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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	Associate professor with tenure Purdue University, West Lafayette, Indiana Department of Biological Sciences/Computer Sciences (joint appointment)
2005.3-present	full member Bindley Bioscience Center at Discovery Park, Purdue University
2003.8-2009.8	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, USA Advisor: Jeffrey Skolnick
2001-2002.9	Senior Postdoctoral Research Associate Donald Danforth Plant Science Center, St. Louis, MO, USA Advisor: Jeffrey Skolnick
1999-2001	Postdoctoral Research Associate Donald Danforth Plant Science Center, St. Louis, MO, USA 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, 2010
- Best paper, Great Lakes Bioinformatics Conference, Athens, Ohio, May 2-4, 2011
- International Structural Genomics Organization Poster Prize, International Conference on Structural Genomics 2011, Toronto, Canada, May 10-14, 2011
- Best paper award, the 21st International Conference on Genome Informatics (GIW 2010), December 16-18, 2010, Hangzhou, China.

Publications

- [70] Detecting Local Ligand-Binding Site Similarity in Non-Homologous Proteins by Surface Patch Comparison.
L. Sael & D. Kihara
Proteins: Structure, Function, and Bioinformatics, in press (2012)
- [69] Constructing patch-based ligand-binding pocket database for predicting function of proteins.
L. Sael & D. Kihara
BMC Bioinformatics, in press (2012)
- [68] Evaluation of multiple docking structures using correctly predicted pairwise subunits.
J. Esquivel-Rodriguez & D. Kihara
BMC Bioinformatics, in press (2012)
- [67] Graphical models for protein function and structure predictions.
M. Tang, K.M. Tan, X.L. Tan, L. Sael, M. Chitale, J. Esquivel-Rodriguez, & D. Kihara
Handbook of Biological Knowledge Discovery, M. Elloumi and A.Y. Zomaya (ed), Wiley, in press. (2012)
- [66] A novel method for protein-protein interaction site prediction using phylogenetic substitution models.
D. La & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 1: 126-141 (2012)
- [65] JnCML-like, an EF-hand motif-containing gene seasonally upregulated in the transition zone of black walnut (*Juglans nigra* L.).
Z. Huang, P. Surana, D. Kihara, R. Meilan, & K. Woeste,
American Journal of Molecular Biology, 1: 140-155 (2011)
- [64] Community-wide assessment of protein-interface modeling suggests improvement to design methodology.
S.J. Fleishman, ..., J. Esquivel-Rodriguez, D. Kihara, ..., & D. Baker (total 96 authors)
J. Mol. Biol. 414: 289-302 (2011)
- [63] Quantification of protein group coherence and pathway assignment using functional association.
M. Chitale, S. Palakodety, & D. Kihara
BMC Bioinformatics, 12: 373 (2011)
- [62] Identification of a novel effector domain of BIN1 for cancer suppression.
G.L. Lundgaard, N.E. Daniels, S. Pyndiah, E.K. Cassimere, K.M. Ahmed, A. Rodrigue, D. Kihara, C. Post, & D. Sakamuro
J. Cell. Biochem. 112: 2992-3001. (2011)
- [61] N-terminal Gly224-Gly411 Domain in *Listeria* Adhesion Protein Interacts with Host Receptor Hsp60.
B. Jagadeesan, A.E. Fleishman Littlejohn, M.A. Amalaradjou, A.K. Singh, K.K. Mishra, D. La, D. Kihara, & A. K. Bhunia,
PLoS ONE, 6:e20694 (2011)
- [60] Molecular surface representation using 3D Zernike descriptors for protein shape comparison and docking.
D. Kihara, L. Sael, R. Chikhi, J. Esquivel-Rodriguez
Curr. Protein and Peptide Science, 12: 520-530 (2011)
- [59] Energetics-based discovery of protein-ligand interactions on a proteomics scale.
Pei-Fen Liu, Daisuke Kihara & Chiwook Park
J. Mol. Biol. 408: 147-162 (2011)
- [58] Protein binding ligand prediction using moment-based methods.
Rayan Chikhi, Lee Sael & Daisuke Kihara
in *Protein function prediction for omics era*, Daisuke Kihara ed., Chapter 8, Springer-Verlag, Chap. 8, pp. 145-163. (2011)

