Julie C. Mitchell

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Research and Professional Experience

2014 -	Professor	Mathematics and Biochemistry, U.W. Madison
2009 - 2014	Associate Professor	Mathematics and Biochemistry, U.W. Madison
2003 - 2009	Assistant Professor	Mathematics and Biochemistry, U.W. Madison
2001 - 2003	Assistant Principal Scientist	San Diego Supercomputer Center, U.C. San Diego
1998 - 2001	Postdoctoral Scientist	San Diego Supercomputer Center, U.C. San Diego

Education and Training

University of California at San Diego	Postdoctoral	1998 - 2001	Computational Biology
University of California at Berkeley	Ph.D.	1998	Mathematics
San Jose State University	B.A.	1992	Mathematics

Professional Activities

Trainer	Computation & Informatics in Biology & Medicine
Trainer	Biotechnology Training Program
Trainer	Biophysics Program
Trainer	Medical Sciences Training Program
Trainer	Khorana Scholars Program
Trainer	Undergraduate Research Program
Program Committee	Great Lakes Bioinformatics Meeting, 2016
Program Committee	Great Lakes Bioinformatics Meeting, 2015
Program Committee	International Society for Computational Biology Meeting, 2016
Program Committee	International Society for Computational Biology Meeting, 2015
Program Committee	International Society for Computational Biology Meeting, 2014
Program Committee	International Society for Computational Biology Meeting, 2013
Session Chair	Society for Industrial and Applied Mathematics, Boston MA, July 2016
Session Chair	Society for Mathematical Biology, Knoxville TN, July 2012
Session Chair	Intl. Conf. on Numerical Analysis and Applied Math., Rhodos, Greece, September 2010
Session Chair	Intl. Conf. on Numerical Analysis and Applied Math., Crete, Greece, September 2009
Session Chair	Math Fest, Madison WI, August 2008
Session Chair	Intl. Meeting of the American Mathematical Society, Rio de Janiero, Brazil, June 2008
Session Chair	Biomedical Engineering Society Meeting, Chicago IL, Oct 2006
Co-Organizer	32nd Annual Steenbock Symposium, Madison WI, May 2006
Organizer	Contemporary Biochemistry Series, Madison WI, Fall 2005
Organizer	Environmental Microbes Workshop, Madison WI, Sep 2005
Co-Organizer	High Performance Biocomputing Workshop, Washington DC, Aug 2005
Co-Organizer	SciDAC Workshop, San Francisco CA, Jun 2005
Co-Organizer	Multiscale Mathematics Workshop, Portland OR, May 2005
Advisory Editor	Journal of Theoretical & Computational Chemistry
Member	American Math Society Liason Committee to AAAS (2010-2012)
Referee	Proteins, Nuc Acids Res, Biophys J, Bioinformatics, PLoS Comput Biol, J Comp Chem
Reviewer	NIH, NSF, DOE

Awards and Honors

2007 Vilas Associates Award
2006 Alfred P. Sloan Research Fellowship in Molecular Biology
2003 Steenbock Faculty Fellow, U.W. Madison
1998 La Jolla Interfaces in Science Postdoctoral Fellow, U.C. San Diego
1997 Achievement Rewards for College Scientists (ARCS) Foundation Fellow
1997 Regents Fellow, U.C. Berkeley

Codes and Websites

KFC: web server for predicting alanine mutagenesis hot spots (over 70,000 jobs since 2011!)
http://kfc.mitchell-lab.org

DBSI: predicts DNA binding sites on proteins
http://dbsi.mitchell-lab.org

CubeZern: creates representations of low-resolution microscopy data using Zernike polynomials
http://cubezern.mitchell-lab.org

CUDESA: method for calculating surface areas and desolvation on using parallel computation on graphics cards
http://cudesa.mitchell-lab.org/

FADE: computes atomic density using Fast Fourier Transforms
http://www.mitchell-lab.org/FADE.php

SOI: calculates statistically uniform samples of 3D rotation groups
http://rotations.mitchell-lab.org

Publications

[1] Cimermancic P, Weinkam P, Rettenmaier JT, Bichmann L, Keedy DA, Woldeyes RA, Schneidman-Duhovny D, Demerdash ONA, Mitchell JC, Wells JA, et al. (2016) CryptoSite: Expanding the druggable proteome by characterization and prediction of cryptic binding sites. (in press).

