

# Nurit Haspel

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## Education

- 2002-2006 **Ph.D.** Computer Science  
Tel Aviv University, Tel Aviv, Israel  
**Advisors:** Prof. Ruth Nussinov and Prof. Haim Wolfson  
**Thesis title:** Computational modeling and prediction of self-assembling beta-sheet rich protein structures
- 1999-2002 **M.Sc.** Structural Bioinformatics at the Department of Human Genetics (Summa Cum Laude)  
Tel Aviv University, Tel Aviv, Israel  
**Advisors:** Prof. Ruth Nussinov and Prof. Haim Wolfson  
**Thesis title:** Computational study of protein folding pathways using the building blocks folding model
- 1995-1998 **B.Sc.** Chemistry and Computer Science (Cum Laude)  
Tel Aviv University, Tel Aviv, Israel

## Employment

- 2022 - present **Professor**, Department of Computer Science  
University of Massachusetts Boston
- 2016-2022 **Associate Professor**, Department of Computer Science  
University of Massachusetts Boston
- 2009-2016 **Assistant Professor**, Department of Computer Science  
University of Massachusetts Boston
- 2007-2009 **Postdoctoral Research Associate**, Department of Computer Science  
Rice University, Houston, TX  
**Advisor:** Prof. Lydia Kavraki
- 2002-2006 **Research and Teaching Assistant**, School of Computer Science  
Tel-Aviv University, Tel-Aviv, Israel
- 2001-2005 **Visiting Researcher**, Center for Cancer Research Nanobiology Program  
National Cancer Institute Frederick, MD
- 1999-2001 **Research Assistant**, Department of Human Genetics, School of Medicine  
Tel-Aviv University, Tel-Aviv, Israel

## Publications

### Peer Reviewed Journal Publications

- Haspel, N., Jang, H., and Nussinov, R. (2024). Allosteric activation of rhoa complexed with p115-rhogef deciphered by conformational dynamics. *Journal of Chemical Information and Modeling*, 64(3):862–873. PMID: 38215280
- Jilani, M., Turcan, A., Haspel, N., and Jagodzinski, F. (2022). Elucidating the structural impacts of protein indels. *Biomolecules*, 12(10)

3. Afrasiabi, F., Dehghanpoor, R., and Haspel, N. (2021). Integrating rigidity analysis into the exploration of protein conformational pathways using rrt\* and mc. *Molecules*, 26(8)
4. Haspel, N., Jang, H., and Nussinov, R. (2021). Active and inactive cdc42 differ in their insert region conformational dynamics. *Biophysical Journal*, 120(2):306–318
5. Campbell, K. L., Haspel, N., Gath, C., Kurniatash, N., (Nouduri) Akkiraju, I., Stuffers, N., and Vadher, U. (2021). Protein hormone fragmentation in intercellular signaling: hormones as nested information systems. *Biology of Reproduction*, 104(4):887–901
6. Joshi, A. and Haspel, N. (2020). A novel data instance reduction technique using linear feature reduction. *Journal of Artificial Intelligence and Systems*, 2(1):191–206
7. Vajdi, A., Zarringhalam, K., and Haspel, N. (2020b). Patch-dca: Improved protein interface prediction by utilizing structural information and clustering dca scores. *Bioinformatics*, 36(5):1460–1467
8. Joshi, A. and Haspel, N. (2019). Clustering of protein conformations using parallelized dimensionality reduction. *Journal of Advances in Information Technology (JAIT)*, 10(4):142–147
9. Dehghanpoor, R., Ricks, E., Hursh, K., Gunderson, S., Farhoodi, R., Haspel, N., Hutchinson, B., and Jagodzinski, F. (2018). Predicting the effect of single and multiple mutations on protein structural stability. *Molecules*, 23(2):251
10. Levy, B., Gable, S., Tsoy, E., Haspel, N., Wadler, B., Wilcox, R., Hess, C., Hogan, J., Driscoll, D., and Hashmi, A. (2017). Machine learning detection of cognitive impairment in primary care. *Alzheimers Disease & Dementia*, 1(2):38–46
11. Luo, D., González, E., and Haspel, N. (2017). Detecting intermediate protein conformations using algebraic topology. *BMC Bioinformatics*, 18(Suppl 15)
12. Farhoodi, R., Akbal-Delibas, B., and Haspel, N. (2017a). Machine learning approaches for predicting protein structure similarity. *J. Comp. Biol.*, 24(1):40–51
13. Akbal-Delibas, B., Farhoodi, R., Pomplun, M., and Haspel, N. (2016). Accurate refinement of docked protein complexes using evolutionary information and deep learning. *J. Bioinf. Comp. Biol.*, 14(3):1642002
14. Akbal-Delibas, B., Pomplun, M., and Haspel, N. (2015a). Accurate prediction of docked protein structure similarity. *J. Comp. Biol.*, 22(9):892–904
15. Murase, S. K., Haspel, N., del Valle, L. J., Perpete, E. A., Michaux, C., Nussinov, R., Puiggali, J., and Aleman, C. (2014). Molecular characterization of l-phenylalanine terminated poly(l-lactide) conjugates. *RSC Advances*, 4(44):23231–23241
16. Akbal-Delibas, B. and Haspel, N. (2013). A conservation and biophysics guided stochastic approach to refining docked multimeric proteins. *BMC Struct. Biol.*, 13(Suppl 1):S7
17. B. Akbal-Delibas, F. Jagodzinski, and Haspel, N. (2013). A conservation and rigidity based method for detecting critical protein residues. *BMC Struct. Biol.*, 13(Suppl 1):S6  
\* – Equal contribution
18. Zanuy, D., Kotla, R., Nussinov, R., Teesalu, T., Sugahara, K. N., Aleman, C., and Haspel, N. (2013). Sequence dependence of c-end rule peptides in binding and activation of neuropilin-1 receptor. *Journal of Structural Biology*, 182(2):78 – 86
19. Haspel, N., Laurent, A. D., David, Z., Ruth, N., Carlos, A., Jordi, P., and Guillem, R.-

