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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

2014.8-present	Full Professor
2015.1-2015.8	Visiting Scientist , Eli Lilly, Indianapolis
2009.8-2014.8	Associate professor
2003.8-2009.8	tenure-track Assistant professor Purdue University, West Lafayette, Indiana Department of Biological Sciences/Computer Sciences (joint appointment)
2002.9-2003.7	Senior Postdoctoral Research Associate Advisor: Jeffrey Skolnick Buffalo Center of Excellence in Bioinformatics, Buffalo, NY, USA
1999-2002.9	Postdoctoral Research Associate Advisor: Jeffrey Skolnick Donald Danforth Plant Science Center, St. Louis, MO, USA
1998-1999	Research Assistant Bioinformatics Center Institute for Chemical Research, Kyoto University, Japan

Awards

- Showalter University Faculty Scholar, Purdue University, 2013-2018
- The Seed of Success Award (earned a grant over \$1M/year), Purdue University, 2005, 2006, 2007, 2008, 2010, 2012, 2014
- Best Oral Presentation Award “Origin of protein superfamily and superfolds”, 3D-SIG 2015, an ISMB satellite meeting on Structural Bioinformatics and Computational Biophysics, Dublin, Ireland, July 10-11, 2015

- Best paper award, Great Lakes Bioinformatics Conference (GLBIO) 2011 (an official conference of the International Society for Computational Biology, ISCB), May 1-3, 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 (GIW2010), December, 2010

Publications

- [145] Computing and visualizing gene function similarity and coherence with NaviGO.
Z. Ding, Q. Wei, & D. Kihara
Methods in Mol. Biol., in press (2018)
- [144] Virtual ligand screening using PL-PatchSurfer2, a molecular surface-based protein-ligand docking method.
W. H. Shin & D. Kihara
Methods in Mol. Biol., in press (2018)
- [143] Recent computational methods for predicting protein-protein interactions using various protein features.
Z. Ding & D. Kihara.
Current Protocols, in press (2018)
- [142] Application of machine learning techniques for prediction of the isoform specificity of cytochrome P450 substrates.
Y. Xiong, Y. Qiao, D. Kihara, H. Y. Zhang, X. Zhu, & D. Q. Wei
Current Drug Metabolism, In revision, (2018)
- [141] Modeling the assembly order of multimeric heteroprotein complexes
L. X. Peterson, Y. Togawa, J. Esquivel-Rodriguez, G. Terashi, C. Christoffer, A. Roy, W. H. Shin, & D. Kihara
PLOS Comp. Biol., in press (2018)
- [140] Protein 3D structure and electron microscopy map retrieval using 3D-SURFER2.0 and EM_SURFER.
X. Han, Q. Wei, & D. Kihara
Current Protocols, 60: 3.14.1-3.14.15 (2017)
- [139] An interactive compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes.
S. Chiba, T. Ishita, K. Ikeda, M. Mochizuki, R. Teramoto, Y.H. Taguchi, M. Iwadate, H. Umeyama, C. Ramakrishnan, A.M. Thangakani, D. Velmurugan, M.M. Gromiha, T.Okuno, K. Kato, S. Minami, G. Chikenji, S.D. Suzuki, K. Yanagisawa, Woong-Hee Shin, Daisuke Kihara, K.Z. Yamamoto, Y. Moriwaki, N. Yasuo, R. Yoshino, S. Zozulya, P. Borysko, R. Stavniichuk, T. Honma, T. Hirokawa, Y. Akiyama, & M. Sekijima
Scientific Reports, 7: 12038 (2017)
- [138] Improved performance in CAPRI round 37 using LZerD docking and template-based modeling with combined scoring functions.
L. X. Peterson, W. H. Shin, H. Kim, & D. Kihara
Proteins: Structure, Function, and Bioinformatics, in press (2017)
- [137] Protein structure model refinement in CASP12 using short and long molecular dynamics simulations in implicit solvent.
G. Terashi & D. Kihara
Proteins: Structure, Function, and Bioinformatics, in press (2017)
- [136] In silico structure-based approaches to discover protein-protein interaction targeting drugs.
W. H. Shin, C. Christoffer, & D. Kihara
Methods, 131: 22-32 (2017)
- [135] SHREC'17 Track: Protein shape retrieval.

