Curriculum Vitae –Sefika Banu Ozkan

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Arizona State University
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EDUCATION

Ph.D. in **Chemical Engineering, 1997-2001**
Bogazici University**,** Istanbul, Turkey
Thesis: Analysis of Folding Kinetics for Simplified Models

M.S. in **Chemical Engineering, 1995-1997**
Bogazici University, Istanbul Turkey
Thesis: Identification of Native Conformations of Proteins Using a Low Resolution Model

B.S. Honors in **Chemical Engineering, 1991-1995**
Bogazici University, Istanbul, Turkey

RESEARCH POSITION HELD

- **2013 – Present Associate Professor** Department of Physics, Arizona State University
- **2006 – 2013 Assistant Professor** Department of Physics, Arizona State University
- **2006 – Present Member** Center for Biological Physics, Arizona State University
- **2003-2006 Postdoctoral Fellow** Department of Pharmaceutical Chemistry University of California San Francisco
  Advisor: Ken A. Dill
- **2001-2003 Research Associate** Department of Computational Biology, University of Pittsburgh, School of Medicine
  Advisor: Hagai Meirovitch

- **2001 Summer Visiting Researcher** Department of Computational Biology, University of Pittsburgh, School of Medicine
  Advisor: Ivet Bahar
- **1999-2001 Visiting Scholar** Department of Pharmaceutical Chemistry University of California San Francisco
  Advisor: Ken A. Dill
- **Summer 1996 Visiting Scholar** Stevens Institute of Technology Department of Chemical and Polymer Engineering
  Advisor : Dilhan Kalyon

AWARDS

- Scialog Fellow, Research Foundation and Moore Foundation , 2014
- Faculty Achievement Young Investigator Award, Arizona State University, 2013
- Best Ph.D. Thesis Prize, awarded by Bogazici University, 2001
- Integrated Ph.D. Program Fellowship from Scientific and Technical Research Council (TUBITAK) of Turkey, 1999 - 2002

PUBLICATIONS

1. **Butler BM, Kumar A** and Kumar S Ozkan SB "Dynamic allosteric residue coupling (DARC spots) reveals disease mechanism for Gaucher disease and nSNVs across the proteome " (2017) *Submitted*

2. **Butler BM, Kazan IC** and Ozkan SB "From Protein Sequence to Dynamics: Utilizing co-evolution to identify positions critical for protein dynamics" (2017) *Nature Scientific Reports* Submitted

3. **Modi T**, Hui Hui J, Ghosh K and Ozkan SB Thioredoxins evolved to modern day stability-function requirement by altering Native State ensemble (2017) *Philosophical Transactions of The Royal Society B* Ancient *Under Review*

4. **Campitelli P**, Guo J, Zhou HX, Ozkan S.B A Hinge-shift Mechanism Modulates Allosteric Regulations in Human Pin1 J. (2017) Phys Chem B Accepted

5. Larrimore KEm **Kazan IC, Bolia A** LKannan L, R Kendle RP,Jamal T, Barcus M, , Stephen Brimijoin S, Gao Y, Zhan CG, Ozkan SB, and Moore TS, "Enhanced nerve agent bioscavenging of cocaine hydrolase mutants of butyrylcholinesterase expressed in plants" (2017) Nature Scientific Reports

6. **Bolia A** and Ozkan SB "Adaptive BP-Dock: An Induced Fit Docking Approach for Full Receptor Flexibility" (2016) *J. Chem Inf. Model* **56**:734-746

7. **Kumar A, Butler BM,** Kumar S and Ozkan SB "Integration of Structural Dynamics and Evolution to Protein Interaction Networks: A New Era in Genomic Medicine" (2015) *Current Opinion in Structural Biology* **35**:135-142

8. **Kumar A, Campitelli P,** Thorpe MF and Ozkan SB " Partial Unfolding and Refolding for Structure Refinement: A Unified Approach of Geometric Simulations and Molecular Dynamics" (2015) *Proteins* **83**: 2279-2292

9. **Li Z, Bolia A,** Maxwell JD, Bobkow AA Ghirlanda G, Ozkan SB and Margulis CM **"**A Rigid Hinge Region is Necessary for High Affinity Binding of Dimannose to Cyanovirin and Associated Constructs" (2015) *Biochemistry* **54** :6951-6960