- L. (2012a). Conformational exploration of two peptides and their hybrid polymer conjugates: Potentialities as self-aggregating materials. *The Journal of Physical Chemistry B*, 116(48):13941–13952
20. Akbal-Delibas, B., Hashmi, I., Shehu, A., and Haspel, N. (2012a). An evolutionary conservation-based method for refining and reranking protein complex structures. *J. Bioinformatics and Computational Biology (JBCB)*, 10(3):1242002
21. Hashmi, I., Akbal-Delibas, B., Haspel, N., and Shehu, A. (2012). Guiding protein docking with geometric and evolutionary information. *J. Bioinformatics and Computational Biology (JBCB)*, 10(3):1242008
22. Haspel, N., Zanuy, D., Nussinov, R., Teesalu, T., Ruoslahti, E., and Aleman, C. (2011d). Binding of a c-end rule peptide to the neuropilin-1 receptor: a molecular modeling approach. *Biochemistry*, 50(10):1755–1762
23. Haspel, N., Moll, M., Baker, M., Chiu, W., and Kavraki, L. E. (2010b). Tracing conformational changes in proteins. *BMC Structural Biology*, Suppl1:S1
24. Haspel, N., Geisbrecht, B., Lambris, J., and Kavraki, L. (2010a). 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
25. Zanuy, D., Ballano, G., Jimenez, A. I., Casanovas, J., Haspel, N., Cativiela, C., Curco, D., Nussinov, R., and Aleman, C. (2009). Protein segments with conformationally restricted amino acids can control supramolecular organization at the nanoscale. *J. Chemical and Information Modeling*, 49(7):1623–1629
26. Haspel\*, N., D. Ricklin\*, Geisbrecht, B., Lambris, J., and Kavraki, L. (2008). Electrostatic contributions drive the interaction between staphylococcus aureus protein efb-c and its complement target c3d. *Protein Science*, 17(11):1894–1906  
\* – Equal contribution
27. Zanuy, D., Rodriguez-Ropero, F., Haspel, N., Zheng, J., Nussinov, R., and Aleman, C. (2007). 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
28. Tsai, C., Zheng, J., Zanuy, D., Haspel, N., and Nussinov, R. (2007). Principles of nanostructure design with protein building blocks. *Proteins: Structure, function and bioinformatics*, 68:245–253
29. Haspel, N., Zanuy, D., Zheng, J., Aleman, C., Wolfson, H., and Nussinov, R. (2007b). Changing the charge distribution of beta-helical based nanostructures can provide the conditions for charge transfer. *Biophys. J.*, 93:245–253
30. Zheng, J., Zanuy, D., Haspel, N., Tsai, C., Aleman, C., and Nussinov, R. (2007). Nanostructure design using protein building blocks enhanced by conformationally constrained synthetic residues. *Biochemistry*, 46(5):1205–1218
31. Aleman, C., Zanuy, D., Jimenez, A., Cativiela, C., Haspel, N., Zheng, J., Casanovas, J., Wolfson, H., and Nussinov, R. (2006). Concepts and schemes for the re-engineering of physical protein modules: generating nanodevices via targeted replacements with constrained amino acids. *Phys. Biol.*, 3(1):S54–62