- N. Song, D. Craciun, C. W. Christoffer, X. Han, D. Kihara, G. Levieux, M. Montes, H. Qin, P. Sahu, G. Terashi, & H. Liu, Eurographics Workshop on 3D Object Retrieval, I. Pratikakis, F. Dupont, & M. Ovsjanikov (Eds.) (2017)
- [134] MPFit: Computational tool for predicting moonlighting proteins.
I.K. Khan, J. McGraw, & D. Kihara
Methods in Mol. Biol. 1611: 45-57 (2017).
- [133] Using PFP and ESG protein function prediction webservers.
Q. Wei, J. McGraw, I. Khan, & D. Kihara.
Methods in Mol. Biol. 1611: 1-14 (2017).
- [132] DextMP: Deep dive into Text for predicting Moonlighting Proteins.
I. K. Khan, M. Bhuiyan, & D. Kihara
Bioinformatics (ISMB 2017), i83-i91 (2017)
- [131] Modeling disordered protein interactions from biophysical principles.
L. X. Peterson, A. Roy, C. Christoffer, G. Terashi, & D. Kihara.
PLOS Comp. Biol., 13: e1005485 (2017)
- [130] Exploring structure-function relationships in moonlighting proteins.
S. Das, I. Khan, D. Kihara, & C. Orengo.
Moonlighting Proteins: Novel Virulence Factors in Bacterial Infections. B. Henderson (ed.) Chapter 2, pp. 21-44, Wiley-Blackwell
- [129] NaviGO: Interactive tool for visualization and functional similarity and coherence analysis with gene ontology.
Q. Wei, I. Khan, Z. Ding, S. Yerneni, & D. Kihara.
BMC Bioinformatics, 18: 177 (2017).
- [128] Variability of protein structural models from electron microscopy.
L. Monroe, G. Terashi, & D. Kihara
Structure, 25: 592-602 (2017)
- [127] Prediction of local quality of protein structure models considering spatial neighbors in graphical models.
W.H. Shin, X. Kang & D. Kihara.
Scientific Reports, 7: 40629 (2017).
- [126] BindML/BindML+: Detecting protein-protein interaction interface propensity from amino acid substitution patterns.
Q. Wei, D. La, & D. Kihara.
Methods in Mol. Biol., 1529: 279-289 (2017)
- [125] Predicting real-valued protein residue fluctuation using FlexPred.
Lenna X. Peterson, Michal Jamroz, Andrzej Kolinski, & Daisuke Kihara
Methods in Mol. Biol., 1484: 175-186 (2017)
- [124] Discovery of nicotinamide adenine dinucleotide binding proteins in the Escherichia coli proteome using a combined energetic- and structural-bioinformatics-based approach.
L. Zeng, W.H. Shin, X. Zhu, S.H. Park, C. Park, W.A. Tao, & D. Kihara
J. Proteome Res. 16: 470-480 (2017)
- [123] Human and server docking prediction for CAPRI round 30-35 using LZerD with combined scoring functions.
L.X. Peterson, H. Kim, J. Esquivel-Rodriguez, A. Roy, X. Han, W.H. Shin, J. Zhang, G. Terashi, M. Lee, & D. Kihara.
Proteins: Structure, Function, and Bioinformatics, 85: 513-527 (2017).
- [122] A study of the Boltzmann sequence-structure channel.
Proceedings of the IEEE Inst. Electr. Electron. Eng. 105: 286-306 (2017)
(Original version) The Boltzmann sequence-structure channel.
A. Magner, D. Kihara, & W. Szpankowski.
IEEE International Symposium on Information Theory, 255-259, (2016).

