Curriculum Vitae

Nurit Haspel

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EDUCATION

Tel-Aviv University, Tel-Aviv, Israel

2002-2006

Ph.D., Structural Bioinformatics (Department of Computer Science)

Advisors: Prof. Haim Wolfson and Prof. Ruth Nussinov

Thesis title: Computational modeling and prediction of self assembling beta-sheet rich

protein structures

Tel-Aviv University, Tel-Aviv, Israel

1999-2002

M.Sc., Structural Bioinformatics (Department of Human Genetics),

Summa Cum Laude

Advisors: Prof. Ruth Nussinov and Prof. Haim Wolfson

Thesis title: Computational study of protein folding pathways using the building blocks

folding model

Tel-Aviv University, Tel-Aviv, Israel

1995-1998

B.Sc., Chemistry and Computer Science, Magna Cum Laude

ACADEMIC EMPLOYMENT

University of Massachusetts Boston, Department of Computer Science

Assistant Professor

Rice University, Houston, TX, Department of Computer Science

2007-2009

2009-present

Postdoctoral research associate, Physical and Biological Computing Group

Advisor: Prof. Lydia Kavraki

Tel-Aviv University, Tel-Aviv, Israel, School of Computer Science

2002-2006

Research and teaching assistant, Structural Bioinformatics Group.

Advisors: Prof. Haim Wolfson and Prof. Ruth Nussinov

National Cancer Institute, Frederick, MD

2001-2005

Visiting researcher, Center for Cancer Research Nanobiology Program

Advisor: Prof. Ruth Nussinov

1999-2002

Research assistant, Structural Bioinformatics Group.

Advisors: Prof. Ruth Nussinov and Prof. Haim Wolfson

SELECTED AWARDS AND SCHOLARSHIPS

- **2009:** Postdoctoral Fellow of NIH Nanobiology Training program of the Gulf Coast Consortia (declined).
- 2004, 2006: Tel Aviv University School of Computer Science PhD fellowship.
- 2005: Don and Sara Marein award for PhD students.
- 2005: Dan David prize for PhD students.
- 2002,2003: Tel Aviv University Rector Scholarship for excellent PhD students.
- 1999-2001: Tel Aviv University School of Medicine MSc Fellowship.
- 1997: Tel Aviv University commemoration fellowship.
- 1997: Undergraduate training scholarship, School of Chemistry, Tel Aviv University
- 1996,1997: Dean's honor list, School of Chemistry, Tel Aviv University.

PUBLICATIONS

PEER REVIEWED JOURNAL ARTICLES

- 1. Akbal-Delibas B., Hashmi I., Shehu A. and **Haspel N.**, An Evolutionary Conservation Based Method for Refining and Reranking Protein Complex Structures. Journal of Bioinformatics and Computational Biology (JBCB), in press, 2012.
- 2. Hashmi I., Akbal-Delibas B., **Haspel N.** and Shehu A., Guiding Protein Docking with Geometric and Evolutionary InformationJournal of Bioinformatics and Computational Biology (JBCB), in press, 2012.
- 3. **Haspel N.,** Zanuy D., Nussinov R., Teesalu T., Ruoslahti E. and Aleman C. Binding of a C-end rule peptide to neuropilin-1 receptor: A molecular modeling approach. Biochemistry 50(10):1755-1762, 2011.
- 4. **Haspel N.,** Moll M., Baker M., Chiu W. and Kavraki L.E. Tracing conformational changes in proteins. *BMC Structural Biology*, 10 Suppl.1 (S1) (2010).
- 5. **Haspel N.**, Geisbrecht B., Lambris J. and Kavraki L.E. Multi-scale Characterization of the Energy Landscape of Proteins with Application to the C3d/Efb-C Complex. *Proteins: Structure, Function and Bioinformatics*, 78(4):1004-1014 (2010).
- 6. Zanuy D., Ballano G., Jimenez A., Casanovas J., **Haspel N.**, Cativiela C., Curcó D., Nussinov R., Aleman C., Protein segments with conformationally restricted amino acids can control supramolecular organization at the nanoscale. *Journal of Chemical Information and Modeling*, 49(7): 1623-1629 (2009). (selected for journal cover).