- [57] Enhanced sequence-based function prediction methods and application to functional similarity networks.
Meghana Chitale & Daisuke Kihara
in *Protein function prediction for omics era*, Daisuke Kihara ed., Chapter 2, Springer-Verlag, Chap. 2, pp. 19-34. (2011)
- [56] Computational protein function prediction: framework and challenges.
Meghana Chitale & Daisuke Kihara
in *Protein function prediction for omics era*, Daisuke Kihara ed., Chapter 1, Springer-Verlag, Chap. 1, pp. 1-17, (2011)
- [55] Effect of using suboptimal alignments in template-based protein structure prediction
H. Chen, & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 79: 315-334 (2011)
- [54] Binding ligand prediction for proteins using partial matching of local surface patches.
Lee Sael & Daisuke Kihara
Int. J. Molecular Sciences, 11: 5009-5026 (2010)
- [53] Protein surface representation for application to comparing low-resolution protein structure data.
L. Sael, & D. Kihara
BMC Bioinformatics 11: S2 (2010)
- [52] SubAQUA: Real-value quality assessment of protein structure models.
Yifeng D. Yang, Preston Spratt, Hao Chen, Changsoon Park, & Daisuke 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.
Troy Hawkins, Meghana Chitale, & Daisuke Kihara
BMC Bioinformatics, 11: 265 (2010)
- [50] Real-time ligand binding pocket database search using local surface descriptors.
Rayan Chikhi, Lee Sael, & Daisuke Kihara
Proteins: Structure, Function, and Bioinformatics, 78: 2007-2028, (2010)
- [49] Application of 3D Zernike descriptors to shape-based ligand similarity searching.
Vishwesh Venkatraman, Padmasini R. Chakravarthy & D. Kihara
J. Cheminformatics, 1: 19. (2009)
- [48] Protein-protein docking using region-based 3D Zernike descriptors.
Viswesh Venkatraman, Yifeng D. Yang, Lee Sael & Daisuke Kihara
BMC Bioinformatics, 10: 407. (2009)
- [47] Error estimation of template-based protein structure models.
Daisuke Kihara, Yifeng D. Yang & Hao Chen
Multiscale approaches to protein modeling: structure prediction, dynamics, thermodynamics and macromolecular assemblies. Andrzej Kolinski ed. , Springer-Verlag, Chapter 13, pp. 295-314. (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, Changsoon 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 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)

Books

- [1] Protein function prediction for omics era, D. Kihara, ed. Springer-Verlag, (2011)

Miscellaneous Publication:

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

Invited Talks

- [94] Functional coherence assessment for protein groups and its application to pathway assignment, Zing conference, IECA (International E. coli Alliance) 2011, Xcaret, Cancun, Mexico, Dec. 5-9, 2011
- [93] Unified Molecular Representation for Protein Shape Comparison and Interaction, Zing conference on Protein and RNA Structure Prediction, Xcaret, Cancun, Mexico, Dec. 3-7, 2011
- [92] Protein surface representation for ligand binding site screening, Eli Lilly, Indianapolis, Oct. 3, 2011
- [91] Next Generation Protein 3D Structure Analysis: Rapid Global/Local Surface Comparison, Docking and Low-Resolution Data, University of Alberta, Edmonton, Canada, Sept. 16, 2011
- [90] Binding ligand prediction by comparing local surface patches of potential pocket regions. Computational Biology Research Center, Tokyo, Japan, September 2, 2011
- [89] Next generation protein structure analysis for structure comparison and interaction prediction. Fukushima Medical University, Fukushima, Japan, September 1, 2011.
- [88] Binding ligand prediction by comparing local surface patches of potential pocket regions. RIKEN, Yokohama, Japan, August 30, 2011
- [87] Unified molecular representation for protein shape comparison and interaction. ICR Symposium to Celebrate the Bioinformatics Center's 10 Year Anniversary and New Restructuring, Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan, August 29, 2011
- [86] Next generation protein 3D structure analysis: rapid global/local surface comparison and low-resolution data. Seoul National University, Dept. of Computer Science and Engineering, August 22, 2011
- [85] Function Prediction for Systems Level: Functional Coherence of Protein Groups and Identification of Missing Genes. M. Chitale & D. Kihara, Automated Function Prediction SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July 15-16, 2011
- [84] Protein-protein docking prediction: from pairwise docking, docking interface prediction, and multiple protein docking. Workshop on "Modeling Biomolecular Structures, Interactions, and Functions, Telluride, Colorado, June 13-17, 2011.
- [79-83] 4 lectures, Faculty of Chemistry, Warsaw University, Poland, May 23-27, 2011
- Template-based structure prediction and quality assessment using suboptimal alignments
 - Sequence-based function prediction: from prediction of single genes to functional coherence for protein groups
 - Protein-protein docking prediction: from pairwise docking, docking using docking interface information, and multiple protein docking

