

Asim Okur

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## EDUCATION

- PhD, Chemistry, May 2007, Stony Brook University, Stony Brook, NY
- BS, Chemical Engineering, May 2000, Bogazici University, Istanbul Turkey

## RESEARCH INTERESTS

- Computational structural biology, peptide and protein folding
- Enhanced conformational sampling algorithms such as Replica Exchange Method
- Free energy calculations, drug binding calculations, loop modeling

## RESEARCH EXPERIENCE

- 2000 – 2007, Graduate Research  
Stony Brook University, Chemistry Department, with Dr. Carlos Simmerling
  - o Determined the transferability of force field parameters using energy comparisons of decoy structures. Worked on further improvements and testing of new parameter sets for AMBER.
  - o Worked on folding kinetics and thermodynamics of  $\beta$ -hairpins through molecular dynamics and Replica Exchange Methods.
  - o Incorporated hybrid explicit/implicit solvation scheme to Replica Exchange Method to reduce the number of replicas required for explicit solvent simulations and tested its performance on short alanine peptides and salt bridged peptides.
  - o Developed a new variant of Replica Exchange Method to increase sampling efficiency and convergence rates by coupling the high temperature replica to a pre-generated structure reservoir
  - o Worked on determining the flap opening and closing events on HIV-1 protease
- 1999 – 2000, Undergraduate Research  
Bogazici University, Chemical Engineering Department, Istanbul, Turkey, Senior research with Prof. Ivet Bahar
  - o Investigated key residues for protein stability using normal mode analysis via Gaussian Network Model on various proteins.

## PUBLICATIONS

1. Roitberg A., Okur A., Simmerling C., “Coupling of Replica Exchange Simulations to a non-Boltzmann structure reservoir”, *Journal of Physical Chemistry B*, 111, p.2415-2418, 2007
2. Roe D., Okur A., Wickstrom L., Hornak V., Simmerling C., “A Detailed Study of Several Implicit Solvent Models: Comparison of Free Energy of Solvent Polarization and Thermodynamics to Explicit Solvent Results”, *Journal of Physical Chemistry B*, 111, p.1846-1857, 2007
3. Okur A., Roe D., Cui G., Hornak V., Simmerling C., “Improving Convergence of Replica Exchange Simulations through Coupling to a High Temperature Structure Reservoir”, *Journal of Chemical Theory and Computation*, 3, p.557-568, 2007
4. Hornak V., Abel R., Okur A., Strockbine B., Roitberg A., Simmerling C., “Comparison of multiple Amber force fields and development of improved protein backbone parameters”, *Proteins: Structure, Function and Bioinformatics*, v65(3),p.712-725, 2006.
5. Wickstrom L., Okur A., Song K., Hornak V., Raleigh D., Simmerling S., “The Unfolded State of the Villin Headpiece Helical Subdomain: Computational Studies of the Role of Locally Stabilized Structure”, *Journal of Molecular Biology*, 360 (5), p.1094-1107, 2006

6. Okur A., Simmerling C., "Hybrid explicit/implicit solvation methods", Annual Reports in Computational Chemistry, v2, p.97-109, 2006.
7. Okur A., Wickstrom L., Layten M., Geney R., Song K., Hornak V., Simmerling C., "Improved efficiency of replica exchange simulations through use of a hybrid explicit/implicit solvation model", Journal of Chemical Theory and Computation, v.2, p.420-433, 2006.
8. Hornak V., Okur A., Rizzo RC., Simmerling C., "HIV-1 Protease Flaps Spontaneously Close to the Correct Structure in Simulations Following Manual Placement of an Inhibitor into the Open State", Journal of American Chemical Society, v.128, p.2812-2813, 2006.
9. Hornak V., Okur A., Rizzo RC., Simmerling C., "HIV-1 protease flaps spontaneously open and recluse in molecular dynamics simulations", PNAS, v.103, no.4, p.915-920, 2006.
10. Okur A., Strockbine B., Hornak V., Simmerling C., "Using PC Clusters to Evaluate the Transferability of Molecular Mechanics Force Fields for Proteins", Journal of Computational Chemistry, v.24, p.21-31, 2003.

## PRESENTATIONS

- 233<sup>rd</sup> ACS National Meeting: General Oral: Molecular Mechanics, Oral Presentation, "Improving Convergence of Replica Exchange Simulations", Chicago, 2007
- 231<sup>st</sup> ACS National Meeting: Computers and Chemistry and SCI-MIX, Poster, "Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model", Atlanta, GA, 2006
- 227<sup>th</sup> ACS National Meeting: Computers and Chemistry, Poster, "Multiple pathways in  $\beta$ -hairpin folding and unfolding simulations", Anaheim, CA, 2004
- 226<sup>th</sup> ACS National Meeting: Computers and Chemistry, Poster, "Folding Kinetics of a  $\beta$  – Hairpin: A molecular dynamics study", NYC, NY, 2003
- Gordon Research Conference: Computational Chemistry, Poster, "Using PC Clusters to Evaluate the Transferability of Molecular Mechanics Force Fields for Proteins", NH, 2002

## TEACHING EXPERIENCE

- Stony Brook University, Chemistry Department, Stony Brook, NY  
Fall 2004, Guest Lecture, AMS 535 Introduction to Computational Structural Biology and Drug Design, Lectures on "Introduction to Molecular Dynamics" and "Replica Exchange Method"
- Fall 2003, Teaching Assistant, CHE 301 Physical Chemistry I
- Spring 2001, Teaching Assistant, CHE 134 General Chemistry Laboratory II
- Fall 2000, Teaching Assistant, CHE 133 General Chemistry Laboratory I

## AWARDS AND AFFILIATIONS

- CCG Excellence Award from COMP Division of American Chemical Society and Chemical Computing Group, "Multiple pathways in  $\beta$ -hairpin folding and unfolding and unfolding simulations", Spring 2004
- First Year Teaching Assistant Award for academic year 2000 – 2001, Stony Brook University Chemistry Department, 2001
- Member of American Chemical Society
- Member of Graduate Chemical Society, Stony Brook University, Stony Brook, NY

## SKILLS

Computational Skills: AMBER, Shell scripting, Fortran, C/C++, Linux system administration, VMD, PovRay, OpenDX, Microsoft Office, Endnote

- Languages: Turkish (native), English and German (fluent in reading, writing and speaking)

## REFERENCES

Dr. Carlos Simmerling  
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