- 7. **Haspel N.***, Ricklin D.*, Geisbrecht B., Kavraki L.E. and Lambris J.D., Electrostatic Contributions Drive the Interaction Between Staphylococcus aureus Protein Efb-C and its Complement Target C3d. *Protein Science*, 17(11):1894-1906 (2008).

 * These authors contributed equally to the work
- 8. **Haspel N.**, Zanuy D., Zheng J., Alemàn C., Wolfson H. and Nussinov R. Changing the charge distribution of beta-helical based nanostructures can provide the conditions for charge transfer. *Biophysical Journal*, 93:245-253 (2007).
- 9. Zheng J., Zanuy D., **Haspel N.**, Tsai C.J., Alemàn C. and Nussinov R. Nanostructure Design using Protein Building Blocks Enhanced by Conformationally Constrained Synthetic Residues. *Biochemistry*, 46(5):1205-1218 (2007).
- 10. Tsai C.J., Zheng J., Zanuy D., **Haspel N.**, Wolfson H., Alemàn C. and Nussinov R. Principles of nanostructure design with protein building blocks. *Proteins: Structure, Function and Bioinformatics* 68(1):1-12 (2007).
- 11. Zanuy D., Rodriguez-Ropero F., **Haspel N.**, Zheng J., Nussinov R. and Alemàn C. Stability of tubular structures based on beta-helical proteins: self-assembled versus polymerized nanoconstructs and wild-type versus mutated sequences. *Biomacromolecules*, 8(10):3135-3146 (2007).
- 12. **Haspel N.**, Zanuy D., Alemàn C., Wolfson H. and Nussinov R. De-novo tubular nanostructure design based on self-assembly of β-helical protein motifs. *Structure*, 14(7):1137-1148 (2006).
- 13. Wainreb G., **Haspel N.**, Wolfson H. and Nussinov, R., A permissive secondary structure guided superposition tool for clustering of protein fragments toward protein structure prediction via fragment assembly. *Bioinformatics* 22: 1343 1352 (2006).
- 14. Aleman C., Zanuy D., Jimenez A.I., Cativiela C., **Haspel N.**, Zheng J., Casanovas J., Wolfson H. and Nussinov R.: Concepts and schemes for the re-engineering of physical protein modules: generating nanodevices via targeted replacements with constrained amino acids. *Physical biology*, 3(1):S54-S62 (2006).
- 15. **Haspel N.**, Zanuy D., Ma B., Wolfson H. and Nussinov R., A comparative study of amyloid fibril formation by residues 15-19 of the human calcitonin hormone: A single β-sheet model with a small hydrohpobic core. *Journal of Molecular Biology* 345(5):1213-1227 (2005).
- 16. Zanuy D.*, **Haspel N.***, Ma B., Kannan G., Wolfson H. and Nussinov R. Side chain interactions determine the amyloid organization: a single layer β-sheet molecular structure of the calcitonin peptide segment 15–19. *Physical Biology*, 1:89-99 (2004). * These authors contributed equally to the work.
- 17. Tsai H. H., Zanuy D., **Haspel N.**, Ma B., Gunasekaran K., Tsai C.J. and Nussinov R., The Stability and Dynamics of the Human Calcitonin Amyloid Peptide DFNKF. *Biophysical Journal*, 87(1),146-158 (2004).
- 18. **Haspel N.**, Tsai C.J. Wolfson H. and Nussinov R., Hierarchical protein folding pathways: A computational study of protein fragments. *Proteins: Structure, Function and Bioinformatics*, 51:203-215 (2003).