- Binding ligand prediction by Comparing Local Surface Patches of Potential Pocket Regions
- [78] Surface Representation for Molecular Global and Local Shape Comparison and Docking. International Institute of Molecular and Cell Biology, Warsaw, Poland, May 25, 2011
- [71-77] 6 selected oral presentations at Great Lakes Bioinformatics Conference 2011, May 2-4, 2011, Ohio University, Athens, Ohio
- Protein-protein Interaction Sites Prediction using Phylogenetic Substitution Models, D. La, & D.Kihara
 - Protein Docking Prediction Using Predicted Protein-Protein Interface, B. Li, & D. Kihara
 - Multi-LZerD: Multiple Protein Docking for Asymmetric Complexes, J. Esquivel-Rodriguez, & D. Kihara
 - Rapid Comparison and Multimeric Protein Complex Fitting for Low-Resolution Electron Microscopy Data", J. Esquivel-Rodriguez, L. Sael, & D. Kihara
 - Patch-Surfer: Alignment Free Surface Patch-Based Ligand Binding Pocket Comparison, L. Sael, & D. Kihara
 - Functional Coherence Assessment for Protein Groups and its Application to Pathway Assignment, M. Chitale, & D. Kihara
- [70] Prediction of protein-protein interaction sites, pair-wise, and multiple protein docking, Academy of Mathematics and Systems Science, Chinese Academy of Science, Beijing, China, December 20, 2010
- [69] Improved Protein Surface Comparison and Application to Low-Resolution Protein Structure Data. L. Sael, & D. Kihara, The 21st International Conference on Genome Informatics, Hangzhou, China, December 16-18, 2010
- [68] Binding ligand prediction using local surface Zernike descriptors. Shanghai Institute of Materia Medica, Chinese Academy of Science, Shanghai, China, December 15, 2010
- [67] Sequence-based function prediction: from prediction of single genes to functional coherence for protein groups. Institute of Biochemistry and Cell Biology, Chinese Academy of Science, Shanghai, China, December 15, 2010
- [66] Protein-protein docking prediction: from pairwise docking, docking using docking interface information, and multiple docking. Shanghai Jiaotong University, Shanghai, China, December 14, 2010
- [65] Sequence-based function prediction: from prediction of single genes to functional coherence for protein groups. Fudan University, Shanghai, China, December 13, 2010
- [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 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.
Univ. 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.
Center for Computational Biology and Bioinformatics, IUPUI, Indianapolis, IN, October 6, 2006.
- [37] Low resolution and uncertainty in protein structure and function prediction.
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, April 1, 2005
- [25] Conserved Small RNA Families in Gamma-Proteobacteria.
Computational Biology Research Center, Tokyo, Japan, December 28, 2004.
- [24] Computational sequence and structure analyses.
Biological Sciences Faculty Research Presentations, Dept. of Biological Sciences, Purdue University, December 9, 2004
- [23] Comparative genomics study of non-coding RNA in Gamma-proteobacteria
Ecolunch, Dept. of Biological Sciences, Purdue University, November 17, 2004
- [22] Genome-scale Protein Structure Assignment to Microbial Genome Sequences.

