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Associate Professor of Biological Sciences/Computer Science
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<http://bio.purdue.edu/people/faculty/index.php?refID=166>
<http://www.cs.purdue.edu/faculty/dkihara.html>
<http://dragon.bio.purdue.edu> (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- **Associate professor**
Purdue University, West Lafayette, Indiana
Department of Biological Sciences/Computer Sciences
2005.3- **full member,**
Bindley Bioscience Center at Discovery Park, Purdue University
2003.8- **tenure-track Assistant professor**
Purdue University, West Lafayette, Indiana
Department of Biological Sciences/Computer Sciences
2002.9-2003.7 **Senior Postdoctoral Research Associate**
Buffalo Center of Excellence in Bioinformatics, Buffalo, NY
Advisor: Jeffrey Skolnick
2001-2002.9 **Senior Postdoctoral Research Associate**
Donald Danforth Plant Science Center, St. Louis, MO
Advisor: Jeffrey Skolnick
1999-2001 **Postdoctoral Research Associate**
Donald Danforth Plant Science Center, St. Louis, MO
Laboratory of Computational Genomics
1998-1999 **Research Assistant**
Bioinformatics Center
Institute for Chemical Research, Kyoto University, Japan

Awards

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

Publications

- [46] Characterization and classification of local protein surfaces using self-organizing map.
Lee Sael & Daisuke Kihara
International Journal of Knowledge Discovery in Bioinformatics, in press. (2009)
- [45] 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)
- [44] ESG: Extended similarity group method for automated protein function prediction.
Meghana Chitale, Troy Hawkins, Changsoon Park & Daisuke Kihara
Bioinformatics, 25: 1739-1745. (2009)
- [43] Protein surface representation and comparison: New approaches in structural proteomics.
Lee Sael & Daisuke Kihara
(A book chapter in) *Biological Data Mining*, J. Chen and S. Lonardi (eds). V. Kumar, (series ed.), Chapman & Hall/CRC Press, Boca Raton, Florida, USA. In Press.
- [42] Quality assessment of protein structure models.
Daisuke Kihara, Hao Chen & Yifeng D. Yang
Current Protein and Peptide Science, 10: 216-228 (2009)
- [41] Limited proteolysis identifies a novel coiled-coil Bin1 BAR peptide that is sufficient to inhibit E2F1 transactivation and tumor growth.
Greta L. Lundgaard, Erica L. Kinney, Satoshi Tanida, Medeleine B. Leake, Nicholas F. Parchim, Joanna K. Johnson, Kazi M. Ahmed, Amelie A. Rodrigue, Melissa D. Zolodz, Daisuke Kihara, Carol B. Post & Daitoku Sakamuro
Submitted, *Experimental Cell Research*, April 2008.
- [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. Elsik, 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 7th 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 Szilagy 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)

Invited Talks

- [57] Global and local protein surface comparison and its applications
 Telluride workshop on “Method development for protein structure prediction and design”
 (organizer: Jianpeng Ma), Telluride, CO
 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 4th 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: 10th 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 21st 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.
 23rd 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

- [95] Local surface-based protein function prediction using Zernike descriptors.
 D. Kihara, Sael Lee, Rayan Chikhi
 Biophysical Society Meeting, March 4, 2009, Boston MA
- [94] Threading without optimizing weighting factors for scoring function.
 Yifeng D Yang, C. Park, D. Kihara.
 Biophysical Society Meeting, March 4, 2009, Boston MA
- [93] Threading without optimizing weighting factors for scoring function.
 Yifeng D Yang, C. Park, D. Kihara.
 Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009
- [92] Improvement of template-based protein structure prediction by suboptimal alignments.
 Hao Chen, D. Kihara.
 Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009
- [91] ESG: Extended similarity group method for automated protein function prediction.
 Meghana Chitale, C. Park, D. Kihara.
 Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009
- [90] Protein Representation for Efficient Comparison of Surface Properties
 Sael Lee, Bin Li, David La, Raif Rustamov, D. Kihara.
 Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009
- [89] 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