10. **Kumar A, Glembo, TJ,** Ozkan SB "Mechanism of Protein Evolution: The Role of Conformational Dynamics and Allostery in Disease Development " (2015) *Biophysica J*ournal **109**:1273-1281

11. Dutta P, Dargahi L,O' Connell KE, **Bolia A**, Ozkan SB and Dev KK"Parkin associated endothelin like receptor (PAELR) interacts with the autophagosomespecific Ub-like protein, GABARAPL2. " (2015) *European Journal of Neoroscie*nce, under review

12. **Butler MA,** Gerek ZN, Kumar S and Ozkan SB "Dynamically critical sites at protein interface are more prone to disease" (2015) *Proteins,* 83:428-435

13. **Zou T,** Risso VA, Gavira JA, Sanchez-Ruiz JM, Ozkan SB "Evolution of Conformational Dynamics Determines the Conversion of a Promiscuous Generalist into a Specialist Enzyme". (2015) *Mol Biol. Evol.* 32:132-143.

14. Kim H**, Zou T,** Modi C, Dorner K, Grunkmeyer TJ, Chen L, Fromme R, Matz MV, Ozkan SB, Wachter RM, "A hinge migration mechanism unlocks the evolution of green-to-red photoconversion in GFP-like proteins". (2015) *Structure* , 23:34-43

15. **Zou T,** Williams N, Ozkan SB, Ghosh K. "Proteome folding kinetics is limited by protein halflife." (2014) *PLoS One*, 9(11):e112701

16. Dutta B, Ozkan SB, Sailer A and Dev KK "PICK1 interacts with and protects against PAEL receptor induced cell death." (2014) *J. Neurochemistry*. 130:360-73

17. **Mielke C,** Cordova J, Border AW, Ozkan SB, Wayne W and Mandarino LW, "Acetylation of Adenine Nucleotide Translocase in Vivo in Human Muscle May Decrease Affinity for ADP and Alter Mitochondrial Function" (2014) *Biochemistry* 53:3817-29

18. ***Bolia A*,** Woodrum B, Cerada A, Ruben MA, Wang X, Ozkan SB***** and Ghirlanda GH* "Dissecting the determinants for dimannose binding in cyanovirin " (2014) *Biophysical J* 10:1142-51

19. Woodrum BW, Maxwell JD, ***Bolia A***, Ozkan SB*, Ghirlanda G. "The antiviral lectin cyanovirin-N: probing multivalency and glycan recognition through experimental and computational approaches." (2013) *Biochem Soc*. 5:1170-1176.

20. **Gerek ZN,** Kumar S and Ozkan SB* Structural dynamics flexibility informs function and evolution at a proteome scale" (2013) *Evol Appl.* 6:4223-4332. doi: 10.1111/eva.12052

21. **Bolia, A**., Gerek Z.N and Ozkan SB* "BP-Dock: a flexible docking scheme for exploring protein-ligand interactions based on unbound structures." (2014) *J. Chem. Inf Model.* 54(3):913-25.

22. Culviner PH, Anders M. Knight AM, Kurt N, ***Zhou T,*** Ozkan SB* and Cavagnero S Electrostatic Effects of the Ribosomal Surface on Nascent Protein Dynamics (2013) *ACS Chem Biol. 6: 1195–1204.*

23. **Glembo, TJ**, Farrell DW, Thorpe MF and Ozkan SB* "Collective dynamics differentiates functional divergence in protein evolution" (2012) *Plos Comp. Biol.* 8(3):e100242

24. Martin DR, Ozkan SB and Matyushov DV "Dissipative electro-elastic network model of protein electrostatic" (2012) *Phys Biol.* 9(3):036004.

25. **Bolia A** Gerek ZN, Dev KK and Ozkan SB*. "The binding affinity ies of proteins interacting with the PDZ domain of PICK1" (2011) *Proteins* 80:1393-408.

26. **Gerek ZN** and Ozkan SB* " (2011) "Change in allosteric network affects binding affinities of PDZ Domains: Analysis through Perturbation Response Scanning *PLoS Comp Biol. 10: e1002154.*

27. **Zou T** and Ozkan SB* "Native local topology shows important features of denatured basin" (2011) *Phys. Biol*. 8(6):06601.