[2] Alsop JD, Mitchell JC (2015) Interolog interfaces in protein docking. Proteins 83:1940–6.

[3] Hatano H, Shaw J, Marquardt KR, Zhang Z, Gauthier L, Chanteux S, Rossi B, Li D, Mitchell JC, Kollnberger S (2015) The D0 immunoglobulin-like domain plays a central role for the stronger binding of KIR3DL2 to B27 free heavy chain dimers. J Immunol 194:1591–601.

[4] Lohman LC, Forouhar F, Beebe ET, Stefely MS, Minogue CE, Ulbrich A, Stefely JA, Sukumar S, Luna-Snchez M, Jochem A, et al. (2014) Mitochondrial COQ9 is a lipid-binding protein that associates with COQ7 to enable coenzyme Q biosynthesis. Proc Natl Acad Sci U S A 111:E4697–705.

[5] Shen QT, Schuh AL, Zheng Y, , Quinney K, Hanna M, Mitchell JC, Otegui MS, Ahlquist P, Cui Q, et al. (2014) Structural analysis and modeling reveals new mechanisms governing ESCRT-III spiral filament assembly. J Cell Biol 206:763–77.

[6] Lensink MF, Moal IH, Bates PA, Kastritis PL, Melquiond ASJ, Karaca E, Schmitz C, van Dijk M, Bonvin AMJJ, Eisenstein M, et al. (2014) Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function, and Bioinformatics 82:620–32.

[7] Zhu X, Ericksen SS, Demerdash ONA, Mitchell JC (2013) Data-driven models for protein interaction and design. Proteins: Structure, Function, and Bioinformatics 81:2221–2228.

[8] Demerdash ONA, Mitchell JC (2013) Using physical potentials and learned models to distinguish native binding interfaces from *de novo* designed interfaces that do not bind. Proteins 81:1919–1930.

[9] Zhu X, Ericksen SE, Mitchell JC (2013) DBSI: DNA binding site identifier. Nucl Acid Res Methods 41:e160.

[10] Moretti R, Fleishman SJ, Agius R, Torchala M, Bates PA, Kastritis PL, Rodrigues JPGLM, Trellet M, Bonvin AMJJ, Cui M, et al. (2013) Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function, and Bioinformatics 81:1980–1987.

[11] Pattnaik BR, Tokarz S, Asuma M, Schroeder T, Sharma A, Mitchell JC, Edwards AO, Pillers DM (2012) Snowflake vitreoretinal degeneration (SVD) mutation of human Kir7.1 (R162W) is a non-functional channel. PLoS ONE 8:e71744.

[12] Demerdash ONA, Mitchell JC (2012) Density-cluster NMA: A new protein decomposition technique for coarse-grained normal mode analysis. Proteins 80:1766–1779.

[13] Fleishman SJ, Whitehead TA, Strauch E, Corn JE, Qin S, Zhou H, Mitchell JC, Demerdash ONA, et al, Baker D (2011) Community-wide assessment of protein-interface modeling suggests improvements to design methodology. J Mol Biol 414:289–302.

[14] Mitchell JC, Rutkoski TJ, Bannen RM, G N Phillips J (2011) Designing thermophilic proteins: A structure-based computational approach. In: Sen S, Nilsson L, editors, Thermostable Proteins: Structural Stability and Design, CRC Press. pp. 105–116.

[15] Zhu X, Mitchell JC (2011) KFC2: A knowledge-based hot spot prediction method based on interface solvation, atomic density and plasticity features. Proteins 79:2671–2683.

[16] Lall R, Donohue T, Marino S, Mitchell JC (2011) Optimizing ethanol production selectivity. Math Comp Modell 53:1363–1373.

[17] Demerdash ONA, Buyan A, Mitchell JC (2010) ReplicOpter: A replicate optimizer for flexible docking. Proteins 78:3156–3165.