- [88] Intelligent Systems for Molecular Biology (ISMB) 2008, July 19-23, 2008, Toronto, Canada
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
- [87] 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
- [86] Ecolihub: Development of the 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, 108th General Meeting, Boston
June 1-5, 2008
- [85] 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.
- [84] Disorder region prediction of E. coli proteins.
Rupal Trivedi, Yifeng Yang, D. Kihara.
Undergraduate Research and Poster Symposium, College of Science, Purdue University,
Purdue Memorial Union, March 31, 2008.
- [83] Computational modeling of ABC transporters.
Priyanka Surana, Yifeng Yang, D. Kihara.
Undergraduate Research and Poster Symposium, College of Science, Purdue University,
Purdue Memorial Union, March 31, 2008.
- [82] 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 52nd Annual Meeting and 16th International Biophysics
Congress, Long Beach, CA
February 2-6, 2008.
- [81] Predicting the error of template-based protein structure modeling by suboptimal alignment
stability.
Hao Chen & D. Kihara
Meeting of the Biophysical Society 52nd Annual Meeting and 16th International Biophysics
Congress, Long Beach, CA
February 2-6, 2008.
- [80] 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
- [79] 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
- [78] Functional enrichment of proteomics datasets with PFP.
T. Hawkins, M. Chitale, S. Luban & D. Kihara.
ISMB 2007, Vienna, Austria.
July 21-25, 2007

- [77] 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.
- [76] 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.
- [75] 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.
- [74] 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.
- [73] 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.
- [72] 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.
- [71] 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.
- [70] 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.
- [69] 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
- [68] Benchmark of new amino acid similarity matrices on recognition of distant protein structures.
Yu-Hsuan Rex Cheng, Hao Chen & Daisuke Kihara.

- 2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.
April 4, 2007.
- [67] Structure modeling of E. coli proteome: Quality evaluation.
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.
2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.
April 4, 2007.
- [66] Structure modeling of E. coli proteome: Homology models.
Steve Krawczyk, Preston Spratt, Yifeng Yang & D. Kihara
2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.
April 4, 2007.
- [65] Structure modeling of E. coli proteome: Quality Evaluation
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.
Dept. of Biological Science Undergraduate Research Presentation, Purdue University,
March 31, 2007.
- [64] 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.
- [63] 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.
- [62] 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.
- [61] 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.
- [60] 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.
- [59] 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
- [58] 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
- [57] 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.
- [56] 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
- [55] 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
- [54] 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
- [53] 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
- [52] Using Neural Network in Protein Domain Prediction.
Yen Hock Tan and Daisuke Kihara
Undergraduate Research & Poster Symposium, College of Science, Purdue University
April 11, 2006
- [51] Using Neural Network in Protein Domain Prediction.
Yen Hock Tan and Daisuke Kihara
14th Annual Undergraduate Research Day, Dept. of Biological Sciences, College of Science, Purdue University
April 1, 2006
- [50] Including natural protein flexibility in predicted protein structure comparisons.
Jairav Desai and Daisuke Kihara
14th Annual Undergraduate Research Day, Dept. of Biological Sciences, College of Science, Purdue University
April 1, 2006
- [49] Protein structure-sequence alignment with a reliability measure.
Hao Chen and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006
- [48] 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
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006

- [47] Bridging geometric protein surface features and phylogenetic information for rapid identification of protein-protein interaction interfaces.
David La, Denis Liversay and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006
- [46] Multi-resolution protein representation.
Sael Lee, Bin Li, David La, Raif Rustamov and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006.
- [45] Ligand Binding Sites Prediction with the Visibility Criteria.
Bin Li, Srinivasan Turuvekere, Manish Agrawal, Karthik Ramani and
Daisuke Kihara.
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006
- [44] EMD: An ensemble algorithm for discovering regulatory motifs in DNA sequences.
Yifeng D. Yang, Jianjun Hu, and Daisuke Kihara.
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 14, 2006
- [43] 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
- [42] 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
- [41] 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
- [40] 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
- [39] Evaluation and development of protein function prediction.
Stan Luban, Troy Hawkins and Daisuke Kihara (Oral presentation)
16th Annual Argonne Symposium for Undergraduates in Science, Engineering and
Mathematics, Argonne National Laboratory, Argonne, Illinois
November 4th, 2005
- [38] Using neural network in protein domain prediction.
Yen Hock Tan, Adolfo Tapia, Otoniel Venezuela, and Daisuke Kihara (Oral presentation)
16th Annual Argonne Symposium for Undergraduates in Science, Engineering and
Mathematics, Argonne National Laboratory, Argonne, Illinois
November 4th, 2005
- [37] BioQ: A 3D Querying Engine for Proteins.
Athurva Gore, Bin Li, Karthik Ramani & Daisuke Kihara

- Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University.
August 2, 2005
- [36] Protein-protein Interaction Data Assessment.
Ei Ei Phyu & Daisuke Kihara
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University.
August 2, 2005
- [35] Comparison of distantly related protein sequence alignments with multiple amino acid similarity matrices.
Yen Hock Tan & Daisuke Kihara
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University.
August 2, 2005
- [34] Comparative study of small RNAs and small peptides in complete genome sequences.
Stan Luban & Daisuke Kihara
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University.
August 2, 2005.
- [33] Protein Structure Prediction with ZDock 2.3.
Luis Avila, Bin Li & Daisuke Kihara
Marc/Aim Research Presentation, Burton Morgan Center for Entrepreneurship, Purdue University.
July 28, 2005
- [32] 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.
- [31] 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
- [30] Comparing Tertiary Structures of Protein Active Sites.
Yuhao Lin and Daisuke Kihara.
Undergraduate Research Day, College of Science & College of Agriculture, Purdue University.
April 11, 2005
- [29] Comparative Study of Small RNA and Small Peptides in Complete Genome Sequences.
Stan Luban and Daisuke Kihara.
Undergraduate Research Day, College of Science & College of Agriculture, Purdue University.
April 11, 2005.
- [28] Computer Graphics Program in Foreign Language Instruction.
Ei Ei Phyu, Kazumi Hatasa and Daisuke Kihara.
Undergraduate Research Day, College of Science & College of Agriculture, Purdue University.
April 11, 2005.
- [27] Comparison of Distantly Related Protein Sequence Alignments with Multiple Amino Acid Similarity Matrices.
Yen Hock Tan and Daisuke Kihara.

- Undergraduate Research Day, College of Science & College of Agriculture ,Purdue University.
April 11, 2005.
- [26] Structure-basis of protein-protein interaction.
Brian Trisler and Daisuke Kihara.
Undergraduate Research Day, College of Science & College of Agriculture ,Purdue University.
April 11, 2005.
- [25] Comparative Study of Small RNA and Small Peptides in Complete Genome Sequences.
Stan Luban and Daisuke Kihara
The 13th Annual Undergraduate Research Day at Dept. of Biological Sciences,
Purdue University.
April 2, 2005
- [24] A structured approach to computational protein function prediction.
Troy Hawkins and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 17, 2005
- [23] Protein Structure-Sequence Alignment with a Reliability Measure.
Hao Chen and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 17, 2005
- [22] A novel method to construct phylogenetic tree based on complete genome sequences.
Bin Li and Daisuke Kihara
Sigma Xi Graduate Student Research Poster Presentation, Purdue University
February 17, 2005
- [21] Conserved structural non-coding RNA families in Gamma-proteobacteria
Stan Luban and Daisuke Kihara (Oral presentation)
15th Annual Argonne Symposium for Undergraduates in Science, Engineering and
Mathematics, Argonne National Laboratory, Argonne, Illinois
November 5th, 2004
- [20] Improvement of protein sequence alignments for better protein structure prediction.
Yen Hock Tan and Daisuke Kihara (Oral presentation)
15th Annual Argonne Symposium for Undergraduates in Science, Engineering and
Mathematics, Argonne National Laboratory, Argonne, Illinois
November 5th, 2004
- [19] Computational Prediction of Protein Structures and Functions.
Otoniel Venezuela, Troy Hawkins, Evans Tapia, Yen Hock Tan and Daisuke Kihara
Faculty Poster Session, Dept. of Computer Sciences, Purdue University
Stewart Center, Purdue University, 20 September, 2004.
- [18] Computational Prediction of Protein Structures and Functions.
Otoniel Venezuela, Troy Hawkins, Evans Tapia, Yen Hock Tan and Daisuke Kihara
PULSE Program retreat, Purdue University
28 August 2004.
- [17] Feature recognition based identification of potential binding sites on the molecular surfaces.
Srinivasan Turuvekere, Manish Agrawal, Daisuke Kihara, and Karthik Ramani.
The Protein Society 18th Symposium. San Diego, August 14-18, 2004.
- [16] 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.
- [15] Real-Time Manipulation of Keyframe Animation.

- Brian Seckinger, Rodney Weaver and Daisuke Kihara
School of Science Undergraduate Research Day, Purdue University
Purdue University, 17 April, 2004.
- [14] A Web-Interface for a Database of Microbial Intergenic Sequences.
Jason Pardieck and Daisuke Kihara
School of Science Undergraduate Research Day, Purdue University
Purdue University, 17 April, 2004.
- [13] Comparative Study of Structural Non-Coding RNAs
Stanislav Luban and Daisuke Kihara
School of Science Undergraduate Research Day, Purdue University
Purdue University, 17 April, 2004.
- [12] Computational prediction and experimental validation of iron and phosphate gene regulatory sites in the Escherichia coli K-12 and Pseudomonas aeruginosa PA01 genomes.
Sam-Il Jung, Kaushik M. Setty, Khurram Siddiqi, Lu Zhou, Barry L. Wanner and Daisuke Kihara
International Workshop for Escherichia coli Towards New Biology in the 21st Century.
Awaji-shima, Japan, 15-17 October, 2003.
- [11] All-against-all protein structure comparison reveals the current database (PDB) is a covering set of small protein structures.
Daisuke Kihara and Jeffrey Skolnick
Corporate Partner Faculty Poster Session, Department of Computer Sciences, Purdue University.
the Buchanan Club at Ross-Ade Stadium, Purdue University, 15 September, 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
18th 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
35th 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
17th 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
33rd 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
17th 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, 06/01/2005-05/31/2010) Role: PI

