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**Daisuke Kihara, Ph.D.**  
**Associate Professor of Biological Sciences/Computer Science**  
**Purdue University**

**Office**

Purdue University  
Department of Biological Sciences  
Lilly Hall, 915 West State St.  
West Lafayette, IN 47907  
Tel: (765) 496-2284 Fax: (765) 496-1189  
E-mail: [dkihara@purdue.edu](mailto:dkihara@purdue.edu)  
<http://bio.purdue.edu/people/faculty/index.php?refID=166>  
<http://www.cs.purdue.edu/faculty/dkihara.html>  
<http://kiharalab.org> (Lab)

**Education**

1999 Ph.D. (Science) in Bioinformatics  
Kyoto University, Faculty of Science, Japan, Advisor: Minoru Kanehisa  
1996 M.S. in Bioinformatics  
Kyoto University, Faculty of Science, Japan  
1994 B.S. in Biochemistry  
The University of Tokyo, College of Arts and Sciences, Japan

**Positions held**

2009.8-present	<b>Associate professor</b> Purdue University, West Lafayette, Indiana Department of Biological Sciences/Computer Sciences (joint appointment)
2005.3-present	<b>full member</b> Bindley Bioscience Center at Discovery Park, Purdue University
2003.8-2009.8	<b>tenure-track Assistant professor</b> Purdue University, West Lafayette, Indiana Department of Biological Sciences/Computer Sciences
2002.9-2003.7	<b>Senior Postdoctoral Research Associate</b> Buffalo Center of Excellence in Bioinformatics, Buffalo, NY, USA Advisor: Jeffrey Skolnick
2001-2002.9	<b>Senior Postdoctoral Research Associate</b> Donald Danforth Plant Science Center, St. Louis, MO, USA Advisor: Jeffrey Skolnick
1999-2001	<b>Postdoctoral Research Associate</b> Donald Danforth Plant Science Center, St. Louis, MO, USA Laboratory of Computational Genomics
1998-1999	<b>Research Assistant</b> Bioinformatics Center Institute for Chemical Research, Kyoto University, Japan

**Awards**

The Seed of Success Award, Purdue University, 2005, 2006, 2007, 2008

## Publications

- [52] SubAQUA: Real-value quality assessment of protein structure models.  
Y.D. Yang, P. Spratt, H. Chen, C. Park, & D. Kihara  
*Protein Engineering Design & Selection*, 23: 617-632 (2010)
- [51] Functional enrichment analyses and construction of functional similarity networks with high confidence function prediction by PFP.  
T. Hawkins, M. Chitale, & D. Kihara  
*BMC Bioinformatics*, 11: 265 (2010)
- [50] Real-time ligand binding pocket database search using local surface descriptors.  
R.C. hkhii, L. Sael, & D. Kihara  
*Proteins: Structure, Function, and Bioinformatics*, 78: 2007-2028, (2010)
- [49] Application of 3D Zernike descriptors to shape-based ligand similarity searching.  
V. Venkatraman, P.R. Chakravarthy & D. Kihara  
*J. Cheminformatics*, 1: 19. (2009)
- [48] Protein-protein docking using region-based 3D Zernike descriptors.  
V. Venkatraman, Y.D. Yang, L. Sael & D. Kihara  
*BMC Bioinformatics*, 10: 407. (2009)
- [47] Error estimation of template-based protein structure models.  
D. Kihara, Y.D. Yang & H. Chen.  
Multiscale approaches to protein modeling: structure prediction, dynamics, thermodynamics and macromolecular assemblies. Andrzej Kolinski (ed.), Springer-Verlag, Chapter 11, in press. (2010)
- [46] 3D-SURFER: software for high throughput protein surface comparison and analysis.  
David La, Juan Esquivel-Rodriguez, V. Venkatraman, B. Li, L. Sael, S. Ueng, S. Ahrendt & Daisuke Kihara  
*Bioinformatics*, 25: 2843-2844. (2009)
- [45] Characterization and classification of local protein surfaces using self-organizing map.  
Lee Sael & Daisuke Kihara  
*International Journal of Knowledge Discovery in Bioinformatics*, in press. (2010)
- [44] Potential for protein surface shape analysis using spherical harmonics and 3D Zernike descriptors.  
Vishwesh Venkatraman, Lee Sael, & Daisuke Kihara  
*Cell Biochemistry and Biophysics*, 54: 23-32(2009)
- [43] ESG: Extended similarity group method for automated protein function prediction.  
Meghana Chitale, Troy Hawkins, Changsoo Park & Daisuke Kihara  
*Bioinformatics*, 25: 1739-1745. (2009)
- [42] Protein surface representation and comparison: New approaches in structural proteomics.  
Lee Sael & Daisuke Kihara  
*Biological Data Mining*, J. Chen and S. Lonardi (eds). V. Kumar, (series ed.), Chapman & Hall/CRC Press, Boca Raton, Florida, USA, Chapter 3, pp. 89-109. (2009)
- [41] Quality assessment of protein structure models.  
Daisuke Kihara, Hao Chen & Yifeng D. Yang  
*Current Protein and Peptide Science*, 10: 216-228 (2009)
- [40] Predicting binding interfaces of protein-protein interactions.  
David La & Daisuke Kihara.  
*Biological Data Mining in Protein Interaction Networks*, X.-L. Li and S.K. Ng (eds), Chapter 5, pp. 64-79, IGI-Global, Hershey, Philadelphia, USA. (2009)
- [39] The emerging world of wikis.  
Hu, J. C., R. Aramayo, D. Bolser, T. Conway, C. G. Elisk, M. Gribskov, T. Kelder, D. Kihara, T. F. Knight, Jr., A. R. Pico, D. A. Siegele, B. L. Wanner, and R. D. Welch.  
*Science* 320 (5881):1289-1290, (2008)