- Ninth Annual Purdue University Biophysics Symposium, October 25, 2003
- [21] PDB is a Covering Set of Small Protein Structures.
Bioinformatics Center, Kyoto University, Japan, October 20, 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, October 15-17, 2003
- [19] Revisiting protein Structure Space – PDB is a Covering Set of Small Protein Structures.
Computational Biology Research Center, Tokyo, Japan, October 14, 2003.
- [18] Revisiting Protein Structure Space for Prediction – PDB is a Covering Set of Small Protein Structures.
Bioinformatics Seminar Series, Purdue University, September 9, 2003.
- [17] Protein Structure/Function Prediction on a Genome Scale.
The Whitney Laboratory/Dept. of Computer Science, University of Florida, Gainesville, Florida, April 7-8, 2003.
- [16] Genome Scale Protein Structure Prediction.
Computer Science Dept., Virginia Polytechnic Institute and State University, Blacksburg, Virginia, April 3, 2003.
- [15] Protein Structure/Function Prediction on a Genome Scale.
Dept. of Biology, The University of Nebraska at Omaha, Omaha, Nebraska, April 1, 2003.
- [14] Protein Structure/Function Prediction on a Genome Scale.
Dept. of Biological Sciences, Purdue University, West Lafayette, Indiana, March 25, 2003.
- [13] Protein Structure/Function Prediction on a Genome Scale.
Dept. of Informatics, Indiana University, Bloomington, Indiana, March 6, 2003.
- [12] Protein Structure/Function Prediction on a Genome Scale.
Dept. of Biology, University of Kentucky, Lexington, Kentucky, February 4, 2003.
- [11] Protein Structure/Function Prediction on a Genome Scale.
Donald Danforth Plant Science Center, St. Louis, Missouri, October 28, 2002.
- [10] Ab initio Protein Structure Prediction Method on a Genome Scale.
Computational Biology Research Center, Tokyo, Japan, October 12, 2001
- [9] An Ab initio Protein Structure Method Using a Lattice Model.
Structural Bioinformatics Division Seminar, Yokohama City University, Japan, October 11, 2001
- [8] A Lattice Model Based Protein Structure Prediction which Does Not Use Template Structures of Homologous Proteins.
Biophysics Department Seminar, Nagoya University, Japan, October 10, 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, October 9, 2001
- [6] Ab initio Protein Structure Prediction Using Restraints Derived from Threading.
Department of Biochemistry, Cambridge University, UK, September 9, 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, January 10-12, 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, December 15, 2000
- [3] Generalized Comparative Modeling of Protein Structures.
Electrotechnical Laboratory, National Inst. of Advanced Industrial Science,

- Tsukuba, Japan, September 18, 2000
- [2] Analyses of Genome Sequences through Internet.
Kansai Medical University, Japan, March 24, 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, July 29-31, 1998

Poster and Other Presentations

- [75] Binding ligand prediction by comparing local surface patches of potential pocket regions.
L. Sael & D. Kihara
International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July
17-19, 2011
- [74] MULTI-LZERD: Multiple protein docking for asymmetric complexes.
J. Esquivel-Rodriguez & D. Kihara
International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July
17-19, 2011
- [73] Functional coherence assessment for protein groups and its application to pathway
assignment.
M. Chitale, S. Palakodety & D. Kihara
International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July
17-19, 2011
- [72] MULTI-LZERD: Multiple protein docking for asymmetric complexes.
J. Esquivel-Rodriguez & D. Kihara
3D-SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB),
Vienna, July 15-16, 2011
- [71] Rapid comparison and multimeric protein complex fitting for low-resolution electron
microscopy data.
D. Kihara, L. Sael & J. Esquivel-Rodriguez
3D-SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB),
Vienna, July 15-16, 2011
- [70] Binding ligand prediction by comparing local surface patches of potential pocket regions.
L. Sael & D. Kihara
3D-SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB),
Vienna, July 15-16, 2011
- [69] Binding ligand prediction by comparing local surface patches of potential pocket regions.
L. Sael & D. Kihara
Automated Function Prediction (AFP) SIG, International Conference on Intelligent Systems
for Molecular Biology (ISMB), Vienna, July 15-16, 2011
- [68] Binding ligand prediction by comparing local surface patches of potential pocket regions.
L. Sael & D. Kihara
International Conference on Structural Genomics, May 10-14, 2011, Toronto, Canada
- [67] Rapid comparison and multimeric protein complex fitting for low-resolution electron
microscopy data.
J. Esquivel-Rodriguez, L. Sael & D. Kihara
International Conference on Structural Genomics, May 10-14, 2011, Toronto, Canada
- [66] Protein-ligand binding prediction by comparing local protein surface patches.
Lee Sael, D. Kihara
The 55th Annual meeting of Biophysical Society, Baltimore Maryland, March 5-9, 2011
- [65] Novel methods for rapid comparison and multimeric protein complex fitting for low-
resolution electron microscopy data.