32. Haspel, N., Zanuy, D., Aleman, C., Wolfson, H., and Nussinov, R. (2006). De-novo tubular nanostructure design based on self-assembly of beta-helical protein motifs. *Structure*, 14:1137–1148
33. Wainreb, G., Haspel, N., Wolfson, H., and Nussinov, R. (2006). A permissive secondary structure-guided superposition tool for clustering of protein fragments toward protein structure prediction via fragment assembly. *Bioinformatics*, 22:1343–1352
34. Haspel, N., Zanuy, D., Ma, B., Wolfson, H., and Nussinov, R. (2005a). A comparative study of amyloid fibril formation by residues 15–19 of the human calcitonin hormone: A single beta-sheet model with a small hydrophobic core. *J. Mol. Biol.*, 345(5):1213–1227
35. Tsai, H., Zanuy, D., Haspel, N., Gunasekaran, K., Ma, B., Tsai, C., and Nussinov, R. (2004). The stability and dynamic of the human calcitonin amyloid peptide dfnkf. *Biophys. J.*, 87(1):146–158
36. Zanuy\*, D., Haspel\*, N., Tsai, H., Ma, B., Kannan, G., Wolfson, H., and Nussinov, R. (2004). Side chain interactions determine the amyloid organization: A single layer beta-sheet molecular structure of the calcitonin peptide segment 15–19. *Phys. Biol.*, 1:89–99  
\* – Equal contribution
37. Haspel, N., Tsai, C., Wolfson, H., and Nussinov, R. (2003b). Reducing the computational complexity of protein folding via fragment folding and assembly. *Protein Science*, 12:1177–1187
38. Haspel, N., Tsai, C., Wolfson, H., and Nussinov, R. (2003a). Hierarchical protein folding pathways: A computational study of protein fragments. *Proteins: Structure, function and bioinformatics*, 51:203–215
39. Schneidman-Duhovny, D., Inbar, Y., Polak, V., Shatsky, M., Halperin, I., Benyamin, H., Barzilai, A., Dror, O., Haspel, N., Nussinov, R., and Wolfson, H. (2003). Taking geometry to its edge: Fast unbound rigid (and hinge-bent) docking. *Proteins: Structure, function and genetics*, 52(1):107–112

## Peer Reviewed Conference Proceedings

1. Jilani, M. and Haspel, N. (2023). Investigating the role of gene body methylation and cpg methylation in cancer subtyping. In *proc. of ICBRA (International Conference on Bioinformatics Research and Applications)*, volume To Appear
2. Dehghanpoor, R., Afrasiabi, F., Fogel, C., Dao, T., Gautam, S., Nehela, A., Nehela, A., Haehn, D., and Haspel, N. (2023). Classifying protein families with learned compressed representations. In *proc. of BICOB (International conference on Bioinformatics and Computational Biology)*, volume 92, pages 47–57
3. Zurrin, R., Goyal, N., Bendiksen, P., Manocha, M., Simovici, D., Haspel, N., Pomplun, M., and Haehn, D. (2023). Outlier detection for mammograms. In *International Conference on Medical Imaging with Deep Learning*
4. Dehghanpoor, R., Afrasiabi, F., and Haspel, N. (2022). Using topological data analysis and rrt to investigate protein conformational spaces. In *proc. of BICOB (International conference on Bioinformatics and Computational Biology)*
5. Jilani, M., Turcan, A., Haspel, N., and Jagodzinski, F. (2021). Assessing the effects of amino acid insertion and deletion mutations. In *proc. of IEEE-BIBM (in CSBW workshop)*