- [38] PFP: Automated prediction of gene ontology function annotations with confidence scores. Troy Hawkins, Meghana Chitale, Stan Luban & Daisuke Kihara  
*Proteins: Structure, Function, and Bioinformatics*, 74: 566-582, (2009).
- [37] Automated prediction of protein function from sequence. Meghana Chitale, Troy Hawkins & Daisuke Kihara  
*Prediction of Protein Structure, Functions and Interactions*, Janusz Bujnicki (ed.), Chapter 3, pp. 64-86, John Wiley & Sons, Ltd. (2009)
- [36] Rapid comparison of properties on protein surface. Lee Sael, David La, Bin Li, Raif Rustamov, & Daisuke Kihara.  
*Proteins: Structure, Function, and Bioinformatics*, 73: 1-10, (2008).
- [35] New paradigm in protein function prediction for large scale omics analysis. Troy Hawkins, Meghana Chitale & Daisuke Kihara.  
*Molecular BioSystems*, 4: 223-231 (2008)
- [34] Fast protein tertiary structure retrieval based on global surface shape similarity. Lee Sael, Bin Li, David La, Yi Fang, Karthik Ramani, Raif Rustamov & Daisuke Kihara.  
*Proteins: Structure, Function, and Bioinformatics*, 72: 1259-1273. (2008).
- [33] Combining sequence similarity scores and textual information for gene function annotation in the literature. Luo Si, D. Yu, Daisuke Kihara & F. Yi.  
*Information Retrieval*, 11: 389-404 (2008)
- [32] Threading without optimizing weighting factors for scoring function. Yifeng D. Yang, Changsoon Park & Daisuke Kihara.  
*Proteins*, 73:581-596, (2008)
- [31] Tracing lineage in multi-version scientific databases. Mingwu Zhang, Daisuke Kihara & Sunil Prabhakar.  
IEEE 7<sup>th</sup> International Symposium on Bioinformatics & Bioengineering (BIBE), 440-447, (2007).
- [30] Estimating quality of template-based protein models by alignment stability. Hao Chen & Daisuke Kihara.  
*Proteins: Structure, Function, and Bioinformatics*, 71: 1255-1274 (2008)
- [29] Salient critical points for meshes. Yu-Shen Liu, Min Liu, Daisuke Kihara & Karthik Ramani  
*Proceedings of the 2007 ACM Solid and Physical Modeling* 277-282. (2007)
- [28] Characterization of local geometry of protein surfaces with the visibility criterion. Bin Li, Srinivasan Turuvekere, Manish Agrawal, David La, K. Ramani & Daisuke Kihara  
*Proteins: Structure, Function, and Bioinformatics*, 71: 670-683. (2008).
- [27] Function prediction for uncharacterized proteins. Troy Hawkins & Daisuke Kihara  
*J. Bioinformatics and Computational Biology* 5: 1-30. (2007)
- [26] Comparative genomics of small RNAs in bacterial genomes. Stan Luban & Daisuke Kihara.  
*Omics*, 11(1), 58-73. (2007)
- [25] EMD: An ensemble algorithm for discovering regulatory motifs in DNA sequences. Jianjun Hu, Yifeng D Yang & Daisuke Kihara  
*BMC Bioinformatics* 7: 342. (2006)
- [24] Protein function prediction in proteomics era. Daisuke Kihara, Troy Hawkins, Stan Luban, Bin Li, K. Ramani & Manish Agrawal.  
*Proceedings of Frontiers of Computational Science*, Y Kaneda et al. eds., pp. 143-148, Springer-Verlag, Berlin, Heidelberg (2007).
- [23] Statistical potential based amino acid similarity matrices for aligning distantly related protein sequences.

- Yen Hock Tan, He Huang & Daisuke Kihara  
*Proteins: Structure, Funct. Bioinformatics*, 64: 587-600. (2006)
- [22] Enhanced automated function prediction using distantly related sequences and contextual association by PFP.  
 Troy Hawkins, Stan Luban & Daisuke Kihara.  
*Protein Science*, 15: 1550-1556. (2006)
- [21] Bioinformatics resources for cancer research with an emphasis on gene function and structure prediction tools.  
 Daisuke Kihara, Yifeng D. Yang & Troy Hawkins  
*Cancer Informatics*, 2: 25-35. (2006)
- [20] The effect of long-range interactions on the secondary structure formation of proteins.  
 Daisuke Kihara  
*Protein Science*, 14: 1955-1963. (2005)
- [19] Limitations and Potentials of Current Motif Finding Algorithms.  
 Jianjun Hu, Bin Li and Daisuke Kihara  
*Nucleic Acid. Res.* 33:4899-4913. (2005)
- [18] Biomolecular Structure Databases.  
 Daisuke Kihara.  
 Genome Function Research Handbook, Chapter 2. pp. 73-81. Yodosha Publishers, Tokyo, Japan. (2004).
- [17] Development and large scale benchmark testing of the PROSPECTOR 3.0 threading algorithm.  
 Jeffrey Skolnick, Daisuke Kihara and Yang Zhang.  
*Proteins: Structure, Funct. Bioinformatics* 56:502-518. (2004)
- [16] Microbial genomes have over 72% structure assignment by the threading algorithm PROSPECTOR\_Q.  
 Daisuke Kihara and Jeffrey Skolnick.  
*Proteins: Structure, Funct. Bioinformatics* 55: 464-473 (2004)
- [15] The PDB is a covering set of small protein structures.  
 Daisuke Kihara and Jeffrey Skolnick.  
*J. Mol. Biol.* 334: 793-802 (2003)
- [14] TOUCHSTONE: a unified approach to protein structure prediction.  
 Jeffrey Skolnick, Yang Zhang, Adrian Arakaki, Andrzej Kolinski, Michael Boniecki, Andras Szilagyi and Daisuke Kihara.  
*Proteins: Structure, Funct. Genet.* 53: Suppl.6: 469-479 (2003)
- [13] TOUCHSTONEX: Protein Structure Prediction Using Sparse NMR Data.  
 Wei Li, Yang Zhang, Daisuke Kihara, Yuanpeng J. Huang, Deyou Zheng, Gaetano T. Montelione, Andrzej Kolinski, and Jeffrey Skolnick.  
*Proteins: Structure, Funct. Genet.* 53: 290-306 (2003)
- [12] Local Energy Landscape Flattening: Parallel Hyperbolic Monte Carlo Sampling of Protein Folding.  
 Yang, Zhang, Daisuke Kihara and Jeffrey Skolnick  
*Proteins: Structure, Funct. Genet.* 48: 192-201 (2002)
- [11] Ab initio Protein Structure Prediction on a Genomic Scale: Application to the *Mycoplasma genitalium* Genome.  
 Daisuke Kihara, Yang Zhang, Hui Lu, Andrzej Kolinski and Jeffrey Skolnick  
*Proc. Natl. Acad. Sci. USA*, 99: 5993-5998 (2002)
- [10] Ab initio Protein Structure Prediction via a Combination of Threading, Lattice Folding, Clustering, and Structure Refinement.  
 Jeffrey Skolnick, Andrzej Kolinski, Daisuke Kihara, Marcos Betancourt, Piotr

- Rotkiewicz and Michael Boniecki  
*Proteins: Structure, Funct. Genet.* 45 (Suppl 5): 149-156 (2001)
- [9] Genome Databases on the Internet.  
 Daisuke Kihara  
*Tanpakushitsu Kakusan Koso (Protein, Nucleic Acid and Enzyme)*  
 46 (16 Suppl): 2639-2645 (2001)
- [8] Prediction of Membrane Proteins in Post-Genomic Era.  
 Daisuke Kihara and Minoru Kanehisa  
*Recent Res. Developments in Protein Engng.* 1: 179-196 (2001)
- [7] TOUCHSTONE: An ab initio Protein Structure Prediction Method that Uses  
 Threading-based Tertiary Restraints.  
 Daisuke Kihara, Hui Lu, Andrzej Kolinski and Jeffrey Skolnick  
*Proc. Natl. Acad. Sci. USA* 98: 10125-10130 (2001)
- [6] Generalized Comparative Modeling (GENECOMP): A Combination of Sequence  
 Comparison, Threading, and Lattice Modeling for Protein Structure Prediction  
 and Refinement.  
 Andrzej Kolinski, Marcos Betancourt, Daisuke Kihara, Piotr Rotkiewicz and Jeffrey Skolnick  
*Proteins: Structure, Funct. Genet.* 44: 133-149 (2001)
- [5] Defrosting the Frozen Approximation: PROSPECTOR – A New Approach to  
 Threading.  
 Jeffrey Skolnick and Daisuke Kihara  
*Proteins: Structure, Funct. Genet.* 42: 319-331 (2001)
- [4] Tandem Cluster of Membrane Proteins in Complete Genome Sequences.  
 Daisuke Kihara and Minoru Kanehisa  
*Genome Res.* 10: 731-743 (2000)
- [3] The Genome Projects and Bioinformatics.  
 Daisuke Kihara and Minoru Kanehisa.  
*Iwanami Kouza (Iwanami Lecture Series): Gendai Igaku no Kiso (The Basis of  
 Modern Medical Science)*, vol.1, Chap.11, pp: 215-235, Iwanami Shoten  
 Publishers, Tokyo Japan (1998)
- [2] Prediction of Membrane Proteins Based on Classification of Transmembrane  
 Segments.  
 Daisuke Kihara, Toshio Shimizu and Minoru Kanehisa  
*Protein Engng.*, 11: 961-970 (1998)
- [1] Internet Resources for Genome Research.  
 Daisuke Kihara, Minoru Kanehisa and Toshihisa Takagi.  
*Tanpakushitsu Kakusan Koso (Protein, Nucleic Acid and Enzyme)*,  
 42(17 Suppl): 3090-3099 (1997)