28. **Glembo, TJ** and Ozkan SB* "Union of geometric constrained based simulations with molecular dynamics for protein structure prediction" (2010) *Biophysical J.* 98:1046-1054

29. **Gerek ZN** and Ozkan SB* " A Flexible docking scheme to explore PDZ Domain's binding selectivity" (2010) *Protein Science* 19:914-928.

30. Atilgan C, **Gerek ZN,** Ozkan SB*, Atilgan AR* "Manipulation of conformational change in proteins by single residue perturbation" (2010) Biophysical J. 99:933-943

31. **Gerek ZN**, Keskin O and Ozkan SB* "Identification of specificity and promiscuity in PDZ domain interactions through their dynamics behavior" (2009) Proteins. 77: 796-811.

32. Shell MS, Ozkan SB, Voelz V, Wu AGH and Dill KA "Blind test of physics-bases prediction of protein structures " (2009) Biophysical. J. 96:917-924.

33. Engen, JR, Wales TR, Hochrein JM, Meyn MA, Ozkan SB, Bahar I, and Smithgall TE, " Structure and dynamic regulation of Src-Famy Kinases (2008) *Cell. Mol. Life* Sci 65: 3058-3073

34. Dill KA, Ozkan SB, Shell MS, Weikl TR "The Protein Folding Problem" (2008) *Annu. Rev. Biopyhs. Biomol. Struct.* 37: 289-316

35. Dill KA, Ozkan SB, Wiekl TR, Chodera JD, Voelz VA, "The protein folding problem: when will it be solved?" (2007) *Curr. Opin. Struct. Biol*. 17: 342-346.

36. Ozkan SB, Wu AGH , Chodera JD, Dill KA "Protein Folding by Zipping and Assembly" (2007) *Proc. Natl. Acad. Sci. USA* 104:11987-11992

37. Ghosh K, Ozkan SB, Dill KA "The Ultimate Speed Limit of Protein Folding is Conformational Searching" (2007) *J. Amer. Chem. Soc*. 129:11920 -11927.

38. Ozkan SB and Meirovitch H "Conformation Search of Peptides and Proteins: The Monte Carlo Minimization with Adaptive Bias Applied to Hepta-Peptide Deltorphin", (2004) J*. Comp Chem*. 25:565-572.

39. Ozkan SB, Kirca S and Haliloglu T "Unfolding Events of Chymotrypsin Inhibitor 2 Revealed by off-lattice Monte Carlo Simulations and their Consistency from Structure-Based Analysis of Conformations", *Polymers (*2004) 45 :581-595

40. Ozkan SB and Meirovitch H, "Efficient Conformational Search Method for Peptides and Proteins: Monte Carlo Minimization with an Adaptive Bias", (2003) J*. Phys Chem*. 107: 9128-9131

41. Ozkan SB, Dill KA and Bahar I, "Computing the Transition State Populations in Simple Protein Models", (2003) *Biopolymers* 68: 35-46

42. Ozkan SB, Dill KA and Bahar I, "Fast-Folding Protein Kinetics, Hidden Intermediates and the Sequential Stabilization Model", (2002) *Protein Science* 11:1958-1970.

43. Ozkan SB, Bahar I and Dill KA, "Nonclassical Phi-values in Protein Folding Kinetics", *Nature Structural Biology* (2001) 98: 765-767.

44. Ozkan B and Bahar I, " Recognition of Native Structure from a Complete Enumeration of Low Resolution Conformation with Constraints" *Proteins* (1998) 32: 211-222.

INVITED PRESENTATIONS

1. Ozkan SB. Allostery Conformational Dynamics and Evolution 62nd Biophysical Society Meeting San Francisco February 2018, *Atoms to Cell Modelling Molecualr Complexity Workshop* ***invited speaker***

2. Ozkan SB. Allostery and Conformatoinal Dynamics in Protein Evolution, *Allostery and Molecular Machine Royal Society Symposion, June 2017 London* ***invited speaker***

3. Ozkan SB. Allostery and Dynamics in Protein Evolution and Disease, Kansas, State University, December 2016, Manhattan, Kansas, Chemistry Colloquium, ***invited speaker***

4. Ozkan SB. Allostery and Dynamics in Protein Evolution and Disease, University of Kansas Medical School, December 2016,Kansas City, KansasBiophysics Seminars ***invited speaker***

5. Ozkan S. B. Role of Conformational Dynamics in Protein Evolution and Disease Development, 1st International Conference on Computational Genomics and Proteomics October 2016 Columbus Ohio ***invited speaker***