6. Afrasiabi, F. and Haspel, N. (2020). Efficient exploration of protein conformational pathways using rrt\* and mc. In *proc. of ACM-BCB (in CSBW 2020 workshop)*
7. Mohebbi, H. R., Quach, J., and Haspel, N. (2020). Fusion transcript detection from rna-seq using jaccard distance. In *proc. of ACM-BCB (in HPC-BOD workshop)*
8. Vajdi, A., Joshi, A., and Haspel, N. (2019). Integrating co-evolutionary information in monte carlo based method for proteins trajectory simulation. In *proc. of ACM-BCB (in CSBW 2019 workshop)*
9. Mohebbi, H., Vajdi, A., Haspel, N., and Simovici, D. (2017). Detecting chromosomal structural variation using jaccard distance and parallel architecture. In *proc. of IEEE-BIBM (in HIBB 2017 workshop)*
10. Farhoodi, R., Akbal-Delibas, B., and Haspel, N. (2017b). Ranking protein-protein binding using evolutionary information. In *CSBW, in proc. of ACM-BCB (International Conference on Bioinformatics, Computational Biology and Health Informatics)*, pages 667–672
11. Farhoodi, R., Shelbourne, M., Hsieh, R., Haspel, N., Hutchinson, B., and Jagodzinski, F. (2017c). Predicting the effect of point mutations on protein structural stability. In *proc. of ACM-BCB (International Conference on Bioinformatics, Computational Biology and Health Informatics)*, pages 247–252
12. Andersson, E., Hsieh, R., Szeto, H., Farhoodi, R., Jagodzinski, F., and Haspel, N. (2016). Assessing how multiple mutations affect protein stability using rigid cluster size distributions. In *proc. of IEEE-ICCAABS (International Conference on Computational Advances in Bio and Medical Sciences)*
13. Vajdi, A. and Haspel, N. (2016). Clustering protein conformations using a dynamic programming based similarity measurement. In *proc. of BICoB (8th international conference on Bioinformatics and Computational Biology)*
14. Vajdi, A., Banaee, H., and Haspel, N. (2015a). A new dp algorithm for comparing gene expression data using geometric similarity. In *Workshop on Computational Regulatory Genomics and Metagenomics, in conjunction with IEEE-BIBM 2015*, pages 1157–1161
15. Farhoodi, R., Akbal-Delibas, B., and Haspel, N. (2015). Accurate prediction of docked protein structure similarity using neural networks and restricted boltzmann machines. In *CSBW (Computational Structural Bioinformatics Workshop), in conjunction with IEEE-BIBM 2015*, pages 1296–1303
16. Akbal-Delibas, B., Pomplun, M., and Haspel, N. (2015b). Accurefiner: A machine learning guided refinement method for protein-protein docking. In *proc. of BICoB (7th international conference on Bioinformatics and Computational Biology)*
17. Vetro, R., Farhoodi, R., Kotla, R., Haspel, N., Weisman, D., Rosen, J., and Simovici, D. (2014). Tide: Inter-chromosomal translocation and insertion detection using embeddings. In *The 2014 Workshop on Big Data in Bioinformatics and Healthcare Informatics (BBH14), held in conjunction with the 2014 IEEE International Conference on Big Data*, pages 64–70
18. Akbal-Delibas, B., Pomplun, M., and Haspel, N. (2014). Accurmsd: A machine learning approach to predicting structure similarity of docked protein complexes. In *proc. of ACM-BCB (5th ACM International conference on Bioinformatics and Computational Biology)*, pages 289–296

19. Jagodzinski, F., Akbal-Delibas, B., and Haspel, N. (2013). An evolutionary conservation & rigidity analysis machine learning approach for detecting critical protein residues. In *CSBW (Computational Structural Bioinformatics Workshop), in proc. of ACM-BCB (ACM International conference on Bioinformatics and Computational Biology)*, pages 780–786
20. Luo, D. and Haspel, N. (2013b). Multi-resolution rigidity-based sampling of protein conformational paths. In *CSBW (Computational Structural Bioinformatics Workshop), in proc. of ACM-BCB (ACM International conference on Bioinformatics and Computational Biology)*, pages 787–793
21. Luo, D. and Haspel, N. (2013a). Efficient coarse-grained geometry-based sampling of protein conformational paths. In *Proc. 5th Int. Conf. on Bioinformatics and Computational Biology (BiCOB)*, Honolulu, HI, USA
22. Haspel, N., Luo, D., and Gonzalez, E. (2013). Detecting intermediate structures in protein conformational pathways. In *Proc. 5th Int. Conf. on Bioinformatics and Computational Biology (BiCOB)*, Honolulu, HI, USA
23. Haspel, N. and Gonzalez, E. (2012). Topological properties of the configuration spaces of proteins. In *Proc. 4th Int. Conf. on Bioinformatics and Computational Biology (BiCOB)*, Las Vegas, NV, USA
24. Vetro, R., Haspel, N., and Simovici, D. (2012). Characterizing intermediate conformations in protein conformational space. In *Proc. of the Ninth International Meeting on Computational Intelligence Methods for Bioinformatics and Biostatistics*, Houston, TX, USA
25. Akbal-Delibas, B. and Haspel, N. (2012b). Refining multimeric protein complexes using conservation, electrostatics and probabilistic selection. In *IEEE Intl Conf on Bioinf and Biomed Workshops (BIBMW)*, pages 102–108
26. B. Akbal-Delibas\*, F. Jagodzinski\*, and Haspel, N. (2012). Towards a hybrid method for detecting critical protein residues. In *IEEE Intl Conf on Bioinf and Biomed Workshops (BIBMW)*, pages 82–85  
\* – Equal contribution
27. Akbal-Delibas, B., Hashmi, I., Shehu, A., and Haspel, N. (2011). Refinement of docked protein complex structures using evolutionary traces. In *2011 IEEE International Conference on Bioinformatics and Biomedicine Workshops (BIBMW)*, pages 400–404. IEEE
28. Hashmi, I., Akbal-Delibas, B., Haspel, N., and Shehu, A. (2011). Protein docking with information on evolutionary conserved interfaces. In *Proc. Computational Structural Biology workshop (CSBW), in conjunction with IEEE Int. Conference on Bioinformatics and Biomedicine (BIBM)*, pages 358–365, Atlanta, GA, USA
29. Haspel, N. (2010). Tracing conformational changes in proteins represented at a coarse level. In *BIONETICS 2010, Bioinformatics track*, Boston, MA, USA
30. Haspel, N., Moll, M., Baker, M., Chiu, W., and Kavraki, L. (2009a). Tracing conformational changes in proteins. In *Proc. Computational Structural Biology workshop (CSBW), in conjunction with IEEE Int. Conference on Bioinformatics and Biomedicine (BIBM)*, pages 120–127, Washington DC, USA

