvent viscosity dependence of the folding rate of a small protein: distributed computing study", *Journal of Computational Chemistry*, 24, 1432-1436.
5. Snow CD, Zagrovic B & Pande VS (2002) "Trp Cage: Folding kinetics and unfolded state topology", *Journal of the American Chemical Society*, 24(49), 14548-14549.
4. Zagrovic B, Snow CD, Khaliq S, Shirts MR & Pande VS (2002) "Native-like mean structure in the unfolded ensemble of small proteins", *Journal of Molecular Biology*, 323 (1), 153-164.
3. Pande VS, Baker I, Chapman J, Elmer S, Khaliq S, Larson SM, Rhee YM, Shirts MR, Snow CD, Sorin EJ & Zagrovic B. (2002) "Atomistic protein folding simulations on the hundreds of microsecond timescale using worldwide distributed computing ", *Biopolymers*, 68 (1), 91-109.
2. 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.
1. Mende U, Zagrovic B, Cohen A, Li Y, Valenzuela D, Fishman MC & Neer EJ (1998) "Effect of deletion of the major brain G-protein α_0 subunit on coordination of G-protein subunits and on adenylyl cyclase activity", *Journal of Neuroscience Research*, 54, 263-272.

Other scholarly contribution

3. Zagrovic B (2008) "The Mediterranean institute for life sciences - An attempt at scientific excellence in Croatia", *IUBMB Life*, 60(5), 262-264. (science policy article)
2. Zagrovic B & Dikic I (2008) "Childhood of a phoenix: modern biology in Eastern and South-Eastern Europe", *Nature Reviews Molecular Cell Biology*, 9(4), 333-336. (science policy article)
1. Zagrovic B & Aldrich RW (1999) "For the latest information, tune to channel Kcsa", *Science*, 285, 59. (scientific commentary)

Submitted articles

1. Müller CL, Sbalzarini IF, van Gunsteren WF, Zagrovic B & Hünenberger PH (2008) "In the eye of the beholder: inhomogeneous distribution of high-resolution shapes within the random-walk ensemble", submitted to *Journal of Chemical Physics*
2. Wlodarski T & Zagrovic B (2009) "Conformational selection and induced fit mechanism underlie specificity in non-covalent interactions with ubiquitin", submitted to *Science Signaling*

Scientific Talks

- 2009. IRB Barcelona, Spain
- 2009. Regional Biophysics Conference, Linz, Austria
- 2009. CCPB Biomolecular Simulation conference, York, UK
- 2008. MedILS summer school on entropy in biomolecular systems, Split, Croatia
- 2008. EMBO YIP meeting, EMBL, Heidelberg, Germany
- 2008. From Solid-state to Biophysics conference, Cavtat, Croatia
- 2008. EMBO meeting on cellular signaling, Cavtat, Croatia
- 2008. Physics Department seminar, PMF Zagreb, Croatia
- 2008. Department of Inorganic Chemistry; University of Zurich, Switzerland
- 2008. BEST - international meeting of electrical engineering students, Zagreb
- 2007. Structural bioinformatics conference, Split, Croatia
- 2007. Chemistry Department, University of Zagreb
- 2007. Computer Science Department Seminar, ETH Zurich
- 2007. The 2nd Opatija Meeting On Computational Solutions in the Life Sciences, Opatija, Croatia
- 2007. Regional Biophysics Conference, Balatonfüred, Hungary
- 2007. EMBO Intrinsically Unfolded Proteins, Budapest, Hungary
- 2007. Chemistry Department seminar, EPFL Lausanne, Switzerland
- 2007. Necker Institute, Paris, France
- 2007. Biophysics Department seminar, Washington University, USA
- 2006. Gordon Conference on Computational Chemistry, Les Diablerets, Switzerland
- 2006. Institute of Physics, Zagreb, Croatia
- 2006. CECAM workshop, Lyon, France
- 2006. BIOMOS meeting, Burg Arras, Germany
- 2006. Medils Institute, Split, Croatia
- 2006. Chemistry Department Seminar, Cambridge University, UK
- 2005. NCCR Report, University of Zurich, Zurich, Switzerland
- 2005. BIOMOS meeting, Burg Arras, Germany
- 2005. Croatian Biophysical Society Meeting, Zagreb, Croatia
- 2005. Workshop on Macromolecular Modeling, Hünfeld, Germany
- 2005. Ludwig Institute, Lausanne, Switzerland
- 2004. Society for Mathematical and Theoretical Biology, Ruđer Bošković Institute, Zagreb, Croatia
- 2004. Pliva Pharmaceuticals, Zagreb, Croatia
- 2003. European Protein Society Meeting, Florence, Italy
- 2003. Gen-Proc Symposium, Tokyo, Japan
- 2002. SAC-CASP, Pacific Grove, CA, USA
- 2002. BCATS Symposium, Stanford University, CA, USA
- 2002. Molecular Biophysics Seminar, Stanford University, CA, USA

Languages

Croatian (native), English (fluent), German (advanced)

Professional and academic activities

- head, Laboratory of Computational Biophysics, Mediterranean Institute for Life Sciences, Split, Croatia
- scientific director, 2007-2008, Mediterranean Institute for Life Sciences, Split, Croatia
- reviewer for BMC Structural Biology, Journal of the American Chemical Society, Journal of Physical Chemistry, European Physical Journal E, Journal of Molecular Biology, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Physica, Croatica Chemica Acta
- 3 undergraduate thesis (completed), 1 master's thesis (completed) and 1 PhD thesis co-advisor ETH Zurich (in progress)
- 1 undergraduate thesis (University of Zagreb, in progress)
- 3 PhD theses advisor (University of Split, Croatia, in progress)
- teaching assistant for Cellular Biophysics (Stanford University), Computational statistical physics, Introduction to Computer Sciences for Scientists, Computational Chemistry (ETH Zurich)
- principal co-organizer of the "MedILS Summer School on Entropy in Biomolecular Systems 2008" with participation of 30 scientists from more than 10 countries (<http://www.medils.org/index.php/summer-schools-2008/entropy-in-biomolecular-systems/>)
- principal co-organizer of the "1st Split Meeting on Development and Applications of Novel Methods and Models in Computational Biophysics and Structural Bioinformatics", Split, Croatia

References

Dr. Vijay S. Pande, Professor, Department of Chemistry, Stanford University, Stanford, CA 94305, USA. Email: pande@stanford.edu. Tel: 001-650-723-3660.

Dr. Wilfred F. van Gunsteren, Professor, Physical Chemistry Institute, ETH, Zurich, CH-8093, Switzerland. Email: wfvgn@igc.phys.chem.ethz.ch. Tel: 0041-44-632-5501

Dr. Sebastian Doniach, Professor, Departments of Physics and Applied Physics, Stanford University, Stanford, CA 94305, USA. Email: doniach@drizzle.stanford.edu. Tel: 001-650-723-4786.

Dr. Kevin W. Plaxco, Professor, Chemistry and Biochemistry Department, UC Santa Barbara, Santa Barbara, CA 93106, USA. Email: kwp@chem.ucsb.edu. Tel: 001-805-893-5558.

Dr. Philippe Hünenberger, Physical Chemistry Institute, ETH, Zurich, CH-8093, Switzerland. Email: phil@igc.phys.chem.ethz.ch. Tel: 0041-44-632-5503