#### **Miscellaneous Publication:**

WWW Homepages for Biophysicists. Part 1-6.  
*Biophysics (Japan)* (1996-1998)  
 (Short columns for bioinformatics tools)

#### **Papers in Revision or in Submission (as of July 25, 2010)**

- [3] Effect of using suboptimal alignments in template-based protein structure prediction.  
 Hao Chen & Daisuke Kihara  
*Proteins: Str. Func. and Bioinformatics*, in revision (2010)
- [2] Protein surface representation for application to comparing low-resolution protein structure  
 data.  
 L. Sael & Daisuke Kihara. Submitted (2010).

- [1] Molecular surface representation using 3D Zernike descriptors for protein shape comparison and docking.  
D. Kihara, L. Sael, R. Chikhi, J. Esquivel-Rodriguez, Submitted (2010)

### **Papers in preparation**

A novel method for protein-protein interaction site prediction using phylogenetic substitution models.  
David La & D. Kihara, in preparation.

### **Invited Talks**

- [64] Real-Time Ligand Binding Pocket Database Search Using Local Surface Zernike Descriptors  
R. Chikhi, L. Sael, D. Kihara  
3D-SIG, ISMB 2010, Boston MA  
July 9-10, 2010
- [63] Protein surface representation for structure-based function prediction and docking.  
Telluride workshop on "Coarse-grained modeling of structure and dynamics of biomacromolecules" Telluride, CO  
July 5-9, 2010
- [62] Molecular surface representation for protein shape comparison and docking  
Korea Institute for Advanced Study (KIAS), Seoul, Korea  
June 30, 2010
- [61] Structure of gene functional space in genomes  
The First International Conference for Industrial Statistics and Bioinformatics, The Research Center for Data Science, Chung-Ang University, Seoul, Korea  
June 29, 2010
- [60] Protein surface representation for fast structure search, docking, and function prediction  
Nara Institute of Science and Technology (NAIST), Nara, Japan  
January 7, 2010
- [59] Protein surface representation for fast structure search, docking, and function prediction  
Dept. of Computer Science, Tokyo Institute of Technology, Tokyo, Japan  
Dec 28, 2009
- [58] Protein structure bioinformatics for predicting structure, docking, and function  
Nanomedicine Development Center, University of Cincinnati  
Nov 5, 2009
- [57] Global and local protein surface comparison and its applications  
Telluride Workshop on "Method development for protein structure prediction and design",  
Telluride Science Research Center, Telluride, Colorado  
June 15-19, 2009
- [56] Protein surface comparison for function prediction and docking  
Dept. of Statistics, Chung-Ang University, Seoul Korea  
May 15, 2009
- [55] Algorithms for biological sequence analysis  
Dept. of Statistics, Chung-Ang University, Seoul Korea  
May 14, 2009
- [54] Novel bioinformatics approaches for studying protein sequence, structure, and function in omics era.  
Division of Bio-Medical Informatics, Center for Genome Science, National Institute of Health, Seoul, Korea  
May 13, 2009
- [53] Annotating protein structures by surface shape comparison", Biochemistry seminar, Dept. of Chemistry, Purdue University, Feb 27, 2009.

- [52] Annotating protein structures by surface shape comparison.  
e-Bioinformatics session in 4<sup>th</sup> IEEE International Conference on e-Science, IUPUI,  
Indianapolis  
Dec. 12, 2008
- [51] Informatics approaches for studying protein sequence, structure, and function in omics era.  
Dept. of Biological Sciences, Purdue University  
October 15, 2008
- [50] Quality assessment of template-based protein structure prediction.  
University of Illinois at Chicago, Department of Bioengineering, Chicago, IL  
February 26, 2008
- [49] Computational protein structure and function prediction.  
Chung-Ang University, Statistics Department, Seoul, Korea  
December 27, 2007
- [48] Template-based protein structure prediction and beyond.  
Korea Institute for Advanced Study (KIAS), Daejeon, Korea.  
December 26, 2007
- [47] Protein function prediction for proteomics era.  
7th KIAS-Soongsil Conference, Soongsil Univ., Seoul, Korea.  
October 4-6, 2007
- [46] A fast method for high throughput comparison of tertiary structure and  
physicochemical properties. (Session chair)  
Biomedical Engineering Society Annual Meeting, Los Angeles, CA  
September 26-29, 2007
- [45] Surface shape-based protein structure classification and search.  
Interface 2007: the 39th Symposium on the interface of statistics, computing science, and  
applications, Doubletree Hotel, Philadelphia  
May 23-26, 2007
- [44] Protein function and structure prediction for proteomics analyses.  
Indiana University, Dept. of Informatics, Bloomington, IN, May 3, 2007.
- [43] Advanced techniques for protein function prediction and protein tertiary structure search for  
proteomics analyses.  
Nara Institute of Science and Technology, Nara, Japan  
December 28, 2006
- [42] Bioinformatics: Introduction and advanced topics.  
Graduate program, Kansai Medical University, Osaka, Japan  
December 25, 2006
- [41] Advanced techniques for protein function prediction and protein tertiary structure search for  
proteomics analyses.  
Ajinomoto Life Science Institute, Kawasaki, Japan  
December 22, 2006
- [40] Round table discussion on function prediction at Critical Assessment of Techniques for  
Protein Structure Prediction (CASP7) Asilomar Conference Center, CA  
November 26-30, 2006
- [39] Enhanced protein function prediction for proteomics analysis.  
Daisuke Kihara & Troy Hawkins.  
Biomedical Engineering Society Annual Meeting 2006, Systems Biology and Bioinformatics  
track, Hyatt Regency Chicago, IL. IUPUI, Indianapolis, IN.  
October 12, 2006.
- [38] Protein function prediction from sequence and structure.  
Daisuke Kihara.  
Center for Computational Biology and Bioinformatics, IUPUI, Indianapolis, IN.