## Books

1. Haspel, N., Jagodzinski, F., and Molloy, K., editors (2022). *Algorithms and Methods in*

*Structural Bioinformatics*. Springer Nature

## Book Chapters

1. Jilani, M. and Haspel, N. (2021). Computational methods for detecting large-scale structural rearrangements in chromosomes. In Nakaya, H. I., editor, *Bioinformatics*, chapter 3, pages 323–352. Exon Publications
2. Haspel, N., Zheng, J., Zanuy, D., Aleman, C., and Nussinov, R. (2017). A protocol for the design of protein and peptide nanostructure self- assemblies exploiting synthetic amino acids. In Samish, I., editor, *Methods Mol. Biol.*, volume on Computational Protein Design, chapter 17, pages 323–352. Springer, NY, USA
3. Haspel, N. and Jagodzinski, F. (2017). Methods for detecting critical residues in proteins. In Reeves, A., editor, *Methods Mol. Biol.*, volume on In Vitro Mutagenesis, pages 227–242. Springer, NY, USA
4. Haspel, N. (2015). Methods for detecting protein binding interfaces. In Zhang, W., editor, *Method in Pharmacology and Toxicology*, volume on Computer aided drug discovery, pages 133–152. Springer, NY, USA
5. Haspel, N., Shell, A., and Deutsch, C. (2012b). Computational approaches to measurement of visual attention: Modeling over-selectivity in intellectual and developmental disability. In Pomplun, M. and Suzuki, J., editors, *Developing and applying biologically inspired vision systems: Interdisciplinary concepts*, pages 31–43. IGI Global, Hershey, PA, USA
6. Haspel, N., Wainreb, G., Inbar, Y., Tsai, H., Tsai, C., Wolfson, H., and Nussinov, R. (2007a). A hierarchical protein folding scheme based on the building block folding model. *Methods Mol. Biol.*, 350:189–204
7. Haspel, N., Zanuy, D., Tsai, H., Ma, B., Wolfson, H., and Nussinov, R. (2005b). Computational approaches and tools for establishing structural models for short amyloid-forming peptides. In *Amyloid Proteins*, volume 1, pages 301–318. Ed. Jean D. Sipe. Wiley-VCH
8. Haspel, N., Tsai, C., Wolfson, H., and Nussinov, R. (2002). From the building blocks folding model to protein structure prediction. In *Protein Structure Prediction: Bioinformatics approach*, chapter 8, pages 201–226. Ed. Tsigelny I
9. Kumar, S., Barzilai, A., Haspel, N., Sham, Y., Tsai, C., Wolfson, H., and Nussinov, R. (2002). Critical building blocks in proteins: a common theme in folding and binding. In *Recent Research Developments in Protein Folding, Stability and Design.*, chapter 15. Gromiha, M. KH. and Selvarage, S., Trivadrum, India

## Refereed Abstracts and Others

1. Vajdi, A., Zaghdian, M. R., Farahmand, S., Rastegar, E., Maroofi, K., Jia, S., Pomplun, M., Haspel, N., and Bayat, A. (2020a). Human gait database for normal walk collected by smart phone accelerometer
2. Campbell, K. L., Haspel, N., and Stuffers, N. (2019b). Coincidence maps of proteolytic cleavage, secondary structure, and exon origins for the soluble human protein hormone proteome: Functional associations? In *Protein Science*, volume 28, pages 52–52. Wiley 111 River st., Hoboken 07030-5774, NJ USA
3. Joshi, A. and Haspel, N. (2018). Clustering of protein conformations using parallelized di-