- 19. **Haspel N.**, Tsai C.J. Wolfson H. and Nussinov R., Reducing the computational complexity of protein folding via fragment folding and assembly. *Protein Science*, 12:1177-1187 (2003).
- 20. Schneidman-Duhovny D., Inbar Y., Polak V., Shatsky M., Halperin I., Benyamini H., Barzilai A., Dror O., **Haspel N.**, Nussinov R. and Wolfson H.J. Taking geometry to its edge: fast unbound rigid (and hinge-bent) docking. *Proteins, Structure, Function and Genetics*. 52(1): 107-112 (2003).

BOOK CHAPTERS

- 1. **Haspel N.**, Wainreb G., Inbar Y., Tsai H.H., Tsai C.J., Wolfson H.J. and Nussinov R., A hierarchical protein folding scheme based on the building block folding model. *Methods Mol. Biol.*, 350:189-204 (2007).
- 2. **Haspel N.**, Zanuy, D., Tsai H.H., Ma B., Wolfson H. and Nussinov R. Computational approaches and tools for establishing structural models for short amyloid-forming peptides. *In Amyloid Proteins. Ed. Jean D. Sipe. Wiley-VCH*, volume 1, pp 301-318 (2005).
- 3. **Haspel N.**, Tsai C. J., Wolfson H. and Nussinov R., From the building blocks folding model to protein structure prediction. *In Tsigelny I.*, (*Ed*): Protein Structure Prediction: Bioinformatics approach. International University Line, chapter 8, 201-226 (2002).
- 4. Kumar S., Barzilai A., **Haspel N.**, Sham Y. Y., Tsai C. J., Wolfson H. and Nussinov R., Critical building blocks in proteins: a common theme in folding and binding. *In Gromiha, M. KH. and Selvarage, S. (Eds): Recent Research Developments in Protein Folding, Stability and Design.* Research Signpost, chapter 15. Trivadrum, India (2002).

PEER-REVIEWED CONFERENCES PROCEEDINGS

- 1. **N. Haspel** and E. Gonzalez, Topological Properties of the Configuration Spaces of Proteins. Proc. of BICoB (4th international conference on bioinformatics and computational biology), March 12-14 2012.
- 2. B. Akbal, I. Hashmi, A. Shehu and **N. Haspel.** Refinement of protein complex structures using evolutionary traces. Proc. of the Computational Structural Biology Workshop (CSBW), in conjunction with IEEE BIBM '11, 400-405, 2011.
- 3. I. Hashmi, B. Akbal, **N. Haspel** and A. Shehu. Protein docking with information on evolutionary conserved interfaces. Proc. of the Computational Structural Biology Workshop (CSBW), in conjunction with IEEE BIBM '11, 358-365, 2011.
- 4. **N. Haspel** Computing Structural changes in proteins represented at a coarse level. in *Proceedings of Bionetics10*, Dec. 2010, Boston MA.
- 5. **Haspel N.**, Moll M., Baker, M.L., Chiu W. and Kavraki L.E. Tracing Conformational Changes in Proteins. *Proceedings of CSBW09* (Computational Structural Biology Workshop), 120-127, part of BIBM09 IEEE international conference on Bioinformatics and Biomedicine, Nov. 2009, Washington DC.

SELECTED PRESENTATIONS

- 1. Conquering the Complexity of Protein Data, Bio-IT conference, Lehigh University, and Bio-IT 2011 (April 2011).
- 2. Haspel, N. (Presenter) Oral Presentation, Affordable departmental supercomputing to calculate protein dynamics, Bio-IT 2011, (April 2011).
- 3. Computing Structural Changes in Proteins, UMass Boston, Biology department seminar, Sep. 2009 (invited talk), George Mason University, CS department seminar, Nov. 2009 (invited talk).
- 4. **Haspel N.,** Moll M. and Kavraki L.E., HPC for Computational Structural Biology. Rice University annual HPC users workshop, 2008 (invited talk).
- 5. "Design of Novel Nano-structures using beta-helical protein segments". University of Illinois at Urbana-Champaign, 2006 (seminar talk).
- 6. "A comparative study of the amyloid structures formed by the hCT peptide". Ben-Gurion University, Beer-Sheva, Israel, 2004 (invited seminar talk).
- 7. "Computational study of protein folding pathways using the building blocks folding model". National Cancer Institute, Frederick, MD, 2000 (invited seminar talk).