- [121] PL-PatchSurfer2: Improved local surface matching-based virtual screening methods that is tolerant to target and ligand structure variation.
W.H. Shin, C. Christoffer, J. Wang, & D. Kihara.
J. Chem. Inf. Model. 56: 1676-1691 (2016).
- [120] Missing gene identification using functional coherence scores.
M. Chitale, I. K. Khan, & D. Kihara
Scientific Reports, 6: 31275 (2016)
- [119] An expanded evaluation of protein function prediction methods shows an improvement in accuracy.
Y. Jian, I. K. Khan, D. Kihara, I. Friedberg, & P. Radivojac. (147 authors)
Genome Biology, 17: 184 (2016).
- [118] Ranking protein-protein docking models using steered molecular dynamics and potential of mean force calculations.
L. J. Kingsley, J. Esquivel-Rodriguez, D. Kihara, & M A. Lill.
J. Comp. Chem., 37: 1861-1865 (2016).
- [117] Genome-scale prediction of moonlighting proteins using diverse protein association information.
I. K. Khan & D. Kihara.
Bioinformatics, 32: 2281-2288 (2016).
- [116] Ensemble-based evaluation for protein structure models.
M. Jamroz, A. Kolinski, & D. Kihara.
Bioinformatics (ISMB 2016), 32: i314-i321 (2016)
- [115] Energetic coupling between ligand binding and dimerization in E. coli phosphoglycerate mutase.
N.W. Gardner, L.K. Monroe, D. Kihara, & C. Park
Biochemistry, 55: 1711-1723 (2016)
- [114] Computational protein function predictions.
D. Kihara
Methods, 93: 1-2 (2016)
- [113] Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: CASP-CAPRI experiment.
M.F. Lensink, L.X. Peterson, H.R. Kim, A. Roy, J. Esquivel-Rodriguez, D. Kihara, & S. J. Wodak. (98 authors)
Proteins: Structure, Function, and Bioinformatics, 84 (Suppl 1): 323-348 (2016).
- [112] PatchSurfers: Programs for local molecular property-based binding ligand prediction.
W.H. Shin, M.G. Bures, & D. Kihara
Methods, 93: 41-50 (2016)
- [111] Combined approach of Patch-Surfer and PL-PatchSurfer for protein-ligand binding prediction in CSAR 2013 and 2014.
X. Zhu, W.H. Shin, H.R. Kim, & D. Kihara
J. Chem. Inf. Model. 56: 1088-1099 (2015)
- [110] Protein structure prediction using residue- and fragment- environment potentials in CASP11.
H.R. Kim & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 84 (Suppl 1): 105-117 (2016).
- [109] IAS: Interaction specific GO term associations for predicting protein-protein interaction networks.
S. Yerneni, I. K. Khan, Q. Wei & D. Kihara
IEEE Transactions on Computational Biology and Bioinformatics, DOI: 10.1109/TCBB.2015.2476809 (2015)
- [108] PFP and ESG protein function prediction methods in 2014: Effect of database updates and ensemble approaches.
I.K. Khan, Q. Wei, S. Chapman, Dukka, B.K.C., & D. Kihara
GigaScience, 4: 43. (2015)