6. Ozkan S.B **"**The State of Pharmacogenomic" June 2016 Gordon Research Conference on Human Single Nucleotide Polymorphisms & Disease Boston, *Chair /Discussion Leader*

7. Ozkan S. B. Role of Conformational Dynamics in Protein Evolution and Disease Development, 3rd International Conference on Mathematical and Computational Medicine May 2016 Columbus Ohio ***invited speaker***

8. Ozkan S. B. Mechanism of Protein Evolution: Conformational Dynamics and Allostery Biology Seminar Series, March 2016, Temple University, Philadelphia PA ***invited Speaker***

9. Ozkan S. B.,Mechanism of Protein Evolution, Conformational Dynamics and Allostery, Albany 21st Conversation, University of Albany, NY June 2015 ***invited speaker***

10. Ozkan S. B. The Role of Conformational Dynamics on Protein Evolution and Mechanism of Disease Development, Department of Pediatrics, Nationwide Children's Hospital Ohio State University, May 2015, ***invited speaker***

11. Ozkan SB The Mechanism of Protein Evolution, Biological Physics Seminar April 2015 ASU, ***invited speaker***

12. Ozkan SB***,*** Sequence-Structure and Function: Folding and Design, July 2015, Koc University, Turkey ***invited speaker***

13. Ozkan S. B. A Physic-based Protein Structure Refinement Approach: Protein and RNA Structure Prediction Conference December 2013 Cancun, Mexico, ***invited speaker***

14. Ozkan S. B. Design of New Sequences Through Zipping and Assembly, American Physical Society Four Corners Meeting October 2013 Denver, Colorado, ***invited speaker***

15. Ozkan S. B. The role of Structural Dynamics in Disease Mutations, Zing Conferences: Mathematical and Computational Medicine Conference December 2012 Cancun, Mexico, ***invited speaker***

16. Ozkan S.B Deciphering the folding code using a physics-based folding approach Gordon Research Conference Biopolymers, June 2012 Salve Regina University Newport, Rhode Island, ***invited speaker***

17. Ozkan SB Protein Folding on Ribosome , Protein and Peptide Interactions in Cellular Environment Workshop June 2012, Telluride Conferences, Telluride Science Research Center, Telluride, Colorado, ***invited speaker***

18. Ozkan SB Protein Binding and Allostery, , Coarse-Grained Modeling of Structure and Dynamics of Bio-macromolecules July 2012, Telluride Conferences ,Telluride, Colorado, ***invited speaker***

19. Ozkan SB "Protein Folding on Ribosome" 243rd American Chemical Society Meeting, San Diego Protein Evolution and Conformational Diversity, 2012 ***invited speaker,***

20. Ozkan SB. " Structural Dynamics and Protein Evolution " Society for Molecular Biology and Evolution (SMBE) Satellite Symposium on Phylomedicine 2012 Arizona ***invited speaker***

21. Ozkan SB "Conformational Diversity, Evolution and Foldability" 2011 11th KIAS Conference on Protein Structure and Function, Seoul, South Korea **invited speaker.**

22. Ozkan SB "Conformational Diversity, Evolution and Foldability invited speaker Zing Conference on Protein and DNA Structure Prediction, December 2011 Mexico, ***invited speaker***

23. Ozkan SB "Perturbation Response Scanning Method for Identifying Allosteric Transitions and Utilizing in Flexible Docking" Albany 2011 17th Conversation, June 2011, ***invited speaker***.

24. Ozkan SB "Conformational Diversity, Evolution and Foldability", University of Chicago, Department of Bioengineering 2011 ***invited speaker*** for seminar series.

25. Ozkan S. B "Protein Foldability and Functional Evolution by Conformational Dynamics" Telluride Conferences 2010, ***invited speaker***

26. Ozkan SB, Adam de Graff, Dan Farrel, Mike Thorpe, Mechanical Aspects of Protein Folding and Unfolding, April 2010, NIH-NSF PI meetings at University of Maryland, ***Invited Speaker***

27. Ozkan S. B "Protein Foldability and Functional Evolution by Conformational Dynamics" University of California Santa Barbara 2010***, invited speaker*** for Biochemistry Seminar Series

28. Ozkan S. B "Protein Foldability and Functional Evolution by Conformational Dynamics" Protein Folding Workshop, Arizona State University, 2010, ***invited speaker***