FUNDING AND RESOURCES

- AF: SMALL: Developing Novel Computational Methods for Investigating Protein Dynamics Using a Multi-Scale Approach, Haspel N. (PI), \$249,774, (September 1, 2011 - August 31, 2014).
- UMass Boston proposal development grant: Towards Rational Design of Amyloid-based Peptides to Self-assemble into Ordered Nano- or Micro-structures with Distinct Morphology. Haspel N. (PI), Zheng J., U. of Akron (Co-PI), April 2010 – December 2011 - \$10000.
- UMass Boston Healey Research grant: Identification and Characterization of Biologically Active Metabolic Fragments of Pituitary Hormones: Has an Entire Area of Cell Signaling Been Missed? Campbell K. (Co-PI), Haspel N. (Co-PI). April 2010 – June 2011, \$12000.
- PII award for instruction innovation: WUMP women undergraduate mentoring program. Ding W. (PI), Haspel N.(Co-PI), O'Neil E. (Co-PI), Jan. 2010 \$5000.

TEACHING

- **2010:** CS624, Analysis of Algorithms, UMass Boston.
- 2009-2011: CS310, Advanced data structures and algorithms, UMass Boston.
- 2008: Teaching assistant, COMP 450, Algorithmic Robotics, Rice University.
- 2006: Lecturer, Programming for engineering students, Tel Aviv University.
- **2005,2006:** Teaching assistant, Introduction to Computer Science in Scheme, Tel Aviv University.
- **2003,2004:** Teaching assistant, Programming for engineering students, Tel Aviv University.
- 2005: Lecturer, Programming for Chemistry students, Tel Aviv University.

MENTORED STUDENTS

- Kit Menlove (graduate student rotation project), Rice University. Advisor Lydia Kavraki.
- Nick Zhu (undergraduate research project), Rice University. Advisor Lydia Kavraki.
- Bahar Akbal (PhD student), UMass Boston.
- Rohith Kotla (PhD student), UMass Boston.
- Uma Vadhar (Msc Student). co-advisor. Main advisor Kenneth Campbell, UMass Boston, department of Biology.
- Alex Jurgens Undergraduate research project.
- Harold Gomez Undergraduate honors thesis.

PROFESSIONAL DEVELOPMENT

CONFERENCE ORGANIZATION

- Computational Structural Biology Workshop (CSBW) 2011, co-chair.
- Bionetics 2010, special track on bioinformatics, chair.
- Bionetics 2010, special track on visualization, PC member.
- International Conference on Recent Advances in Technology, Engineering, Management and Science (ICRATEMS-2011) advisory committee.

REVIEWER

- Proceedings of the National Academy of Science (PNAS).
- Computational Systems in Bioinformatics conference (CSB).
- RECOMB conference.
- Biopolymers: Peptide science.
- Journal of Bioinformatics and Computational Biology special guest editor for the Bioinformatics track in BIONETICS 2010.
- IEEE/ACM transactions on Computational Biology and Bioinformatics.
- Journal of Organic Chemistry.
- PLoS Computational Biology.
- PLoS one.
- International Journal of Data Mining and Bioinformatics (IJDMB).
- Editorial board member of the book "Developing and Applying Biologically-Inspired Vision Systems: Interdisciplinary Concepts" to be published by IGI Global. Editors: Marc Pomplun and Jun Suzuki.
- Guest editor for a special issue in JBCB, June 2011 (associated with Bionetics).

MEMBER

- International Society for Computational Biology (ISCB).
- Association for Computing Machinery (ACM).
- Protein Society.
- Biophysical Society.
- IEEE, IEEE Women in Engineering.