- [107] Tuning of pectin methylesterification: PECTIN METHYLESTERASE INHIBITOR 7 modulates the processive activity of co-expressed PME3 in a pH-dependent manner. F. Sénéchal, M. L'Enfant, J. M. Domon, E. Rosiau, M. J. Crépeau, O. Surcouf, J. Esquivel-Rodriguez, P. Marcelo, A. Mareck, F. Guérineau, H. R. Kim, J. Mravec, E. Bonnin, E. Jamet, D. Kihara, P. Lerouge, M. C. Ralet, J. Pelloux, & C. Rayon. *J. Biol. Chem.* 290: 23320-23335 (2015)
- [106] Three-dimensional compound comparison methods and their application in drug discovery. W.-H. Shin, X. Zhu, M.G. Bures, & D. Kihara. *Molecules*, 20: 12841-12862. (2015)
- [105] Navigating 3D electron microscopy maps with EM-SURFER. J. Esquivel-Rodriguez, Y. Xiong, X. Han, S. Gang, C. Christoffer, & D. Kihara *BMC Bioinformatics*, 16: 181 (2015)
- [104] On the origin of protein superfamily and superfolds. A. Magner, W. Szpankowski, & D. Kihara *Scientific Reports*, 5: 8166 (2015)
- [103] Structure and inhibition of EV-D68, a virus that causes respiratory illness in children. Y. Liu, J. Sheng, A. Fokine, G. Meng, W.-H. Shin, F. Long, R.J. Kuhn, D. Kihara, & M.G. Rossmann *Science* 347: 71-74 (2015)
- [102] GenoBase: comprehensive resource database of Escherichia coli K-12. Y. Otsuka, A. Muto, R. Takeuchi, M. Ishikawa, K. Nakamura, N. Yamamoto, H. Dose, K. Nakahigashi, S. Tanishima, S. Suharnan, W. Nomura, T. Nakayashiki, W.G. Aref, B.R. Bochner, T. Conway, M. Gribskov, D. Kihara, K.E. Rudd, Y. Tosato, B.L. Wanner, & H. Mori *Nuc. Acid. Res.* 43: D606-D617 (2015)
- [101] Large-scale binding ligand prediction by improved patch-based method PatchSurfer2.0 X. Zhu, Y. Xiong, & D. Kihara *Bioinformatics*, 31: 707-713 (2015)
- [100] PFP/ESG: Automated protein function prediction servers enhanced with Gene Ontology visualization tool. I. Khan, Q. Wei, M. Chitale, & D. Kihara *Bioinformatics*, 31: 271-272 (2015)
- [99] Genome-scale identification and characterization of moonlighting proteins. I. Khan, Y. Chen, T. Dong, X. Hong, R. Takeuchi, H. Mori, & D. Kihara *Biology Direct*, 9:30 (2014)
- [98] Computational characterization of moonlighting proteins. I. Khan & D. Kihara *Biochem Soc. Trans.* 42: 1780-1785 (2014)
- [97] A proteomic strategy for global analysis of plant protein complexes. U.K. Aryal, Y. Xiong, Z. McBride, D. Kihara, J. Xie, M.C. Hall, & D.B. Szymanski *Plant Cell*, 26: 3867-3882 (2014)
- [96] PL-PatchSurfer: A novel molecular local surface-based method for exploring protein-ligand interactions. B. Hu, X. Zhu, L. Monroe, M. Bures, & D. Kihara *International Journal of Molecular Science*, 15: 15122-15145 (2014)
- [95] Small-angle x-ray scattering reveals three-dimensional surface structures of dimers of the catalytic and zinc-finger domains of cellular synthase. A.T. Orek, C. J. Rayon, L. Makowski, P. Ciesielski, L. Paul, H.R. Kim, S. Ghosh, D. Kihara, M. Crowkey, M. Himmel, J. Bolin, & C. Carpita. *Plant Cell*, 26: 2996-3009 (2014).
- [94] Detecting local residue environment similarity for recognizing near-native structure models. H.R. Kim & D. Kihara. *Proteins: Structure, Function, and Bioinformatics*, 82: 3255-3272 (2014).

- [93] Comparison of image patches using local moment invariants.
A. Sit & D. Kihara
IEEE Transactions on Image Processing, 23: 2369-2379 (2014)
- [92] Protein side-chain conformation prediction accuracy in different residue environments.
L.X. Peterson, X. Kang & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 82: 1971-1984 (2014)
- [91] Pairwise and multimeric protein-protein docking using the LZerD program suite.
J. Esquivel-Rodriguez, V. Filos-Gonzalez, B. Li & D. Kihara.
Methods in Molecular Biology, 1137: 209-234 (2014)
- [90] 3D-SURFER 2.0. Web platform for real-time search and characterization of protein surfaces.
Y. Xiong, J. Esquivel-Rodriguez, L. Sael, & D. Kihara.
Methods in Molecular Biology, 1137: 105-117 (2014)
- [89] Efficient strategy for detecting gene x gene joint action and its application in schizophrenia.
S. Won, M.S. Kwon, M. Mattheisen, S. Park, C. Park, D. Kihara, S. Chichon, R. Ophoff, M.M. Nothen, M. Rietschel, M. Baur, & C. Lange.
Genet Epidemiology 38: 60-71 (2014)
- [88] Structure-function analysis of the DNA translocating portal of the bacteriophage T4 packing machine.
V. Padilla-Sanchez, S. Gao, H.R. Kim, D. Kihara, L. Sun, M.G. Rossmann, & V.B. Rao.
J. Mol. Biol. 426: 1019-1038 (2014)
- [87] Computational methods for constructing protein structure models from 3D electron microscopy maps.
J. Esquivel-Rodríguez & D. Kihara.
J Struct Biol. 184: 93-102 (2013)
- [86] Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions.
R. Moretti, ,, J. Esquivel-Rodriguez, D. Kihara, ,,, D. Baker (70 authors)
Proteins: Struct, Funct., Bioinformatics, 81: 1980-1987 (2013)
- [85] Ligand binding site identification.
Y. Xiong, X. Zhu, & D. Kihara
In silico Drug Discovery and Design Techniques. M. Lill (eds), Chapter 16, pp. 204-220, Future Science, London, UK (2013)
- [84] Characterization and prediction of human protein-protein interactions.
Y. Xiong, D. Syzmanski, & D. Kihara
Biological Data Mining and Its Applications in Healthcare, X.-L. Li, S.-K. Ng, & J.T.L. Wang (eds), Chapter 9, pp. 237-261, World Scientific, New Jersey, USA, (2013)
- [83] A large-scale evaluation of computational protein function prediction.
P. Radivojac,,, M. Chitale, D. Kihara, ,, & I. Friedberg (100 authors)
Nature Methods, 10: 221-227 (2013)
- [82] In-depth performance evaluation of PFP and ESG sequence-based function prediction methods in CAFA 2011 experiment.
M. Chitale, I. Khan, & D. Kihara
BMC Bioinformatics, 14 (Suppl 3): S2 (2013)
- [81] Predicting permanent and transient protein-protein interfaces.
D. La, M. Kong, W. Hoffman, Y.I. Choi & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 81: 805-818 (2013)
- [80] 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, Chapter 9, pp. 191-224, Wiley. (2013)
- [79] Effective inter-residue contact definitions for accurate protein fold recognition.
C. Yuan, H. Chen, & D. Kihara