- Lee Sael, Juan Esquivel-Rodriguez, D. Kihara
The 55th Annual meeting of Biophysical Society, Baltimore Maryland, March 5-9, 2011
- [64] Protein Docking Prediction Using Predicted Protein-Protein Interface.
Bin Li, D. Kihara
The 21st International Conference on Genome Informatics, Hangzhou, China, Dec. 16-18, 2010
- [63] Performance of SUPRB Threading Method in CASP9.
Chao Yuan, Mateusz Kurcinski, Hao Chen, D. Kihara
The 21st International Conference on Genome Informatics, Hangzhou, China, Dec. 16-18, 2010
- [62] Multiple Protein Docking for Asymmetric Hetero Oligomeric Complexes.
Juan Esquivel-Rodriguez, Yifeng D Yang, D. Kihara
The 21st International Conference on Genome Informatics, Hangzhou, China, Dec. 16-18, 2010
- [61] Functional coherence for protein groups by considering associations between Gene Ontology terms.
Meghana Chitale, S. Palakodety, D. Kihara
The 21st International Conference on Genome Informatics, Hangzhou, China, Dec. 16-18, 2010
- [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 Siegele, 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 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
- [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 52nd Annual Meeting and 16th 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 52nd Annual Meeting and 16th 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, Dec. 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, Dec. 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, Dec. 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, Dec. 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 18th 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-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, October 15-17, 2003.
- [10] PDB is a covering set of a single-domain protein structures.
Daisuke Kihara and Jeffrey Skolnick
Frontiers in Bioinformatics Symposium, Buffalo NY, June 5-8, 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:

Identification of protein-metabolite interactome.

(NIH, R01, 9/1/2011-05/31/2015, \$1,118,554, total), PI

Surface shape based screening of large protein databases.

(Agency: NIH, R01, Total: \$1,408,659 direct cost, 09/01/2005-08/31/2012) Role: PI

III: Small: Quality assessment of computational protein models.

(NSF, IIS, \$327,606, 09/01/2009 – 08/31/2012) 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)

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, 6/1/2010-5/31/2012) Role: co-PI, (PI: Yuk Fai Leung)

TRGP: Novel quantitative proteomic methods to discover and localize endogenous protein complexes.

(NSF, IOS, 09/01/2011-08/31/2015, \$3,458,824 total) Role: co-PI (PI: D. Szymanski)

Development of RAVAT: the tool that uncovers the roles of rare variants and their functions on common diseases with next generation sequencing data.

(Global Research Network Program, 2012-2015, 3 million Korean Won, total) Role: co-PI (PI: C. Park)

Pending

The ROC Project: Development of Robust and Optimized Chassis for making Safe and Secure Biofactories.

(DARPA, 04/01/2012-09/30/2014, \$6M, total) Role: co-PI (PI: Wanner)

III: Small: Elucidating protein functional sites using sequence variation.

(NSF, IIS, 07/01/2012-06/30/2015, \$489,805 total) Role: PI

Comprehensive mapping of Enterobacteriaceae transcriptomes.
(NIH, R01, \$3,045,928 total 04/01/2012 – 03/31/2016). Role: co-PI (PI: B. Wanner)

Past

Protein 3D Structure-based rational drug discovery.
(Purdue Res. Foundation, \$1,6750, 09/01/09 – 08/31/10), Role: PI

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)

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 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

Hyungrae Lee, September 2011 - current

Sael Lee (PhD in CS, Purdue) August 2010 – July 2011, currently researcher at Samsung, Korea

Mateusz Kurcinski, March 2010 – March 2011

Hao Chen (PhD, Biol, Purdue) September-December, 2010 – currently bioinformatics analyst at Craig Venter Institute

Vishwesh Venkatraman September 2007 – July 2009, Currently research scientist at LORIA, France

Jianjun Hu 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, January 3, 2008 – Feb 28 2008