- mensionality reduction. In *ICSB Rocky 2018 Abstract + Oral presentation*
4. Campbell, K., Haspel, N., and Stuffers, N. (2019a). Sat-048 a map of predicted proteolytic cleavage products for the soluble human protein proteome: Intriguing patterns. *Journal of the Endocrine Society*, 3(Supplement 1). SAT-048
  5. Hall, B., Anwar, M., Cheng, D., Hoang, J., Haspel, N., and Campbell, K. (2018). Possible functional roles for proteolytic products of protein hormones. In *Protein Science*, volume 27, pages 106–107. Wiley 111 River st., Hoboken 07030-5774, NJ USA
  6. Gath, C., Stuffers, N., Hasaba, A., Nouduri, I., Haspel, N., and Campbell., K. L. (2017). Protein hormone transcripts are nested information systems: Co-alignment of dna exon boundaries, protein domain borders, and predicted transcribed protein hormone cleavage sites. In *Annual Society for the Study of Reproduction Meeting*, page 272 (Abstract + poster)
  7. Campbell, K., Nouduri, I., and Haspel, N. (2016). Protein hormones as nested information systems: Computational analysis of interleukins and cxc chemokines reveal alignments of family domains and proteolytic cleavage sites. In *Endocrine Society Meeting* (Abstract + poster)
  8. Vajdi, A., Banaee, H., and Haspel, N. (2015b). A new dp algorithm for comparing gene expression data using geometric similarity. In *IEEE Intl Conf on Bioinf and Biomed (BIBM)*, page To appear (abstract+poster, selected for oral presentation)
  9. Campbell, K., Haspel, N., Ford, V., and Gabriel-Richards, T. (2015). Hormone signal modulators among protein hormone pro-peptides and hormone fragments. In *47th Annual Society for the Study of Reproduction Meeting*, page 690 (Abstract + poster)
  10. Campbell, K., Haspel, N., Dominas, B., Mason, B., Calixte, W., Bigos, R., Taguzem, G., Vadher, U., Palmstrom, N., Stenbruck, J., Solchenberger, S., and Diallo, F. (2014). Protein hormone proteolysis in target cell endosomes and lysosomes and release of previously unrecognized signaling information. In *World Congress of Reproductive Biology Meeting* (Abstract + poster)
  11. B. Akbal-Delibas, M. P. and Haspel, N. (2014). An artificial neural network to predict rmsds of docked protein complexes. In *Intelligent Systems in Molecular Biology (ISMB)* (Abstract + poster)
  12. Akbal-Delibas, B. and Haspel, N. (2012a). An evolutionary-guided iterative refinement approach for protein multimers. In *IEEE Intl Conf on Bioinf and Biomed (BIBM)* (Abstract + poster)
  13. Akbal-Delibas, B., Jagodzinski, F., and Haspel, N. (2012b). Combining conservation and rigidity methods to detect critical residues in proteins. In *IEEE Intl Conf on Bioinf and Biomed (BIBM)* (Abstract + poster)
  14. Diallo, F. B., Campbell, K., and Haspel, N. (2012). Discovering proteins potentially participating in novel protein hormone signal transduction pathways. In *ABRCMS (Annual biomedical research conference for minority students)* (Abstract + oral presentation)
  15. Campbell, K., Haspel, N., Palmstrom, N., Steinbruck, J., Vadher, U., and Solchenberger, S. (2012a). Progress in identifying possible targets for a novel signal transduction pathway for protein hormones involving products of  $\beta$  cathepsin proteolysis of the hormones. In *Society for the Study of Reproduction (SSR) meeting* (Abstract + poster)