- BMC Bioinformatics*, 13: 292 (2012)
- [78] Effect of conformation sampling strategies in genetic algorithm for multiple protein docking.
J. Esquivel-Rodriguez & D. Kihara
BMC Proceedings, 7:S6 (2012)
- [77] Evaluation of function predictions by PFP, ESG, and PSI-BLAST for moonlighting proteins.
I. Khan, M. Chitale, C. Rayon, & D. Kihara
BMC Proceedings, 7:S5 (2012)
- [76] Protein domain recurrence and order can enhance prediction of protein functions.
M.A. Messih, M. Chitale, V.B. Bajic, D. Kihara*, & X. Gao* (* co-corresponding authors)
Bioinformatics, 28: i440-i450 (2012)
- [75] Multi-LZerD: Multiple protein docking for asymmetric complexes.
J. Esquivel-Rodriguez, Y.D. Yang, & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 80: 1818-1833. (2012)
- [74] Fitting multimeric protein complexes into electron microscopy maps using 3D Zernike descriptors.
J. Esquivel-Rodriguez, & D. Kihara
Journal of Physical Chemistry B, 116: 6854-6861 (2012)
- [73] Formyl-coenzyme A (CoA):oxalate CoA-transferase from the acidophile *Acetobacter acetii* has a distinctive electrostatic surface and inherent acid stability.
E.A. Mullins, C.M. Starks, J.A. Francois, L. Sael, D. Kihara, & T.J. Kappock,
Protein Science, 21: 686-696 (2012)
- [72] Structural features that predict real-value fluctuations of globular proteins.
M. Jamroz, A. Kolinski, & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 80: 1425-1435 (2012)
- [71] Structure- and sequence-based function prediction for non-homologous proteins.
L. Sael, M. Chitale, & D. Kihara
Journal of Structural and Functional Genomics, 13: 111-123 (2012)
- [70] Protein docking prediction using predicted protein-protein interface.
B. Li & D. Kihara
BMC Bioinformatics, 13: 7 (2012)
- [69] Detecting local ligand-binding site similarity in non-homologous proteins by surface patch comparison.
L. Sael & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 80: 1177-1195 (2012)
- [68] Constructing patch-based ligand-binding pocket database for predicting function of proteins.
L. Sael & D. Kihara
BMC Bioinformatics, 13: S7 (2012)
- [67] Evaluation of multiple docking structures using correctly predicted pairwise subunits.
J. Esquivel-Rodriguez & D. Kihara
BMC Bioinformatics, 13: S6 (2012)
- [66] A novel method for protein-protein interaction site prediction using phylogenetic substitution models.
D. La & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 80: 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, pp. 145-163. Springer-Verlag
(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, pp. 19-34Springer-Verlag
(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, , pp. 1-17, Springer-Verlag
(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] Improved protein surface comparison and application to low-resolution protein structure data.
L. Sael, & D. Kihara
BMC Bioinformatics 11: S2 (2010)
- [52] Sub-AQUA: Real-value quality assessment of protein structure models.
Y.D. Yang, P. Spratt, H. Chen, C. Park, & D. Kihara
PEDS: Protein Engineering Design & Selection, 23: 617-632 (2010)
- [51] Functional enrichment analyses and construction of functional similarity networks with high
confidence function prediction by PFP.
T. Hawkins, M. Chitale, & D. Kihara
BMC Bioinformatics, 11: 265 (2010)
- [50] Application of 3D Zernike descriptors to shape-based ligand similarity searching.
V. Venkatraman, P.R. Chakravarthy & D. Kihara
J. Cheminformatics, 1: 19. (2009)
- [49] Real-time ligand binding pocket database search using local surface descriptors.