- October 6, 2006.
- [37] Low resolution and uncertainty in protein structure and function prediction.  
Daisuke Kihara.  
Symposium on Protein functional and folding motion, Institute for Protein Research, Osaka Univ., Osaka, Japan.  
September 28-29, 2006.
- [36] PFP: sequence-based annotation of sequences and local sequence motifs with contextual GO term associations.  
Troy Hawkins, Stan Luban, Daisuke Kihara.  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [35] Bridging geometric protein surface features and phylogenetic information for rapid identification of protein-protein interaction interfaces.  
David La, Dennis Liversay, Daisuke Kihara.  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [34] Enhanced Automated Function Prediction for Proteomics Analysis.  
Bioinformatics Seminar Series, Dept. of Statistics, Purdue University  
January 24, 2006
- [33] Protein Function Prediction in the Structural Genomics Era.  
International Symposium, From Genomics to Chemical Genomics: 10<sup>th</sup> Anniversary of KEGG. PALULU Plaza, Kyoto, Japan  
December 15-16, 2005
- [32] Protein Function Prediction in the Proteomics Era.  
International Symposium on Frontiers of Computational Science 2005  
Noyori Conference Hall, Nagoya University, Japan  
December 12-13, 2005
- [31] Protein function prediction methods beyond BLAST search.  
Structural Biology Seminar Series, Dept. of Biological Sciences, Purdue University  
November 16, 2005
- [30] Protein function prediction in structural genomics era.  
Computing Research Institute, CS&E Seminar Series, Purdue University  
October 19, 2005
- [29] Protein function prediction from sequence and structure.  
Mini-Workshop on Computational Studies on Proteins, Children's Hospital Research Foundation, Cincinnati, Ohio, Sep. 8, 2005
- [28] The use of context-based functional association in automated protein function prediction methods.  
Automated Function Prediction – Special Interest Group, (AFP-SIG), ISMB (International Conference on Intelligent Systems for Molecular Biology), Detroit, Michigan, 24, June, 2005.
- [27] Voxelized Protein Model for Fast Protein Docking and Function Prediction.  
Midwest Computational Structural Biology Workshop Brook Lodge,  
Michigan State University, Augusta, Michigan  
April 30 – May 1, 2005
- [26] Toward a better template-based protein structure prediction.  
Dept. of Chemistry, Biochemistry Division seminar, Purdue University  
1 April, 2005
- [25] Conserved Small RNA Families in Gamma-Proteobacteria.  
Computational Biology Research Center, Tokyo, Japan

- 28 December 2004.
- [24] Computational sequence and structure analyses.  
Biological Sciences Faculty Research Presentations, Dept. of Biological Sciences, Purdue University  
9 December, 2004
- [23] Comparative genomics study of non-coding RNA in Gamma-proteobacteria  
Ecolunch, Dept. of Biological Sciences, Purdue University  
17 November, 2004
- [22] Genome-scale Protein Structure Assignment to Microbial Genome Sequences.  
Ninth Annual Purdue University Biophysics Symposium  
25 October 2003
- [21] PDB is a Covering Set of Small Protein Structures.  
Bioinformatics Center, Kyoto University, Japan  
20 October 2003.
- [20] Genome-scale protein structure assignment to microbial genomes.  
International Workshop for Escherichia coli towards New Biology in the 21<sup>st</sup> Century.  
Awaji-shima, Japan  
15-17 October, 2003
- [19] Revisiting protein Structure Space – PDB is a Covering Set of Small Protein Structures.  
Computational Biology Research Center, Tokyo, Japan  
14 October 2003.
- [18] Revisiting Protein Structure Space for Prediction – PDB is a Covering Set of Small Protein Structures.  
Bioinformatics Seminar Series, Purdue University  
9 September 2003.
- [17] Protein Structure/Function Prediction on a Genome Scale.  
The Whitney Laboratory/Dept. of Computer Science, University of Florida, Gainesville, Florida  
7-8 April, 2003.
- [16] Genome Scale Protein Structure Prediction.  
Computer Science Dept., Virginia Polytechnic Institute and State University, Blacksburg, Virginia  
3 April, 2003.
- [15] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biology, The University of Nebraska at Omaha, Omaha, Nebraska  
1 April, 2003.
- [14] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biological Sciences, Purdue University, West Lafayette, Indiana  
25 March, 2003.
- [13] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Informatics, Indiana University, Bloomington, Indiana  
6 March, 2003.
- [12] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biology, University of Kentucky, Lexington, Kentucky  
4 February, 2003.
- [11] Protein Structure/Function Prediction on a Genome Scale.  
Donald Danforth Plant Science Center, St. Louis, Missouri  
28 October, 2002.
- [10] Ab initio Protein Structure Prediction Method on a Genome Scale.  
Computational Biology Research Center, Tokyo, Japan  
12 October, 2001

- [9] An Ab initio Protein Structure Method Using a Lattice Model.  
Structural Bioinformatics Division Seminar, Yokohama City University, Japan  
11 October, 2001
- [8] A Lattice Model Based Protein Structure Prediction which Does Not Use  
Template Structures of Homologous Proteins.  
Biophysics Department Seminar, Nagoya University, Japan  
10 October, 2001
- [7] TOUCHSTONE: Ab initio Structure Prediction Method Using Restraints  
Derived from Threading.  
Research Society of Computational Genomics, the Biophysical Society of Japan  
Institute for Protein Research, Osaka University, Japan  
9 October, 2001
- [6] Ab initio Protein Structure Prediction Using Restraints Derived from Threading.  
Department of Biochemistry, Cambridge University, UK  
9 September, 2001
- [5] Toward Genome Scale Ab initio Protein Folding Prediction.  
Conference on “Experimental & Theoretical Approach for Protein Folding”,  
sponsored by Mirai Kaitaku Kenkyukai (Frontier Research Society)  
Okazaki Conference Center, Institute for Molecular Science, Okazaki, Japan  
10-12 January, 2001
- [4] Prediction of Protein Structure and Function on a Genome Scale.  
Jeffrey Skolnick, Andrzej Kolinski, Daisuke Kihara and Piotr Rotkiewicz.  
23<sup>rd</sup> Annual Meeting of Molecular Biology Society of Japan, Kobe, Japan  
15 December, 2000
- [3] Generalized Comparative Modeling of Protein Structures.  
Electrotechnical Laboratory, National Inst. of Advanced Industrial Science,  
Tsukuba, Japan.  
18 September, 2000
- [2] Analyses of Genome Sequences through Internet.  
Kansai Medical University, Japan  
24 March, 1998
- [1] Current Aspect of Prediction of Transmembrane Segments in Proteins and  
Application to Genome Sequences.  
Summer School of Biophysical Society of Japan for Young Scientists (Under sponsorship by  
The Biophysical Society of Japan) P.40, Kobe, Japan  
29-31 July, 1998

### **Poster and Other Presentations**

- [60] A novel method for protein-protein interaction site prediction with phylogenetic substitution  
models.  
David La, D. Kihara  
The 24th Annual Symposium of the Protein Society, San Diego, CA, USA. August 1-5, 2010,
- [59] Multiple protein docking prediction based on genetic algorithms and physics based scoring.  
Juan Esquivel-Rodriguez, D. Kihara  
18th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB),  
Boston, MA, July 11-13, 2010
- [58] Multiple Protein Docking Prediction Method Which Can Handle Asymmetric Hetero  
Oligomeric Complexes.  
J. Esquivel-Rodriguez, Y. Yang, D. Kihara  
3D-SIG, ISMB 2010, Boston, MA, July 9-10, 2010