[18] Dufour YS, Wesenberg GE, Tritt AJ, Glasner JD, Perna N, Mitchell JC, Donohue TJ (2010) chipD: A web tool to design oligonucleotide probes for high-density tiling arrays. Nuc Acid Res 38:W321–W325.

[19] Demerdash ONA, Daily M, Mitchell JC (2009) Structure-based predictive models for allosteric hot spots. PLoS Comp Biol 5:e1000531.

[20] Dynerman D, Butzlaff EA, Mitchell JC (2009) CUSA and CUDE: GPU-accelerated methods for estimating solvent accessible surface area and desolvation. J Comp Biol 16:523–537.

[21] Yershova A, Jain S, LaValle SM, Mitchell JC (2009) Generating uniform incremental grids on $SO(3)$ using the Hopf fibration. International Journal of Robotics Research :doi:10.1177/0278364909352700.

[22] Bannen RM, Suresh V, Wright SJ, G N Phillips J, Mitchell JC (2008) Optimal design of thermostable proteins. Bioinformatics 24:2339–2343.

[23] Mitchell JC (2008) Discrete uniform sampling of rotation groups using successive orthogonal images. SIAM J Sci Comp 30:525–547.

[24] Darnell SJ, Legault L, Mitchell JC (2008) KFC server: Interactive forecasting of protein interaction hot spots. Nuc Acid Res 36:W265–W269.

[25] Lall R, Mitchell JC (2007) Metal-reduction kinetics in *Shewanella*. Bioinformatics 23:2754–2759.

[26] Darnell SJ, Page D, Mitchell JC (2007) Automated decision-tree approach to predicting protein-protein interaction hot spots. Proteins 68:813–823.

[27] Marcia RF, Mitchell JC, Rosen JB (2007) Multi-funnel optimization using Gaussian underestimation. Journal of Global Optimization 39:39–48.

[28] Marcia RF, Mitchell JC, Wright SJ (2007) Global optimization in protein docking using convex underestimation and semidefinite programming. Optimization Methods and Software 22:803–811.

[29] Lynch KL, Gerona RRL, Larsen EC, Marcia RF, Mitchell JC, Martin TFJ (2007) Synaptotagmin C2A loop 2 mediates Ca2+-dependent SNARE interactions essential for Ca2+-triggered vesicle exocytosis. Mol Biol Cell 18:4957–4968. **(Feature article)**.

[30] Kedlaya RH, Bhat KMR, Mitchell JC, Darnell SJ, Setaluri V (2006) Trp1 interacting PDZ-domain protein GIPC forms oligomers and is localized to intracellular vesicles in human melanocytes. Arch Bioc Biophys 454:160–169.

[31] Rutkoski TJ, Kurten EL, Mitchell JC, Raines RT (2005) Disruption of shape-complementarity markers to create cytotoxic variants of ribonuclease A. J Mol Biol 354:41–54.

[32] Marcia RF, Mitchell JC, Rosen JB (2005) Iterative convex quadratic approximation for global optimization in protein docking. Comp Opt Appl 32:285–297.

[33] Zbilut JP, Giuliani A, Colosimo A, Mitchell JC, Colafranceschi M, Marwan N, Jr CLW, Uversky VN (2004) Charge and hydrophobicity patterning along the sequence predicts the folding mechanism and aggregation of proteins: A computational approach. J Proteome Res 3:1243–1253.

[34] Zbilut JP, Mitchell JC, Giuliani A, Colosimo A, Marwan N, Webber Jr CL (2004) Singular hydrophobicity patterns and net charge: A mesoscopic principle for protein aggregation/folding. Physica A 343:348–358.

[35] Mitchell JC, Shahbaz S, Ten Eyck LF (2004) Interfaces in molecular docking. Molecular Simulation 30:97–106.

[36] Law DH, Ten Eyck LF, Katzenelson O, Tsigelny I, Roberts VA, Pique ME, Mitchell JC (2003) Finding needles in haystacks: Re-ranking dot results using shape complementarity, cluster analysis and biological information. Proteins 52:33–40.