- R.Chikhi , L. Sael, & D. Kihara
Proteins: Structure, Function, and Bioinformatics, 78: 2007-2028, (2010).
- [48] Protein-protein docking using region-based 3D Zernike descriptors.
 V. Venkatraman, Y.D. Yang, L. Sael & D. Kihara
BMC Bioinformatics, 10: 407. (2009)
- [47] Error estimation of template-based protein structure models.
 D. Kihara, Y.D. Yang & H. Chen.
 Multiscale approaches to protein modeling: structure prediction, dynamics, thermodynamics and macromolecular assemblies. Andrzej Kolinski (ed.) , Springer-Verlag, Chapter 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, 1: 32-47. (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.
*Omic*s, 11(1), 58-73. (2007)
- [25] EMD: An ensemble algorithm for discovering regulatory motifs in DNA sequences.
Jianjun Hu, Yifeng D Yang & Daisuke Kihara
BMC Bioinformatics 7: 342. (2006)
- [24] Protein function prediction in proteomics era.
Daisuke Kihara, Troy Hawkins, Stan Luban, Bin Li, K. Ramani & Manish Agrawal.
Proceedings of Frontiers of Computational Science, Y Kaneda et al. eds., pp. 143-148,
Springer-Verlag, Berlin, Heidelberg (2007).
- [23] Statistical potential based amino acid similarity matrices for aligning distantly related protein sequences.
Yen Hock Tan, He Huang & Daisuke Kihara
Proteins: Structure, Funct. Bioinformatics, 64: 587-600. (2006)
- [22] Enhanced automated function prediction using distantly related sequences and contextual association by PFP.
Troy Hawkins, Stan Luban & Daisuke Kihara.
Protein Science, 15: 1550-1556. (2006)
- [21] Bioinformatics resources for cancer research with an emphasis on gene function and structure prediction tools.
Daisuke Kihara, Yifeng D. Yang & Troy Hawkins
Cancer Informatics, 2: 25-35. (2006)
- [20] The effect of long-range interactions on the secondary structure formation of proteins.
Daisuke Kihara
Protein Science, 14: 1955-1963. (2005)
- [19] Limitations and Potentials of Current Motif Finding Algorithms.
Jianjun Hu, Bin Li and Daisuke Kihara