- [57] Fitting Multimeric Complexes into Cryo-EM Maps Using Protein Docking Procedure and 3D Zernike Descriptors  
D. Kihara, J. Esquivel-Rodriguez, L. Sael  
3D-SIG, ISMB 2010, Boston, MA, July 9-10, 2010
- [56] A unified protein docking procedure with a shape complementarity screening using 3D Zernike descriptors  
D. Kihara, V. Venkatraman, YD Yang, L. Sael  
Biophysical Society meeting, San Francisco, CA, Feb 20-24, 2010
- [55] A unified protein docking procedure with a shape complementarity screening using 3D Zernike descriptors and ranking by physics-based scoring.  
D. Kihara, J. Esquivel-Rodriguez, V. Venkatraman, D. La, Y.D. Yang, L. Sael, B. Li, S. Ueng, S. Ahrendt.  
CAPRI Critical Assessment of Predicted Interactions 4th Evaluation Meeting, Barcelona, Spain, Dec 9-11, 2009
- [54] www.EcoliHub.org: An information resource for experimentation and modeling of E. coli K-12  
BL Wanner, WG Aref, T. Conway, KA Datsenko, SC Ess, MR Gribskov, JC Hu, D Kihara, H Mori, D Siegle, DR Whitaker  
American Society for Microbiology, May 17-21, 2009, Philadelphia, PA
- [53] N terminal Gly224-Gly411 domain in Listeria adhesion protein (LAP) interacts with receptor Hsp60  
B. Jagadessan, D La, D Kihara, AK. Bhunia  
American Society for Microbiology, May 17-21, 2009, Philadelphia, PA
- [52] Local surface-based protein function prediction using Zernike descriptors.  
D. Kihara, Sael Lee, Rayan Chikhi  
Biophysical Society Meeting, March 4, 2009, Boston MA
- [51] Threading without optimizing weighting factors for scoring function.  
Yifeng D Yang, C. Park, D. Kihara.  
Biophysical Society Meeting, March 4, 2009, Boston MA  
Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009
- [50] EcoliHub: An information resource for experimentalists and modelers.  
D.R. Whitaker, W. G. Aref, K.A. Datsenko, S. Ess, M.R. Gribskov, D. Kihara, S. Kim, H. Mori, A. Roumani, B.L.Wanner  
Intelligent Systems for Molecular Biology (ISMB) 2008, July 19-23, 2008, Toronto, Canada
- [49] ESG: Extended Similarity Group Method for improved automated protein function prediction.  
M. Chitale, T. Hawkins, C. Park, D. Kihara  
Invited oral presentation at Automated function prediction special Interest Group at ISMB 2008 (AFP/Biosapiens 2008), July 18-19, Toronto, Canada
- [48] Automated protein function prediction using Extended Similarity Group (ESG) of sequences.  
M. Chitale, T. Hawkins, C. Park & D. Kihara  
Intelligent Systems for Molecular Biology (ISMB) 2008, July 19-23, 2008, Toronto, Canada
- [47] Ecolihub: Development of the [www.ecolicommunity.org](http://www.ecolicommunity.org) Information resource. B.L. Wanner, W.G. Aref, K. Datsenko, S. Ess, M.R. Gribskov, D. Kihara, S. Kim, H. Mori, D. R. Whitaker  
American Society for Microbiology, 108<sup>th</sup> General Meeting, Boston  
June 1-5, 2008
- [46] A fast methodology for high throughput comparison of tertiary structure and physicochemical properties  
Sael Lee, Bin Li, David La, Raif Rustamov, Daisuke Kihara  
The Computer Research Institute Poster Session, Purdue-Industry High Performance Computing Workshop, Purdue Memorial Union, Purdue Univ., April 6, 2008.

- [45] A fast methodology for high throughput comparison of tertiary structure and physicochemical properties.  
D. Kihara, Sael Lee, Bin Li, David La & Raif Rustamov  
Meeting of the Biophysical Society 52<sup>nd</sup> Annual Meeting and 16<sup>th</sup> International Biophysics Congress, Long Beach, CA  
February 2-6, 2008.
- [44] Predicting the error of template-based protein structure modeling by suboptimal alignment stability.  
Hao Chen & D. Kihara  
Meeting of the Biophysical Society 52<sup>nd</sup> Annual Meeting and 16<sup>th</sup> International Biophysics Congress, Long Beach, CA  
February 2-6, 2008.
- [43] High-throughput function assignment for proteomics datasets with PFP.  
T. Hawkins, M. Chitale & D. Kihara.  
The 21st Symposium of the Protein Society, Boston, MA  
July 21-25, 2007
- [42] Protein surface representation for fast comparison of tertiary structure and physicochemical properties.  
S. Lee, B. Li, D. La, R. Rustamov & D. Kihara.  
The 21st Symposium of the Protein Society, Boston, MA  
July 21-25, 2007
- [41] Functional enrichment of proteomics datasets with PFP.  
T. Hawkins, M. Chitale, S. Luban & D. Kihara.  
ISMB 2007, Vienna, Austria.  
July 21-25, 2007
- [40] Using sequence similarity scores for automatic gene function annotation in the biomedical literature.  
L. Si, D. Yu, D. Kihara & Y. Fang  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [39] Estimating quality of template-based protein models by alignment stability (selected for oral presentation).  
H. Chen & D. Kihara  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [38] Threading without training weighting factors for scoring functions.  
Y.D. Yang & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [37] EcoliPredict: structure modeling of E. coli proteome.  
P. Spratt, S. Krawczyk, Y.D. Yang & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [36] Local geometry characterization of protein surfaces with the visibility criteria.  
B. Li, S. Turuvekere, M. Agrawal, K. Ramani & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.

- May 31-June 2, 2007.
- [35] A fast methodology for high throughput comparison of tertiary structure and physicochemical properties.  
Sael Lee, David La, Bin Li, Raif Rustamov & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [34] Development of methods for missing enzyme/gene prediction with PFP.  
Meghana Chitale, Troy Hawkins, & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [33] Function prediction for proteomics datasets using PFP.  
Troy Hawkins, Meghana Chitale, & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [32] Structure modeling of E. coli proteome: Quality evaluation.  
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.  
The Computer Research Institute Poster Presentation, Atrium of MSEE building, Purdue University.  
April 5, 2007
- [31] PFP: Sequence-based annotation of sequences and local sequence motifs with contextual GO term association  
Troy Hawkins, Stan Luban, David La & Daisuke Kihara  
Automated Function Prediction meeting, 2006, UC San Diego, San Diego, CA.  
Aug 30 – Sep 1, 2006.
- [30] EMD: an ensemble DNA regulatory motif discovery algorithm for Grid computing.  
Yifeng D. Yang, Jianjun Hu & Daisuke Kihara.  
TeraGrid '06, Indianapolis University Purdue University Indianapolis, Indianapolis, IN,  
June 12-15, 2006.
- [29] Template-based protein structure prediction with a reliability measure for structural genomics era.  
Hao Chen, Yen Hock Tan, & Daisuke Kihara.  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [28] Ligand binding site prediction with the visibility criteria.  
Bin Li, S. Thruvekere, M. Agrawal, K. Ramani & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [27] Multi-resolution protein representation for fast protein structure searching.  
Sael Lee, Bin Li, David La, Raif Rustamov, & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [26] On the effect of long-range interactions on the secondary structure formation of proteins.  
Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.