[37] Mandell JG, Roberts VA, Pique ME, Kotlovyi V, Mitchell JC, Nelson E, Tsigelny I, Ten Eyck LF (2001) Protein docking using continuum electrostatics and geometric fit. Protein Engineering 14:105–113.

[38] Mitchell JC, Kerr R, Ten Eyck LF (2001) Rapid atomic density methods for molecular shape characterization. J Mol Graph Model 19:324–329.

[39] Mitchell JC, Phillips AT, Rosen JB, Ten Eyck LF (2000) A coupled scanning and optimization scheme for molecular docking. In: Floudas CA, Pardalos PM, editors, Optimization in Molecular Biology and Computational Chemistry. Klewer Academic Publishers, pp. 190–207.

[40] Mitchell JC, Phillips AT, Rosen JB, Ten Eyck LF (1999) Coupled optimization in protein docking. In: Istrail S, Pevzner P, Waterman M, editors, Proceedings of the Third Annual Conference in Computational Biology (RECOMB99). ACM Press, New York, pp. 180–184.

Invited Presentations (Since Fall 2009)

Data-Driven Models for Protein Binding and Mutagenesis Effects
IMPA Biomath Workshop, Rio de Janiero, Brazil, March 2015

Data-Driven Models for Biophysics
UCLA, February 2015

Data-Driven Models for Biophysics
USC, February 2015

Interologs in Protein Docking
Modeling Protein Interactions, October 2014

Data-Driven Models for Protein Binding and Mutagenesis Effects
Bio-X Meeting, Recife, Brazil, November 2013

Kicking and Swinging: Collective Motion at the Local Scale
Gordon Research Conference: Computational Approaches to NMR, July 2013

Knowledge-Based Structural Approaches to Protein Modeling
Telluride Workshop on Protein Modeling, July 2013

DBSI: DNA Binding Site Identifier
Rules of Protein-DNA Recognition: Computational and Experimental Advances, Banff, Canada, June 2013

Using Knowledge-Based Models to Predict Mutagenesis Effects
Critical Assessment of Predicted Interactions (CAPRI), Utrecht, Netherlands, April 2013

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
International Conference Frontiers in Systems and Synthetic Biology, March 2013

Structure-Based Predictive Models for Mutagenesis Effects
Modeling of Protein Interactions, November 2012

Density Cluster NMA: Protein Decomposition for Normal Mode Analysis
Kansas State University, November 2012

Density Cluster NMA: Protein Decomposition for Normal Mode Analysis
American Math Society Meeting, October 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Society for Mathematical Biology, July 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Computational Biology to Systems Biology, June 2012

The Geometry of Molecules
Massachussetts Institute of Technology, March 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Colorado State University, February 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Indiana State University, February 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Michigan State University, January 2012

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
Rush University, November 2011

Uniform Deterministic Sampling of Rotation Groups and Applications to Biology
SIAM Conference on Geometric Modeling, October 2011

ReplicOpter: A Replicate Optimizer for Flexible Docking
Mathematical Biosciences Institute, April 2011

Predictive Models for Flexible Protein Docking and Allostery
University of Illinois - Chicago, January 2011

Uniform Deterministic Sampling of Rotation Groups and Applications to Biology
IMPA Biomath Workshop, Foz do Iguazu, Brazil, March 2011

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
UC Berkeley, May 2010

Knowledge-Based Structural Approaches for Predicting Hot Spots of Protein Binding and Allostery
UC San Francisco, April 2010

Using Numerical Tools to Gain Insight into Protein-Protein and Protein-DNA Interactions
UC San Francisco, March 2010

Using Clustering and Optimization in Flexible Protein Docking
International Conference on Operations Research, Havana, Cuba, February 2010

Replicopter: A Replica Optimizer for Flexible Docking
Critical Assessment of Predicted Interactions (CAPRI), Barcelona, Spain, December 2009

GPU-Enabled Calculations for Molecular Simulation
Intl Conference on Numerical Analysis and Applied Mathematics, Crete, Greece, September 2009