16. Campbell, K., Haspel, N., Palmstrom, N., Steinbruck, J., Vadher, U., and Solchenberger, S. (2012b). Proteomic exploration of potential bioactivities of proteolytic peptides of protein hormones. In *ENDO 2012: The Endocrine Society's 94th Annual Meeting & Expo* (Abstract + poster)
17. Diallo, F. B., Gonzalez, E., and Haspel, N. (2011a). Analyzing the conformational space of proteins using mathematical and computational tools. In *ABRCMS (Annual biomedical research conference for minority students)* (Abstract + oral presentation)
18. Diallo, F. B., Gonzalez, E., and Haspel, N. (2011b). Analyzing the conformational space of proteins using mathematical and computational tools. In *NURDS(4th Annual Northeast Undergraduate Research and Development Symposium)* (Abstract + poster)
19. Haspel, N., Zanuy, D., Aleman, C., and Nussinov, R. (2011c). Binding of a c-end rule peptide to neuropilin-1 receptor: A molecular modeling approach and computational mutant study. In *Protein Society 25th meeting* (Abstract + poster)
20. Haspel, N., Campbell, K., and Vadher, U. (2011a). Proteolytic fragments of follicle stimulating hormone (fsh) show homologies to transducers and metabolic proteins: Are the peptide fragments biologically active? In *11th Hunter meeting* (Abstract + poster)
21. Haspel, N., Revilla-Lopez, G., Zanuy, D., Zheng, J., R, N., and Aleman, C. (2011b). Towards rational design of amyloid-based peptides to self-assemble into ordered nano- or micro-structures with distinct morphology. In *Biophysical Society 55th meeting* (Abstract + poster)
22. Haspel, N., Moll, M., Chiu, W., and Kavraki, L. (2009b). Tracing conformational changes in medium resolution protein structures. In *26th annual houston conference on biomedical engineering research (HSEMB)* (Abstract + poster)
23. Ricklin, D., Ricklin-Lichtsteiner, S. K., Sfyroera, G., Chen, H., Tzekou, A., Magotti, P., Wu, Y.-Q., Garcia, B. L., McWorther, W. J., Haspel, N., Kavraki, L. E., Geisbrecht, B. V., and Lambris, J. D. (2008). Novel insights into target specificities and molecular mechanisms for two potent complement evasion proteins from staphylococcus aureus. In *Biophysical Society 55th meeting*, pages 4114–4115 (Abstract + oral presentation)
24. Gunasekaran, K., Haspel, N., Tsai, C., Kumar, S., Wolfson, H., and Nussinov, R. (2003). Extended disordered proteins: An elegant solution to having large intermolecular interfaces, yet keeping smaller genome and cell sizes. In *Biophysical Society 47th meeting*, volume 84(2), page S163A (Abstract + poster)
25. Haspel, N., Wolfson, H., and Nussinov, R. (2001). A study of protein folding pathways using the building block folding model. In *Protein Society 15th meeting* (Abstract + poster)

## Teaching

### UMass Boston

- CS187SL,CS188SL (Science Gateway Seminar)
- CS220 (Applied Discrete Mathematics)
- CS450 (Structure of Higher Level Languages)
- MOOC about Molecular Dynamics simulations      March 2013 (guest lecture)
- CS612 (Algorithms in Bioinformatics)
- CS697 (Topics in Bioinformatics – Special topics)      Spring 2011
- CS624 (Analysis of Algorithms)
- CS310 (Advanced data structures and algorithms)      INTRD-601 (Inter-departmental seminar)

### Rice University

- COMP 450 (Algorithmic Robotics)      Fall 2008, Teaching assistant

### Tel Aviv University

- Programming for engineering students (lecturer)      2006
- Introduction to Computer Science in Scheme (Teaching assistant)      2005–2006
- Programming for engineering students (TA)      2004-2005
- Programming for Chemistry students (lecturer)      2005

## Graduate Student Mentoring

PhD students: Bahar Akbal-Delibas (2010-2014, graduated with PhD), Rohith Kotla (2011-2014, graduated with MSc), Dong Luo (2012-2015, graduated with MSc), Roshanak Farhoodi (2013-2017), Amir Vajdi (2015–2019), Ramin Dehghanpoor (2016-2022), Fatemeh Afrasiabi (2018-2023) Arpita Joshi (2016–2020), Hamid Reza Mohebbi (2018–2020), Muneeba Jilani (2020–present)

## Grants and Sponsored Research

- **UMB Proposal development grant** “Towards Developing Deep Learning Approaches for Protein-Protein Interaction Detection”. N. Haspel (PI), D. Haehn (Co-PI), \$20,000, (June 2021 – December 2022).
- **MLSC Bits-to-bytes** “Using bioinformatics, machine learning-based computational modeling of peptide-target binding and subsequent screening to aid the development of a bispecific antibody for the treatment of solid tumors targeting EGFR and NRP1”. J. Evans (PI), N. Haspel (Co-PI), \$1,687,000 total. (June 2021 – December 2022).
- **NSF-IIS-2031260** ”EAGER: III: Collaborative Research: In silico Algorithm for Assessing the Effects of Amino Acid Insertion and Deletion Mutations” (Co-PI. PI – Filip Jagodzinski, WWU), \$72,784 (total \$150,000) (July 1 2020–December 31, 2021)
- **MLSC Bits-to-bytes** ”The Oregon-Massachusetts Mammography Database (OMAMA-DB)” (Co-PI. PI - Daniel Haehn, CS. Greg Sorensen, DeepHealth Inc.).
- **NIH R43 DA050383-01A1** ”Discovering Therapeutic Agents for the Treatment of Opioid Use Disorder by Targeting Negative Allosteric Modulators of the mu-Opioid Receptor” (Con-

sultant, PI – Kimberly Stieglitz, Richard Anderson, Symmetric Computing) \$217,405 (April 2020 – October 2020)