- May 19-20, 2006
- [25] Coiled-coil structures in *E. coli* interactome.  
Stan Luban, Akiyasu Yoshizawa & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [24] Neural network based protein domain prediction.  
Yen Hock Tan, Otoniel Venezuela, Evans A. Tapia & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [23] Statistical potential-based amino acid similarity matrices for aligning distantly related protein sequences.  
Yen Hock Tan, He Huang & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [22] Accounting for natural flexibility in protein structure prediction comparisons.  
Jairav Desai & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [21] EcoliPredict: bioinformatics prediction resource for EcoliHub.  
Barry Wanner, Daisuke Kihara, Troy Hawkins & Yifeng D. Yang  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [20] EcoliPredict: bioinformatics prediction resource for EcoliHub  
Barry Wanner, Daisuke Kihara, Troy Hawkins and Yifeng D. Yang  
American Society for Microbiology ASM-FEMS Conference on Protein Traffic in Prokaryotes, Crete, Greece  
May 6-10, 2006
- [19] A New Perspective on an Old Tool: Extending the Coverage of Sequence Similarity-Based Function Prediction with PFP.  
Troy Hawkins, Stan Luban and Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [18] Ligand Binding Sites Prediction with the Visibility Criteria.  
Bin Li, Srinivasan Turuvekere, Manish Agrawal, Karthik Ramani and Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [17] Protein-Protein Docking Algorithm Using Preidentified Binding Site Patches.  
Daisuke Kihara, Sael Lee, Karthik Ramani, Srinivasan Turuvekere, Manish Agrawal, And Bin Li  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [16] Dependence of the Accuracy of Protein Secondary Structure Prediction on Long-Range Interactions.  
Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan

- December 19-21, 2005
- [15] PFP: Automatic annotation of protein function by relative GO association in multiple function prediction methods.  
Troy Hawkins & Daisuke Kihara  
ISMB, Detroit, Michigan, June 25 – 29, 2005.
- [14] Protein Structure-Sequence Alignment with a Reliability Measure.  
Hao Chen, Yen Hock Tan & Daisuke Kihara.  
Midwest Computational Structural Biology Workshop, Brook Lodge,  
Michigan State University, Augusta, Michigan  
April 30 – May 1, 2005
- [13] Feature recognition based identification of potential binding sites on the molecular surfaces.  
Srinivasan Turuvekere, Manish Agrawal, Daisuke Kihara, and Karthik Ramani.  
The Protein Society 18<sup>th</sup> Symposium. San Diego, August 14-18, 2004.
- [12] Comparative Study of Structural Non-coding RNAs in Microbial Genomes.  
Stanislav Luban and Daisuke Kihara  
First Annual Indiana Bioinformatics Conference.  
IUPUI, Indianapolis, 27 May, 2004.
- [11] Computational prediction and experimental validation of iron and phosphate gene regulatory sites in the Escherichia coli K-12 and Pseudomonas aeruginosa PA01 genomes.  
Sam-II Jung, Kaushik M. Setty, Khurram Siddiqi, Lu Zhou, Barry L. Wanner and Daisuke Kihara  
International Workshop for Escherichia coli Towards New Biology in the 21<sup>st</sup> Century.  
Awaji-shima, Japan, 15-17 October, 2003.
- [10] PDB is a covering set of a single-domain protein structures.  
Daisuke Kihara and Jeffrey Skolnick  
Frontiers in Bioinformatics Symposium, Buffalo NY  
5-8 June, 2003
- [9] Classification and Analysis of Eukaryotic ABC Transporters in Complete Eukarya Genomes.  
Yoshinobu Igarashi, Daisuke Kihara and Minoru Kanehisa  
Genome Informatics 11: pp .274-275, Universal Academy Press, Tokyo (2000)
- [8] Classification and Analysis of Eukaryotic ABC Transporters in Complete Eukarya Genomes.  
Yoshinobu Igarashi, Daisuke Kihara and Minoru Kanehisa  
The Cold Spring Harbor Laboratory Meeting (New York, May 2000)
- [7] Detection of Membrane Proteins in the Whole Genome Sequences.  
Daisuke Kihara and Minoru Kanehisa  
Genome Informatics 1997, pp.300-301, Universal Academy Press, Tokyo (1997)
- [6] Systematic Analysis of Enzyme Structures and Metabolic Pathways.  
Daisuke Kihara and Minoru Kanehisa  
18<sup>th</sup> Annual Meeting of Molecular Biology Society of Japan (1997)
- [5] Prediction Method of Transmembrane Segments in Proteins Using Multiple Discrimination Functions.  
Daisuke Kihara and Minoru Kanehisa  
35<sup>th</sup> Annual Meeting of the Biophysical Society of Japan. P.172 (1997)
- [4] A Prediction Method for Transmembrane Segments in Proteins Utilizing Multiple Discrimination Functions.  
Daisuke Kihara, Toshio Shimizu and Minoru Kanehisa  
Genome Informatics 1996, pp.244-245, Universal Academy Press, Tokyo (1996)
- [3] Prediction of Transmembrane Segments in Proteins Using Characteristics by their Numbers and Positions.

- Daisuke Kihara and Minoru Kanehisa  
17<sup>th</sup> Annual Meeting of Molecular Biology Society of Japan, p.140 (1996)
- [2] Analysis of Transmembrane Helices by the Number, Hydrophobicity and Amphipathy.  
Daisuke Kihara and Minoru Kanehisa  
33<sup>rd</sup> Annual Meeting of the Biophysical Society of Japan p.175 (1995)
- [1] Preparation and Characterization of Monoclonal Antibodies Specific for  
N-terminal Fatty Acids of Transducin Alpha-Subunits.  
Koichi Kokame, Osamu Shono, Daisuke Kihara, Yoshitaka Fukada, Masasuke  
Araki, Toshifumi Takao, Yasutsugu Shimonishi, and Toru Yoshizawa  
17<sup>th</sup> Annual Meeting of the Japanese Biochemical Society, p.1067 (1994)

## Research Support

### Current:

Surface shape based screening of large protein databases.

(Agency: NIH, R01, Total: \$1,408,659 direct cost, 09/01/2005-08/31/2011, no-cost extension to 2011)

Role: PI

III: Small: Quality assessment of computational protein models.

(NSF, IIS, \$327,606, 09/01/2009 – 08/31/2011) Role: PI

Template-based protein structure prediction beyond sequence homology.

(NSF, ABI, \$716,001, 06/01/2009-05/31/2013) Role: PI

Information Transfer in Biological Systems.

(NSF, DMS, 06/01/2008-05/31/2012, \$480,000) Role: co-PI, (PI: Wojciech Szpankowski)

Protein 3D Structure-based rational drug discovery.

(Purdue Res. Foundation, \$1,6750, 09/01/09 – 08/31/10), Role: PI

Comprehensive mapping and annotation of the E. coli Transcriptome.

(NIH, Challenge Grant RC1, \$100,000 total 10/01/2009 – 09/30/2011). Role: co-PI (PI: B. Wanner)

Elucidating genetic pathways for curing retinal degeneration

(Showalter Trust, \$75,000, 6/1/2010-5/31/2011) Role: co-PI, (PI: Yuk Fai Leung)

### Pending

Identification of protein-metabolite interactome

(NIH, 2011-2015, \$1,000,000, direct), PI

### Past

Recovery Act administrative Supplement. Parent grant: U24 GM077905-03 Development of the [www.EcoliCommunity.org](http://www.EcoliCommunity.org) Information Resource.