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

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, a grad RA, 09/01/09 – 08/31/10)

Past

Computational proteomics approaches for rational drug design. (Computing Research Institute, Purdue University, CRI PRF-SIRG, \$16,375, (7/1/2008- 6/30/2009))

Recovery Act administrative Supplement. Parent grant: U24 GM077905-03 Development of the www.EcoliCommunity.org Information Resource. (NIH, 4/1/09 – 6/30/09, \$410,000 direct) Role: co-PI, (PI: Barry Wanner)

Development of the 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

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; Currently assistant professor at Univ. of South Carolina) Sept. 2004 – August 2005

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 -

Supervised Technician

Yen Hock Tan: June - August 2004

Stan Luban: January 2006 – June 2006

Supervised Students

Current Graduate Students:

Bin Li (CS)

Hao Chen (BMB)

Yifeng Yang (PULSe)

Sael Lee (CS)

David La (Biol)

Meghana Chitale (CS)

Juan Esquivel (CS)

Padmasini Chakravarthy (ECE)

Former Graduate Students:

Troy Hawkins (Biol, Ph.D. Oct 08)

Khurram Siddiqi (Electrical Engineering)

Fall 2003, Co-supervised with B. Wanner

Chad Pitschka (rotation student, BIOL)

Spring 2004

Srinivasan S. Turuvekere (ME)

Kyle Krull (Biochem./Molecular Biology,
Spring 2004)

Evans Adolfo Tapia (CS, Summer 2004)

He Huang (PULSe, rotation, Fall 2004)

Manish Agrawal (Mechanical Engineering)

Chetak Sirsat (CS, Fall 2004)

Hyun Chul Lee (PULSe) rotation, spring 2005

Otoniel Venezuela (CS), Summer 04-Summer05

Greg Ziegler (Bio) rotation, spring 2006

Prasad Siddavatam (Bio) rotation, spring 2006

Justin Gaylor (CS), Fall 05

Mingwu Zhang (CS), Fall 04 – Fall06

co-supervised with Sunil Prabhakar (CS)

Aditi Gupta (Bio) rotation, Fall 06

Rayan Chikhi (summer intern, 2007, Ecole
Normale, France)

Current Undergraduate Students:

Priyanka Surana (Bio) Fall 07 –

Matt Herron (Animal Sci/CS) Summer 08 –

Gregg Thomas (Bio) Summer 08 -

Paul Tuck (CS) Summer 09

Shen Liang (CS) Summer 09

Former Undergraduate Students:

Stan Luban (CS/Biol) 04 Spring – 06 Spring
Hughes Summer Internship, 04, 05
Ei Ei Phyu (CS) Spring 2005- Fall 2005
Hughes Summer Internship (2005)
Jasmine Williams (MARC/AIM,
Grambling University), Summer 2004
Rodney Weaver (CS), Spring, Fall 2004
Brian Seckinger (CS), Spring 2004
Chanon Sujjapong (Comp. Eng.) Summer 04
Jennifer Susanne Reeve (CS), Summer 04
Jonathan Williford (CS), Fall 2004
Yuhao Lin (Computer Engng), Spring 2005
Howard Chang (CS), Summer 06

Rex Cheng (CS) Spring07
De'Rael Darling (SROP minority) Summer 07

Preston Spratt (Biol), Fall 06 – Spring 08
Emily Flynn (Biol), Fall 08
Devin Lockett (Biol) Fall 08 – Spring 09
En-Husn Liu (CS) Summer 09

Yen Hock Tan (CS) Summer 04 – Spring 06
Hughes Summer Internship 05
Jairav Desai (CS) DURi program
Fall05/Spring 06
Luis Avila (Marc/Aim, St. Edwards Univ,
Texas) Summer 2005
Danny Varghese (CS), Spring 2004
Jason Pardieck (CS), Spring 2004
Irvan Sutiono (CS), Summer 2004
Joel Hayhurst (CS), Fall 2004
Brian Trisler (CS), Spring 2005
Jiyoung Lee (Biol), Fall 2005
Robert Helms (Biol) Fall 06