- **NSF-CCF 1421871** “AF: SMALL: Computational Framework for Characterizing Protein Conformational Landscapes” (PI), \$320,000, (July 1, 2014 - December 31, 2018)
- **MGHPC (Massachusetts Green High Performance Computing Center) seed grant** “Genome-scale Characterization of Chromosomal Aberrations Using Parallelizable Compression Algorithms”. PI’s: N. Haspel, D. Simovici, D. Weisman D. (Biology) and J. Rosen (BU Medical School). \$60,000, (January 1 2013– December 31 2014)
- **NSF-CCF 1116060** “AF: SMALL: Developing Novel Computational Methods for Investigating Protein Dynamics Using a Multi-Scale Approach” (PI), \$249,774, (September 1, 2011 - December 31, 2014)
- **UMB Healey Grant** “Computational and Mathematical Analysis of Protein Conformational Spaces” – N. Haspel (PI), Eduardo Gonzalez, Math department(Co-PI) \$11,000 (July 1 2013 – December 31 2014)
- **UMB Proposal development grant** “Towards Rational Design of Amyloid-based Peptides to Self-assemble into Ordered Nano- or Micro-structures with Distinct Morphology”. N. Haspel (PI), Z. Zheng, U. of Akron (Co-PI), \$10,000, (April 2010 – December 2011).
- **UMB Healey grant** dentification and Characterization of Biologically Active Metabolic Fragments of Pituitary Hormones: Has an Entire Area of Cell Signaling Been Missed? K. Campbell (Co-PI), N. Haspel (Co-PI), \$12,000 (April 2010 – June 2011).
- **UMB PII award for instruction innovation** “WUMP – women undergraduate mentoring program”. W. Ding (PI), N. Haspel (Co-PI), E. O’Neil (Co-PI), \$5,000, (Jan. 2010-Dec. 2010)
- **TeraGrid** Structural properties of peptides that penetrate cells and tissues through binding to the neuropilin-1 (NRP-1) receptor, (December 15, 2010 - December 14, 2011). Allocated 150,000 CPU cycles in the Texas Advanced Computing Center (TACC)

## Awards and Fellowships

- 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 Marejn 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.

## Conference Organization

- ACM-BCB 2022 (international conference on Bioinformatics, Computational biology and health informatics), PC chair.

- ACM-BCB 2017 (international conference on Bioinformatics, Computational biology and biomedicine), general co-chair.
- BiCOB (International conference on Bioinformatics and Computational Biology), Publicity chair since 2014.
- CSBW (Computational Structural Bioinformatics Workshop), co-chair and organizer. Held in conjunction with IEEE BIBM (International Conference on Bioinformatics and Biomedicine) or ACM-BCB (ACM international conference on Bioinformatics and Computational Biology), co-chair or steering committee member since 2013, involved in organization since 2011.
- Robotics in Structural Biology tutorial co-organizer, ACM-BCB (2013)
- Conference PC member: BIONETICS spceial track on bioinformatics (2010), BIONETICS special track on visual systems (2010), BiCOB (2014), CSBW (2011-2016), ACM-BCB (2014-2016), IEEE-BIBM (2014-2016)
- Conference session chair: BIO-IT (2011), CIBB (2012), CSBW (2011-2013), BIBM (2012), BIONETICS spceial track on bioinformatics (2010)
- BIONETICS 2010, chair of a Bioinformatics special track, 2010

### **Journal and Book Editorial**

- IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB), Journal editorial board (2017-present)
- Int. J. of Data Mining and Bioinformatics (IJDMB), journal editorial board (2017-present)
- Advances in Bioinformatics, Hindawi, journal editorial board (2013-2018, journal no longer exists)
- MDPI Molecules, Special issue for CSBW 2017, 2019, guest editor.
- JBCB Special issue for BICoB 2015, guest editor (2015)
- JCB (Journal of Computational Biology) Special issue for the Computational Structural Bioinformtcs Workshop (CSBW 2014, held in conjunction with ACM-BCB), guest editor (2015)
- BMC Structural Biology Special issue for the Computational Structural Bioinformtcs Work- shop (CSBW 2012, held in conjunction with IEEE BIBM), guest editor (2013)
- JBCB Special issue for the Computational Structural Bioinformtcs Workshop (CSBW 2011, held in conjunction with IEEE BIBM), guest editor (2012)
- JBCB Special issue for The 5th International Conference on Bio-Inspired Models of Network, Information and Computing Systems (BIONETICS 2010) special track on bioinformatics, guest editor (2011)
- Developing and Applying Biologically-Inspired Vision Systems: Interdisciplinary Concepts. Editors: M. Pomplun and J. Suzuki. Publishers: IGI Global (2011). Editorial review board member, reviewed 2 chapters.

### **Community and Outreach**

- UMB Women in Science club (WINS) co-organizer and faculty advisor.