Hangchang Lee, Associate Professor, Dept. of Multi-media Engineering, Hangsung University, Seoul, Korea, Jan. 1. 2009 – May 2009

Supervised Technicians

Michael Gillogly (graduate from CS, Purdue) : August 2009 – April 2010

Stan Luban (graduate from Biol/CS, Purdue): January 2006 – June 2006

Yen Hock Tan (graduate from CS, Purdue): June - August 2004

Supervised Students

Graduated with PhD

Bin Li (CS, Dec, 2011) moved on to postdoc at La Jolla Institute for Allergy & Immunology
David La (Biol, Dec. 2011) moved on to postdoc at Univ. Washington (D. Baker lab)
Sael Lee (CS, July 2010), continued as postdoc, and moved on to researcher at Samsung, Korea
Hao Chen (Biol, May, 2010) moved on to bioinformatics analyst at Craig Venter Institute
Yifeng Yang (Biol, May 2010)
Troy Hawkins, (Biol, October, 2008), move on to currently research assistant professor at IUPUI, Indianapolis
Mingwu Zhang (CS, Fall 2006, co-supervised with Sunil Prabhakar), moved on to Microsoft

Current Graduate Students

Chao Yuan (PULSe, Purdue Life Science Program) 2009-
Meghana Chitale (CS) 2006-
Ishita Khan (CS) 2011-
Juan Esquivel-Rodriguez (CS) 2008-
Mingjie Tang (CS) 2010-
Muyi Liu (PULSe) 2011-

Current Undergraduate Students

Shing Jay Ong (CS) Fall 2011-
Yingfei Ma (Stat) Spring 2011-
Shucong Zhang (CS) Fall 2011-
Pratik Mathran (CS) Fall 2011-
Su Lin Ooi (CS) Fall 2011-
Mi-sun Kong (Biol) Fall 2011-

Former Undergraduate Students

Over 65 students (2003-current)

Former Undergraduate Students who entered bioinformatics graduate program

Stan Luban (Biol/CS, graduated 2006) UC San Diego
Steven Ahrendt (CS, graduated 2009) UC Riverside
Priyanka Surana (Biol, graduated 2010) Iowa State University
Sangwook Lee (Biol, graduated 2010) Georgetown University
Satwica Yersini (intern, Vellore Inst Tech, India, 2011) Indiana University

Former Intern graduate students

Mario Alfy Messih, July-August 2011, King Abdullah University, Saudi Arabia
Michal Jamroz, Nov. 2010 – May 2011, Dept. of Chemistry, Warsaw University, Poland.
Through the International PhD Study in Chemistry Program of Dept. of Chemistry,
Warsaw University
Rayan Chikhi, Summer 2007, MS in Computer Science, Ecole Normale, France

K-12 Students

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

Student Awards

- Meghana Chitale (CS) AFP/CAFA 2011 travel fellowship, for attending Automatic Function Prediction Special Interest Group (SIG), Vienna, Austria, May, 2011
- Meghana Chitale (CS), ISMB 2011 travel fellowship for attending ISMB/ECCB, Vienna, Austria, May 2011.
- Juan Esquivel-Rodriguez (CS), ISMB 2011 travel fellowship for attending ISMB/ECCB, Vienna, Austria, May 2011.
- Meghana Chitale (CS), Bilsland Dissertation Fellowship by the Purdue Graduate School, April, 2011.
- Meghana Chitale (CS), travel grant from the Women in Science Programs, Purdue University, for attending the Critical Assessment of Function Annotations (CAFA) at ISMB, Vienna, Austria, July 2011.
- 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), 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), 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). 2nd place in 2004 Purdue University's Burton D. Morgan Entrepreneurship Competition

Courses Taught

CS590 Computing for Life Sciences, core course in the Computing in Life Science CLS Specialization for graduate program (Fall 2011)

CS590-006 Computing for Life Sciences II (Fall 2009, Fall 2010)

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 2006-2010, 2012)

BIOL696E Seminar Crystallography (Spring 2006)

Other Teaching Activities

- Guest lecture at CS591, honor research course (Fall 2011)
- Selected as a participating lab for the International PhD Study in Chemistry Program of Dept. of Chemistry, Warsaw University, Poland (2010).
- Guest lecture at Japanese graduate student association, Purdue University, March 15, 2011
- Coordinator, CS497 honors research, Fall 2010
- 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