(NIH, 4/1/09 – 6/30/09, \$410,000 direct) Role: co-PI, (PI: Barry Wanner)

Computational proteomics approaches for rational drug design.

(Computing Research Institute, Purdue University, CRI PRF-SIRG, \$16,375, (7/1/2008- 6/30/2009)

Bayesian models and Monte Carlo strategies in identifying protein or DNA sequence motifs.

(Agency, NSF, Dev. of Math. Sci, \$ 160,246, 7/1/2006-6/30/2009, PI: Jun Xie) Role: co-PI

Development of the [www.ecolicommunity.org](http://www.ecolicommunity.org) Information Resource (Agency: NIH, Direct cost: \$1,499,521, 4/01/2006-3/30/2009, PI: Barry Wanner) Role: co-PI

Protein Structure Prediction (Agdia Inc., direct cost: \$993.0, 3/1/2006-4/30/2006) Role: PI

Development of a Protein Sequence-Structure Alignment Method for Distantly Related Proteins. (PRF Summer Faculty Grant, Total \$7,000 direct cost, 06/01/2005-08/31/2005) Role: PI

Structure Basis of Protein-Protein Interactions. (Purdue Alumni Association, Incentive Grants Program, Total \$500 direct cost, 6/01/2005-12/31/2005) Role: PI

### **Supervised Postdocs**

Sael Lee (PhD in CS, Purdue) starts from August 2010

Mateusz Kurcinski (Dept. of Chemistry, Warsaw Univ., Poland) March 2010 - current

Vishwesh Venkatraman (Ph.D. in Comp. Chem., Univ. of Portsmouth, UK) September 2007 – July 2009

Jianjun Hu (Ph.D. in Computer Science from Michigan State University) Sept. 2004 – August 2005  
Currently assistant professor in Dept. of Computer Science and Engineering, University of South Carolina

### **Visiting Professor**

Changsoon Park, Full Professor at Statistics Dept., Chung-Ang University, Seoul, Korea  
Jan 3, 2008 – Feb 28 2008

Hangchang Lee, Associate Professor, Dept. of Multi-media Engineering, Hangeung University, Seoul, Korea, Jan. 1. 2009 - present

### **Supervised Technicians**

Michael Gillogly: August 2009 – April 2010

Stan Luban: January 2006 – June 2006

Yen Hock Tan: June - August 2004

### **Supervised Students**

#### **Graduated with PhD**

Sael Lee (CS, July 2010), continuing to work as postdoc

Hao Chen (Biol, May, 2010)

Yifeng Yang (Biol, May 2010)

Troy Hawkins, (Biol, October, 2008)

Mingwu Zhang (CS, Fall 2006, co-supervised with Sunil Prabhakar)

#### **Current Graduate Students**

David La (Biol)

Chao Yuan (PULSe, Purdue Life Science Program)

Bin Li (CS)

Meghana Chitale (CS)

Juan Esquivel-Rodriguez (CS)

#### **Current Undergraduate Students**

Matt Herron (Animal Sci/CS) Summer08 –

Abram Magner (CS/Math) Spring 09-  
Roshna Agrawal (CS) Spring 2010-  
Sanmeet Kanhere (CS) Summer 2010-

### **Former Undergraduate Students**

Over 43 students (2003-current)

### **Former Summer Intern**

Rayan Chikhi, Computer Science, Ecole Normale, France (Summer 2007)

### **K-12 Students**

Summer 2005, Katie Kranjak (high school student, summer intern from the Indiana Academy of Science)

### **Student Awards**

- Yifeng Yang (Biol), Student Travel Grant to the 53rd Annual Meeting of the Biophysical Society from Biophysical Society, November 2008.
- Yifeng Yang (Biol), PULSe Travel Award, Purdue University, October 2008
- Priyanka Surana (Biol), 2008 Summer Howard Hughes Undergraduate Research Internship.
- Hao Chen, (Biol), YeungKyung Woo Achieve Excellence travel award from Dept. Biological Sciences, Purdue University, November 2007.
- Hao Chen, (Biol), Student Travel Grant to the 52nd Annual Meeting of the Biophysical Society from Biophysical Society, November 2007.
- Preston Spratt (Biol), High Performance Computing Community Poster Session, Honorable mention, Purdue University, April 2007.
- Troy Hawkins (Biol), Umbarger Outstanding Graduate Student in Research, Dept. of Biological Sciences, Purdue University, Spring, 2007
- Preston Spratt (Biol), 2007 Summer Howard Hughes Undergraduate Research Internship.
- Preston Spratt (Biol), DURl, Discovery Park Undergraduate Research Internship, Fall 2006, Spring 2007, Fall 2007.
- David La (Biol), 1<sup>st</sup> Place, Sigma Xi Graduate Poster Competition, February 14, 2006
- Yen Hock Tan (CS). Nominated for the Computing Research Association's (CRA) Outstanding Undergraduate Award for 2006 from Dept. of Computer Science
- Jairav Desai (CS), DURl, Discovery Park Undergraduate Research Internship, Fall 2005, Spring 2006.
- Stan Luban (CS/Biol), DURl, Discovery Park Undergraduate Research Internship, 2005
- Athurva Gore (ME) Top Poster Award at the Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University, August 2, 2005
- Stan Luban (CS/Biol). Outstanding Research Award at the Undergraduate Research Day of College of Science & College of Agriculture, Purdue University. April 11, 2005.
- Otoniel Venezuela (CS). Graduate School Incentive Grant. School of Science, Purdue University. April 8, 2005.
- Yen Hock Tan (CS). Hewlett-Packard Fellowship. April, 2005.
- Ei Ei Phyu (CS). 2005 Howard Hughes Fellowship for Undergraduate Research in Bioinformatics.
- Stan Luban (CS/Biol). 2005 Summer Howard Hughes Undergraduate Research Internship.
- Yen Hock Tan (CS). 2005 Summer Howard Hughes Undergraduate Research Internship.
- Stan Luban (CS/Biol). Honorable Mention in the Computing Research Association's (CRA) Outstanding Undergraduate Award for 2005

- Stan Luban (CS/Biol). 2004 Summer Howard Hughes Undergraduate Research Internship.
- Manish Agrawal and Srinivasan S. Turuvekere (Mechanical Engineering). 2<sup>nd</sup> place in 2004 Purdue University's Burton D. Morgan Entrepreneurship Competition

### **Courses Taught**

CS490B/Biol495S Introduction to Bioinformatics (senior undergraduate level)

Spring 2004/Spring & Fall 2005/Fall 2006/Fall 2007/Fall 2008

- Elected for a permanent course in Biology and renumbered to BIOL478 from Fall 2006)
- Also used as BIOL 595 Special Assignment in Computational Life Science (CLS) Master Program