29. Ozkan SB "Promiscuity and Selectivity of Peptide Binding, University of California Santa Barbara ,Department of Biochemistry, Seminar Series, January 2010 ***invited speaker.***

30. Ozkan SB " Protein folding by Zipping and Assembly, Department of Chemical Engineering, Seminar Series, Koc University Turkey, July 2009 ***invited speaker***

31. Ozkan SB "PDZ Domains Selectivity " Center for Innovation in Medicine, Biodesign Institute, ASU March 2009 ***invited speaker***

32. Ozkan SB "PDZ Domains Selectivity " Barrow Neurological Institute March 2008 ***invited speaker***

33. Ozkan SB and Dill KA " Protein Folding Principles" Second Symposium on Proteins Universidad Autonoma Metropolitana Iztapalapa, October 19-21 2008 Mexico City Mexico ***invited speaker.***

34. Ozkan SB and Dill KA "Using the Physics of Protein Folding to Guide Protein Folding" Biochemistry Seminars, April 18, 2005 San Francisco State University San Francisco. ***invited speaker.***

35. Ozkan SB and Dill KA "Using the Physics of Protein Folding to Guide Conformational Searching" 2nd Biological Language Conference, November 18-19, 2004 Carnegie Mellon University, Pittsburgh ***(invited speaker).***

36. Ozkan SB , Folding Kinetics of Proteins, at NIH, Maryland June 2002 (***invited speaker).***

37. Ozkan SB and Dill KA " Protein Folding by Zipping October 29 2006 Molecular Dynamics Discussion University of California San Francisco, San Francisco ***invited speaker).***

38. Atilgan, C, Ozkan SB, Atilgan AR "Conformational Multiplicity and Landscape Shifts in Native Proteins" 51st Biophysical Society Meeting, Long Beach February 2008 (***oral presentation).***

39. Ozkan SB, Shell MS, Wu AG, Voelz VA, Dill KA, "Protein Folding by Zipping and Assembly" 50th Biophysical Society Meeting, Baltimore March 2007 (***oral presentation)***

40. Ozkan SB and Bahar I, " Recognition of Native Structure from a Complete Enumeration of Low Resolution Conformation with Constraints", Statistical Physics IV , July 1997, Istanbul Technical University, Istanbul, Turkey (***Invited Talk***).

41. Ozkan SB, Dan Farrell, Adam De Graff and Michal Thorpe "Protein Folding and Unfolding by Geometric Simulation Methods" Frontiers in Mathematical Biology NSF-NIH PI meeting, University of Maryland, March 2010 (poster presentation)

42. Zou T and Ozkan S.B. "A physics-based approach for protein foldability" 53rd Biophysical Society Meeting, San Francisco February 2010 (Poster Presentation)

43. Glembo T. J. and Ozkan S. B. " Ancient Protein Structure Prediction" " 53rd Biophysical Society Meeting, San Francisco February 2010 (Poster Presentation)

44. Gerek ZN, Ozkan SB, "Flexible Docking in PDZ Domains using Elastic Network Model and Replica Exchange Molecular Dynamics" 52st Biophysical Society Meeting, Boston February 2009 (poster presentation).

45. Shell, M.S., Ni X.,Ozkan S.B. Protein Structure Refinement Using Physics-Based Models And Sampling" 52st Biophysical Society Meeting, Boston February 2009 (poster presentation)

46. Ghosh K, Ozkan SB "The role of pressure in protein folding" 52st Biophysical Society Meeting, Boston February 2009 (poster presentation)

47. Gerek. ZN, Kesin O, Ozkan SB, "How Dynamics Govern the Role of Selectivity in PDZ domains?" 51st Biophysical Society Meeting, Long Beach February 2008 (poster presentation)

48. Glembo T, Wells SA. Thorpe MF, Ozkan SB "A New Search Principle for Protein Structure Prediction: Zipping and Assembly Method Using FRODA" 51st Biophysical Society Meeting, Long Beach February 2008 (poster presentation)

49. Ozkan SB, Gerek ZN, Keskin O "Promiscuity and protein-protein interaction dynamics in PDZ Domains" 50th Biophysical Society Meeting, Baltimore March 2007 (poster presentation).

50. Ozkan SB, Ghosh K, Dill KA "Ultimate Speed Limit of Protein Folding" 50th Biophysical Society Meeting, Baltimore March 2007 (poster presentation).