Steve Krawczyk (Bio), Fall06, Spring07
Stephen Ueng (CS) Fall 07

Rupal Trivedi (Bio) Fall 07-Spring 08
Jared Bannister (CS/Math), Fall 08
Steven Ahrendt (Bio/CS) Fall 08 - Spring 09

K-12 Students

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

Student Awards

- Gregg Thomas (Biol) Sandy Ostroy Undergraduate Summer Internship, Dept. of Biological Sciences, Purdue University, Summer 2009
- 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), DURi, Discovery Park Undergraduate Research Internship, Fall 2006, Spring 2007, Fall 2007.
- David La (Biol), 1st 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), DURi, Discovery Park Undergraduate Research Internship, Fall 2005, Spring 2006.
- Stan Luban (CS/Biol), DURi, 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). 2nd place in 2004 Purdue University's Burton D. Morgan Entrepreneurship Competition

Courses Taught Spring 2004/Spring & Fall 2005/Fall 2006:

CS490B/Biol495S Introduction to Bioinformatics

- 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

Spring 2006, 2007, 2008, 2009: BIOL595A/(CS590B) Protein Bioinformatics

Spring 2006: BIOL696E Seminar Crystallography

Other Teaching Activities

- Gave a 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). 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)
- Guest lecture on bioinformatics research at CS 197 Honors Seminar, Feb 16, 2009
- 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-)
- The Open Proteomics Journal (November 2007 -)

Review of Grants

- Ad hoc reviewer of NIH Recovery Challenge Grant (June, 2009)
- Ad hoc reviewer of the National Science Foundation, MCB (February, 2009)
- Ad hoc reviewer of the National Science Foundation, Division of Chemistry (February, 2008)
- Ad hoc reviewer of the National Science Foundation, Division of Chemistry (September, 2007)
- Ad hoc reviewer of the National Science Foundation, Division of Chemistry (March, 2007)

- Ad hoc reviewer of the National Science Foundation, the Biological Database and Informatics Program (September, 2006)
- 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

- reviewed a draft manuscript of a textbook on bioinformatics planned to be published from Elsevier Inc. (March 2009)
- Editorial Advisory Review Board, “Biological Data Mining in Protein Interaction Networks” Edited by See-Kiong Ng & Xiao-Li Li, IGI Global Press (March 2008)
- Reviewed a draft manuscript of a book on Computational Approaches for Protein Function Prediction planned to be published from Cambridge University Press (July 2006)
- Reviewed a draft manuscript for a bioinformatics textbook planned to be published from Brooks/Cole. (December 2005)

Program Committee

- PC member, GIW 2009: 20th International Conference on Genome Informatics, Yokohama, Japan, December 14-16, 2009
- PC member, 24th International Symposium on Computer and Information Sciences (ISCIS2009), Bioinformatics and Bioengineering track, September 14-16, 2009
- PC member, ISIBM International Joint Conference on Bioinformatics, Systems Biology and Computational intelligence, Shanghai, China, August 3-6, 2009
- PC member, IEEE 9th International Symposium on Bioinformatics & BioEngineering (BIBE09), Taichung, Taiwan, June 22-24, 2009

- Workshop organizer, 4th IEEE International Conference on e-Science, eBioinformatics, Indianapolis, Dec. 12, 2008
- PC member, 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
- Program Committee, 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.
- Program Committee, IEEE 7th International Symposium on Bioinformatics & BioEngineering (BIBE07), Boston, MA, October 14-17, 2007
- Program Committee, the 7th International Workshop on Data Mining in Bioinformatics (BIOKDD ’07), August 12th 2007, San Jose, CA, USA
- Program Committee, 2nd VLDB (Very Large DataBases) Workshop on Data Mining in Bioinformatics, September 23-28 2007, University of Vienna, Austria
- Program Committee, 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
- Program Committee, HiCOMB 2007: Sixth IEEE International Workshop on High Performance Computational Biology, Renaissance Long Beach Hotel, Long Beach, California, March 26, 2007
- Program Committee, 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

- Bioinformatics and Biotechnology Advisory, 2005-6, 2006-7
- Biology Department Graduate School Admission Committee 2005-6
- Umbarger Outstanding Graduate Student Award Review Committee 2005-6
- Bioinformatics search committee, CS department 2004-5, 2005-6, 2006-7
- Graduate Study Committee, CS dept, 2007-9

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