BIOL595A/(CS590B) Protein Bioinformatics

Spring 2006, 2007, 2008, 2009, 2010

CS590-006 Computing for Life Sciences II

Fall 2009

BIOL696E Seminar Crystallography

Spring 2006

### **Other Teaching Activities**

- Guest lecture on bioinformatics research at CS 197 Honors Seminar, Feb 16, 2009
- Guest lecture in SCI190 (Instructor: Bos David, Biology), (11/14/2008)
- Panel discussion, SECANT (Science Education in Computational Thinking)workshop, Purdue University, LWSN building (11/15/2008)
- Preparation discussion lecture to structural biology group in Biology Department for a seminar given by a famous professor in the field, Janet Thornton (3/18/2008).
- Faculty panel of the graduate student board of the Department of Computer Science. Discussion about “how to be successful in their job-hunt “, Nov. 22, 2004

### **Services**

#### Editorial Board

- Associate Editor, International Journal of Knowledge Discovery in Bioinformatics (IJKDB) (January 2009- present)
- The Open Proteomics Journal (November 2007 - present)

#### Review of Grants

Ad hoc reviewer

- National Science Foundation, Advances in Bioinformatics (DBI) (October 2009)
- National Science Foundation, Molecular Cellular Biosciences (MCB) (September 2009)
- National Institutes of Health, Challenge Grant, RC1 (June 2009)
- National Science Foundation, MCB (February, 2009)
- National Science Foundation, Division of Chemistry (February, 2008)
- National Science Foundation, Division of Chemistry (September, 2007)
- National Science Foundation, Division of Chemistry (March, 2007)
- National Science Foundation, Biological Database and Informatics Program (September, 2006)
- Luxembourg National Research Fund (FNR), CORE programme (August 2010)
- Louisiana Board of Regents' Research Competitiveness Subprogram, EPSCoR-style grants program (November, 2009)
- External reviewer of the Council for the Earth and Life sciences, Netherlands Organization for Scientific Research, Netherlands. (March, 2006)

### Review of Papers

- reviewer of  
Bioinformatics  
BMC Bioinformatics  
Protein Science  
Nucleic Acid Research  
Proteins: Structure, Function, Bioinformatics  
Biophysical Journal  
BMC Structural Biology  
ISMB (International Conference on Intelligent Systems for Molecular Biology)  
The Pacific Symposium on Biocomputing (PSB)  
DNA Research  
Biophysics (Japan)  
Journal of Computational Chemistry  
Annals of Biomedical Engineering  
FEBS Letters  
PLoS Computational Biology  
Cancer Informatics  
IEEE Transactions on Information Technology in Biomedicine  
Journal of Bioinformatics and Computational Biology  
Parallel Computing  
International Journal of Data Mining and Bioinformatics (IJDMB)  
Briefings in Bioinformatics  
Briefings in Functional Genomics and Proteomics  
Amino Acids

### Review of Books

- Editorial Advisory Review Board, “Biological Data Mining in Protein Interaction Networks”  
Edited by See-Kiong Ng & Xiao-Li Li, IGI Global Press (March 2008)

### Textbook reviews

- Proposal for a second edition of a bioinformatics textbook to be published from Garland Science (Sep. 2009)
- a draft manuscript of a textbook on bioinformatics planned to be published from Elsevier Inc. (March 2009)
- a draft manuscript of a book on Computational Approaches for Protein Function Prediction planned to be published from Cambridge University Press (July 2006)
- a draft manuscript for a bioinformatics textbook planned to be published from Brooks/Cole. (December 2005)

### Program Committee

- BIOTECHNO2011: The Third International Conference on Bioinformatics, Biocomputational Systems and Biotechnologies, Venice, Italy, May 22-27, 2011.
- ICDM the IEEE International Conference on Data mining, Workshop on “Biological Data mining and its applications in healthcare”, Sydney, Australia, Dec 13, 2010
- The European Conference on Computational Biology 2010, Ghent, Belgium, Sep. 26-29, 2010
- 2010 ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB), Niagara Falls, NY, August 4, 2010

- BIOTECHNO 2010: The second International Conference on Advances in Biotechnologies, Cancun, Mexico, March 7-13, 2010
- GIW 2009: 20th International Conference on Genome Informatics, Yokohama, Japan, December 14-16, 2009
- 24th International Symposium on Computer and Information Sciences (ISCIS2009), Bioinformatics and Bioengineering track, September 14-16, 2009
- ISIBM International Joint Conference on Bioinformatics, Systems Biology and Computational intelligence, Shanghai, China, August 3-6, 2009
- IEEE 9<sup>th</sup> International Symposium on Bioinformatics & BioEngineering (BIBE09), Taichung, Taiwan, June 22-24, 2009
- Workshop organizer, 4<sup>th</sup> IEEE International Conference on e-Science, eBioinformatics, Indianapolis, Dec. 12, 2008
- GIW 2008: 19th International Conference on Genome Informatics, Brisbane, Australia, December 1-3, 2008
- Area chair, 2008 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, November 7-9, 2008
- BIBM Workshop on Data Mining in Functional Genomics (DMFG), 2008 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, November 5-7, 2008
- Program Committee and session co-chair, Biomedical Engineering Society Annual Meeting 2007, "Systems Biology and Bioinformatics" track, Los Angeles, CA, September 26-29, 2007.
- IEEE 7<sup>th</sup> International Symposium on Bioinformatics & BioEngineering (BIBE07), Boston, MA, October 14-17, 2007
- 7<sup>th</sup> International Workshop on Data Mining in Bioinformatics (BIOKDD '07), August 12th 2007, San Jose, CA, USA
- 2nd VLDB (Very Large DataBases) Workshop on Data Mining in Bioinformatics, September 23-28 2007, University of Vienna, Austria
- 15th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) & 6th European Conference on Computational Biology (ECCB) (ISMB/ECCB) 2007, area "Bioinformatics of Disease", July 21-25, 2007
- HiCOMB 2007: Sixth IEEE International Workshop on High Performance Computational Biology, Renaissance Long Beach Hotel, Long Beach, California, March 26, 2007
- Interface 2007: the 39th Symposium on the interface of statistics, computing science and applications. Doubletree Hotel, Philadelphia on May 23- 26, 2007.
- Program Committee and session co-chair, Biomedical Engineering Society Annual Meeting 2006, "Systems Biology and Bioinformatics" track, Chicago, IL, October 12-14, 2006.
- Scientific Committee, Special Session on Computer Infrastructure for Systems Biology, part of the 18th International Conference on Systems Engineering 2005 (ICSEng'05). August 16-18 2005, Las Vegas, NV.

## Internal Services

### Department

#### Biological Sciences:

- Bioinformatics and Biotechnology Advisory 2005-6, 2006-7
- Graduate School Admission Committee 2005-6, 2009-2010
- Umbarger Outstanding Graduate Student Award Review Committee 2005-6

#### Computer Science:

- Undergraduate Committee 2009-2010
- Graduate Study Committee 2007-9

- Bioinformatics search committee 2004-5, 2005-6, 2006-7

#### School

- Member of Bioinformatics Steering Committee (Chair: Rebecca Doerge) 2005-6
- Member of COALESCE bioinformatics & systems biology search committee 2003-4/2004-5/2005-6/2006-7(both Informatics and CS Subcommittee)
- Member of COALESCE systems biology search committee (Chair: Michael Gribskov), 2005-6

#### **Professional Societies**

The Biophysical Society

The Protein Society

The International Society of Computational Biology

Biomedical Engineering Society

The Biophysical Society of Japan

The Molecular Biology Society of Japan

Japanese Society of Bioinformatics