51. Ozkan SB, Ghosh K and Dill KA "Mining the Energy Landscape of Parameters, from Two-State Protein Folding Experiments" 49th Biophysical Society Meeting, Long Beach, February, 2005 (poster presentation).

52. Ozkan SB and Dill KA, "Folding of Simple Protein Models: Relating Micro-paths to Macro paths" 48th Annual Biophysical Society Meeting, Baltimore February 2004 (poster presentation).

53. Ozkan SB and Meirovitch H, “Efficient Conformational Search Method for Peptides and Proteins, Science 2002 Meeting in the University of Pittsburgh, Pittsburgh, September 2002 (poster presentation).

54. Ozkan SB, Kirca S and Haliloglu T. “Unfolding of Chymotrypsin Inhibitor 2 by Coarse Grain Simulations”4th International Conference on Molecular Structural Biology, Vienna Austria, September 2001 (poster presentation).

55. Ozkan SB, Dill KA, Bahar I, “"Sub cooperative Folding Events Revealed by Complete Analysis of Folding Kinetics for Simplified Model Proteins", in Protein Society Meeting, San Diego, USA, August, 2000 (poster presentation).

56. Ozkan SB and Bahar I, “"Vibrational Dynamics of cAMP Kinases", Computational Biophysics 2000, Nice, France, July, 2000 (poster presentation).

57. Ozkan SB, Keskin O, and Bahar I, " Recognition of Native Structure from a Complete Enumeration of Low Resolution Conformation with Constraints”, ", 8th European Congress on Biotechnology, August 1997, Budapest, Hungary. (poster presentation)

58. Ozkan SB and Bahar I, “Vibrational Dynamics of CAMP Kinase Proteins by Gaussian Network Model” International Chemical Physics III October 1998, Bogazici University, Istanbul, Turkey (oral presentation).

59. Keskin O, Ozkan SB, and Bahar I, "Side Chain Packing in Protein Structures", 8th European Congress on Biotechnology, August 1997, Budapest, Hungary. (poster presentation).

GRANTS

Ongoing Research Support

NIH/NIADD Ozkan (PI) 08/01/2016-07/31/2017

New Tools for Glycoscience: Engineering Targeted Lectins by Computer- Guided Directed Evolution

This is multi-PI R21 grant. The application of natural lectins and antibodies in glycoscience is currently hindered due to their low binding affinity and poor specificity. We propose to develop a class of rationally designed high affinity, high specificity reagents targeted to glycans by integrating rational design of lectins using computational methods with guided directed evolution. These new reagents will be integrated into available platforms such as lectin microarrays, and address an urgent need in for robust, reliable, and inexpensive tools to identify glycans

NSF-MBC Ozkan (PI) 8/1/2017-7/31/2019

Mapping Sequence-Structure Function Landscape by Integrating Evolutionary Landscape Inference with Folding and Dynamics

The major goal of this project is utilize protein evolution to elucidate the critical interactions that contributes to folding and also binding specificities of peptide binding domain proteins

Gordon-Betty MooreFoundation (Scialog Award) Ozkan (PI) 8/1/2017-7/31/2018
Unraveling the second secret of life:Are All Proteins Allosteric
The major goal of this project is to understand the mechanism by which distant protein residues communicate, or how prevalent allostery is in proteome. Here, we will combine recently-developed theoretical and experimental methods to answer the question: *how well can we create allostery*

1 R01 GM118772-01 Beckstein (PI) 4/1/2016 – 3/31/2021
NIH-NIGMS
Molecular Mechanisms of Secondary Active Transporters
The major goal of this project is to understand and provide molecular mechanisms of membrane proteins which are secondary active transporters, and our role is to use our BP-docking approach to model the interaction of different ligands with targeted membrane transporter proteins in their different states.
Role: Co-investigator

Completed Research Support

Temple University (NIH/NLM) Ozkan (PI) 08/01/2010 -7/31/2016

NIH/NLM
Computational diagnosis of non-synonymous variations using structural dynamics
We collaborate on integrating protein structural dynamics with functional biological knowledge into human genetics which will lead to a better diagnosis and mechanistic understanding of the structural features of sequence variations implicated in human health.