- Journal of Data Mining in Genomics & Proteomics (November 2010 -)
- 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

Domestic:

- National Science Foundation, Molecular Cellular Biosciences (MCB) (November 2011)
- National Science Foundation, Molecular Cellular Biosciences (MCB) (April 2011)
- National Science Foundation, Molecular Cellular Biosciences (MCB) (March 2011)
- 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)
- Louisiana Board of Regents' Research Competitiveness Subprogram, EPSCoR-style grants program (November, 2009)

International:

- The Wellcome Trust, UK/Dept. of Biotechnology India Alliance, Intermediate fellowship (September 2011)
- National Science Centre, Polish Narodowe Centrum Nauki, Poland (August 2011)
- Agency of Science, Research & Technology (A*STAR), Singapore (August 2011)
- Agency of Science, Research & Technology (A*STAR), Singapore (November, 2010)
- Luxembourg National Research Fund (FNR), CORE programme (August 2010)
- External reviewer of the Council for the Earth and Life sciences, Netherlands Organization for Scientific Research, Netherlands. (March, 2006)

Review of Papers

- reviewer of
Annals of Biomedical Engineering, Amino Acids
Bioinformatics, Biophysical Journal, Biopolymers, Biophysics (Japan)
Briefings in Bioinformatics, Briefings in Functional Genomics and Proteomics
BMC Bioinformatics, BMC Structural Biology, BMC Systems Biology
Cancer Informatics, Cell Research, Current Protein and Peptide Science, DNA Research
FEBS Letters, Future Medicinal Chemistry, Genetica,
Journal of Computational Chemistry, Journal of Bioinformatics and Computational Biology
IEEE Transactions on Information Technology in Biomedicine
International Journal of Data Mining and Bioinformatics (IJDMB)
ISMB (International Conference on Intelligent Systems for Molecular Biology)
Nucleic Acid Research, Neural Computing & Applications,
Parallel Computing, Protein Science, Proteins: Structure, Function, Bioinformatics
PLoS Computational Biology, PLOS ONE
Statistical applications in Genetics and Mol Biol.
The Pacific Symposium on Biocomputing (PSB)
- Number of reviewed papers: 2008: 20, 2009: 21, 2010: 21, 2011 (August): 35

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 bioinformatics textbook to be published from Garland Science (Nov. 2011)
- Proposal for a third edition of a bioinformatics textbook to be published from Wiley (Nov. 2010)
- 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

- Advisory Committee, Great Lakes Bioinformatics Conference 2012, Univ. of Michigan, Ann Arbor, Michigan, May 15-17, 2012
- BIOTECHNO2012: The Fourth International Conference on Bioinformatics, Biocomputational Systems and Biotechnologies, St. Maarten, Netherlands Antilles, March 25-29, 2012.
- ICDM 2011 the IEEE International Conference on Data mining, Workshop on “Biological Data mining and its applications in healthcare”, Vancouver, Canada, Dec 11-14, 2011
- ACM Conference on Bioinformatics, Computational Biology and Biomedicine, Chicago, IL, August 1-3, 2011
- 11th IEEE International Symposium on Bioinformatics and Bio Engineering (BIBE 2011), Taichung, Taiwan, October 24-26, 2011
- Session chair, 3D-SIG, ISMB, Vienna, Austria, July 15-16, 2011
- Steering committee member, Great Lakes Bioinformatics Conference 2011, Athens, Ohio, May 2-4, 2011
- 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
- Organizer (with Barry Wanner, Michael Gribskov, Dawn Whitaker), IECA Functional Genomics Mini-symposium, Purdue University, April 17, 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 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
- 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 7th International Symposium on Bioinformatics & BioEngineering (BIBE07), Boston, MA, October 14-17, 2007
- 7th 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:

- Departmental representative for Computational Life Sciences (CLS) program (2010-)
- Graduate School Admission Committee 2005-6, 2009-2010, 2011-2012
- Graduate and advanced studies committee, 2011-2012
- Review committee of Biophysics Training Grant, June, 2011
- Bioinformatics and Biotechnology Advisory 2005-6, 2006-7
- 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