1U54GM094599-0 Fromme (PI) 01/01/2010 – 04/30/2016
NIH/NIGMS
Center for Membrane Proteins in Infectious Diseases, MPID
This work is concerned with 3-D structure determination of membrane proteins involved in infectious diseases. Our role includes prediction of flexible loops of the structure and all-atom refinement of low resolution experimental structures.

NSF-BMC Ghirlanda (PI) 08/01/2010- 07/31/2016

Collaborative Research: A General Approach to the Design of Tailor-Made Glycan Recognition Protein Modules.
This project aims to investigate the binding specificity of cyanovirin–N (CVN), a small and extremely robust lectin that binds Manα(1,2)Manα with high affinity and specificity. Our role is to explore the sequence space that supports high-affinity binding to the target glycan through our flexible docking methods in parallel to directed evolution by phage display on the experimental side.

2R01DK047936-16m Mandorino (PI) 01/02/2012-12/31/2016
NIH/NIDDK
Molecular Regulation of Muscle Glucose Metabolism in Man
We collaborate on modeling structure of acetylated mitochondrial proteins identified in mitochondrial from insulin resistant obese and type 2 diabetic patients.

ASU-Mayo Ozkan (PI) 01/01/2012 – 05/01/2013
Identifying Disease-Associated Genome Variants through Computational Prediction of Functional Sites in Protein Structures
The goal of this project is to develop a novel *in silico* method for predicting whether a particular non-synonymous single nucleotide variants within a protein coding region of the human genome contributes to disease risk and, if so, what is the probable molecular mechanism.

MPS-NSF Ozkan (PI)
06/01/2010 – 05/31/2011 NSF-MPS
Workshop on Protein Folding
This funding is used to organize a workshop on protein folding and folding pathways where we invite the leading theoretical and experimental expert in the field.

NSF-BMC and U. Wisconsin Ozkan (PI) 03/15/201002/28/2011
Biophysical Aspects of Co-translational folding
This project is concerned with molecular understanding of the nascent chain dynamics, which the protein is being synthesized on ribosome. We provide all-atom molecular dynamics of nascent chain coupled with ribosomal surfaces using multi-scale computational methods. The results are used to set new set of experiments for our experimental collaborator Dr. Cavagnero at University of Wisconsin, Madison.

COLLABORATORS AND OTHER AFFILIATIONS

Collaborators
Ali Rana Atilgan (Sabanci University, Turkey)
Canan Atilgan (Sabanci University, Turkey)
Andrew Bordner (Mayo Clinic)
John Chaput (ASU, Biodesing)
Silvia Cavagnero (University of Wisconsin, Madison)
Kumlesh Dev (Trinity College, Institute of Neuroscience, Ireland)
Petra Fromme (ASU)
Giovanna Ghirlanda (ASU)
Brenda Hogue (ASU)
Ozlem Keskin (Koc University, Turkey)
Sudhir Kumar (ASU, Biodesign)
Lawrence Mandarino (Mayo Clinic)
Michael F. Thorpe (ASU)
Michael Rosenberg (ASU, Biodesign)

Jose Manuel Sancherz Ruiz (University of Granda, Spain)
Jieping Ye (ASU, Biodesign)

TEACHING

Courses Taught

PHY 498/598 Advance topics in Biophysics I developed a graduate level biophysics course about the theoretical modeling of biological systems that was designed to bridge theory with application in order to evoke students' interest towards quantitative research.

PHY 441 Statistical and Thermal Physics New simulation package (MD applications) has been be taught along with other simulation methods.

PHY 241 University Physics III for engineers: Thermodynamics, kinetic theory, physical and wave optics, relativity, photons, matter waves, atomic physics.

BME 595 Modeling and Simulations of Physiological Systems offered by Bioengineering Department, I taught a two-week module on molecular modeling

BDE 701/BCH598 Biological Design Program Major Graduate Course, Guest Lecturer on Computer Models of Proteins

Post-Doctoral Mentoring

Avishek Kumar (2013-present, ASU)
Z. Nevin Gerek (2006-2013, ASU)
Pooja Narang (2010-2011 , ASU)

Graduate Students Mentoring

As Research Advisors (Chair)

PhD Students:
Tyler Glembo (2007 -2011, Department of Physics, ASU)
Taisong Zou (2007 -2013, Department of Physics, ASU)
Ashini Bolia (2010-2015Fall-current Department of Biochemistry, ASU)
Brandon Butler (2012-2016, Department of Physics, ASU)
Paul Campitelli (2014-present, Department of Physics, ASU)
Tushar Modi (2014-present, Department of Physics, ASU)
Ismail Kazan (2015-present School of Molecular Science ASU)

Mentoring Rotation Students Under PhD Program
Nicholas Ose
Brandon Butler (2011 Fall Rotation Student Department of Physics, ASU)
David Dotson (2012 Spring Rotation Student Department of Physics, ASU)
Jaimy Tomlinson (2011 Spring Rotation Student Department of Physics, ASU)
Yao Ji (2010. Fall Rotation Student Department of Physics, ASU)
Sara Sizemore (2009 Fall Rotation Student Department of Physics, ASU)
Rui Wang (2008 Spring, Rotation Student Department of Physics, ASU)

Xuan Ni (2008 Spring-2009 Spring, Department of Physics, ASU)
Veysi Demir (2007 Fall, Rotation Student Department of Physics, ASU)
Yun Zhao (2011 Fall-2012 Spring, Department of Physics, ASU)

Master Students
Ashini Bolia (2009-2010 Computational Biosciences Program, ASU)
John Penn (2008 -2010 Computational Biosciences Program, ASU)
Lohith Madireddy (2007 spring-summer Computational Biosciences Program, ASU)
Jaimy Tomlinson (2010-2012 Physics, ASU)

As Committee Member
David Department of Physics, ASU) Committee Member
Sarah Sizemore (Department of Physics, ASU) Committee Member
Adam De Graff (Department of Physics, ASU) Committee Member
Adam Mott (Department of Physics, ASU) Committee Member
Dan Farrell, (Department of Physics, ASU) Committee Member,
Xiang Chen (Department of Physics, ASU)) Committee Member,
Stephanie Cope (Department of Physics, ASU) Committee Member
Guo Zhu (Department of Physics, ASU) Committee Member
Billie Joe Harvey /9Department of Biochemistry, ASU)Master Thesis Committee Member
Padmini Surapaneni Computational Biosciences Internship Committee Member, Fall 2008
Lohith Madireddy Computational Biosciences Internship Committee Member, Fall 2008
Robert Lawrence (Department of Biochemistry, ASU) Committee Member, Spring, 2008
Ashley Kimbel (Department of Physics, ASU) Committee Member Fall, 2007
Craig Jolley (Department of Physics, ASU) Committee Member Fall, 2007

SERVICE

Professional Service

Organized a workshop on protein folding with Dr. Thorpe at Arizona State University May 2010,

Organizes Tuesday Chalk Talk Series For Center for Biological Physics 2009-2011

Mentoring high school student Arjun Chandrasekhar from Corona Del High School in his science project, Rom Zarchi from t he Center for Research in Engineering, Science, and Technology (CREST) which is a specialty program offered at Paradise Valley High School -

Active participant in Math &Science Teacher Fellow Program (MSTF). She hosted high school teachers in her lab and work together to develop a teaching module that offers the latest in science. Within the program, the teacher taught protein folding in their course and I have visited two high schools (Runyon and Canyon High school) and gave a

seminar about protein folding. I will continue to participate in in Math &Science Teacher Fellow Program (MSTF) this summer.

Lecturer October 20th 2007 Arizona High School Teachers Program.

Lecturer in the Symposium of the IEEE in Monterey, Mexico (SIEEM), organized by the graduate students of Monterey Institute of Technology Monterey Mexico November 2007.

Member of Biophysical Society, Protein Society and American Chemical Society

External Referee for NSF and NIH proposals

Served in the NSF-Math Bio Review Panel twice in April 2009 and 2012

Reviewers for several papers including PNAS, JACS, Biophysical J, Plos Comp Bio, Plos One, Proteins, Protein Science, BMC Bioinformatics, Journal of Chemical Physics, Physical Biolgy

Department Service
Undergraduate Biophysics Program Director (2014-present)
Undergraduate Program Director 2010-2012
Undergraduate Committee Member 2010-2012
Physics Colloquium Member 2010- current
Committee on Committee Member 2010-2011
Chair of Committee on Committee on Committee 2009-2010
Personal Committee Member 2007-2009
Biophysics Faculty Search Committee in 2007 and in 2010 (the committees successfully hired Sara Vaiana, in 2007 and Oliver Beckstein in 2010)