- Nucleic Acid. Res.* 33:4899-4913. (2005)
- [18] Biomolecular Structure Databases.
Daisuke Kihara.
Genome Function Research Handbook, Chapter 2. pp. 73-81. Yodosha Publishers, Tokyo, Japan. (2004).
- [17] Development and large scale benchmark testing of the PROSPECTOR 3.0 threading algorithm.
Jeffrey Skolnick, Daisuke Kihara and Yang Zhang.
Proteins: Structure, Funct. Bioinformatics 56:502-518. (2004)
- [16] Microbial genomes have over 72% structure assignment by the threading algorithm PROSPECTOR_Q.
Daisuke Kihara and Jeffrey Skolnick.
Proteins: Structure, Funct. Bioinformatics 55: 464-473 (2004)
- [15] The PDB is a covering set of small protein structures.
Daisuke Kihara and Jeffrey Skolnick.
J. Mol. Biol. 334: 793-802 (2003)
- [14] TOUCHSTONE: a unified approach to protein structure prediction.
Jeffrey Skolnick, Yang Zhang, Adrian Arakaki, Andrzej Kolinski, Michael Boniecki, Andras Szilagyi and Daisuke Kihara.
Proteins: Structure, Funct. Genet. 53: Suppl.6: 469-479 (2003)
- [13] TOUCHSTONEX: Protein Structure Prediction Using Sparse NMR Data.
Wei Li, Yang Zhang, Daisuke Kihara, Yuanpeng J. Huang, Deyou Zheng, Gaetano T. Montelione, Andrzej Kolinski, and Jeffrey Skolnick.
Proteins: Structure, Funct. Genet. 53: 290-306 (2003)
- [12] Local Energy Landscape Flattening: Parallel Hyperbolic Monte Carlo Sampling of Protein Folding.
Yang, Zhang, Daisuke Kihara and Jeffrey Skolnick
Proteins: Structure, Funct. Genet. 48: 192-201 (2002)
- [11] Ab initio Protein Structure Prediction on a Genomic Scale: Application to the *Mycoplasma genitalium* Genome.
Daisuke Kihara, Yang Zhang, Hui Lu, Andrzej Kolinski and Jeffrey Skolnick
Proc. Natl. Acad. Sci. USA, 99: 5993-5998 (2002)
- [10] Ab initio Protein Structure Prediction via a Combination of Threading, Lattice Folding, Clustering, and Structure Refinement.
Jeffrey Skolnick, Andrzej Kolinski, Daisuke Kihara, Marcos Betancourt, Piotr Rotkiewicz and Michael Boniecki
Proteins: Structure, Funct. Genet. 45 (Suppl 5): 149-156 (2001)
- [9] Genome Databases on the Internet.
Daisuke Kihara
Tanpakushitsu Kakusan Koso (Protein, Nucleic Acid and Enzyme)
46 (16 Suppl): 2639-2645 (2001)
- [8] Prediction of Membrane Proteins in Post-Genomic Era.
Daisuke Kihara and Minoru Kanehisa
Recent Res. Developments in Protein Engng. 1: 179-196 (2001)
- [7] TOUCHSTONE: An ab initio Protein Structure Prediction Method that Uses Threading-based Tertiary Restraints.
Daisuke Kihara, Hui Lu, Andrzej Kolinski and Jeffrey Skolnick
Proc. Natl. Acad. Sci. USA 98: 10125-10130 (2001)
- [6] Generalized Comparative Modeling (GENECOMP): A Combination of Sequence Comparison, Threading, and Lattice Modeling for Protein Structure Prediction and Refinement.
Andrzej Kolinski, Marcos Betancourt, Daisuke Kihara, Piotr Rotkiewicz and Jeffrey Skolnick
Proteins: Structure, Funct. Genet. 44: 133-149 (2001)

- [5] Defrosting the Frozen Approximation: PROSPECTOR – A New Approach to Threading.
Jeffrey Skolnick and Daisuke Kihara
Proteins: Structure, Funct. Genet. 42: 319-331 (2001)
- [4] Tandem Cluster of Membrane Proteins in Complete Genome Sequences.
Daisuke Kihara and Minoru Kanehisa
Genome Res. 10: 731-743 (2000)
- [3] The Genome Projects and Bioinformatics.
Daisuke Kihara and Minoru Kanehisa.
Iwanami Kouza (Iwanami Lecture Series): Gendai Igaku no Kiso (The Basis of Modern Medical Science), vol.1, Chap.11, pp: 215-235, Iwanami Shoten Publishers, Tokyo Japan (1998)
- [2] Prediction of Membrane Proteins Based on Classification of Transmembrane Segments.
Daisuke Kihara, Toshio Shimizu and Minoru Kanehisa
Protein Engng., 11: 961-970 (1998)
- [1] Internet Resources for Genome Research.
Daisuke Kihara, Minoru Kanehisa and Toshihisa Takagi.
Tanpakushitsu Kakusan Koso (Protein, Nucleic Acid and Enzyme), 42(17 Suppl): 3090-3099 (1997)

Books

- [3] Protein function prediction, *Methods in Molecular Biology*, D. Kihara (ed.) Springer, (2017)
- [2] Protein structure prediction (3rd Edition), *Methods in Molecular Biology*, D. Kihara (ed.) Springer, (2014)
- [1] Protein function prediction for omics era, D. Kihara, (ed.) Springer, (2011)

Miscellaneous Publication:

- [2] The International Society of Computational Biology presents: the Great Lakes Bioinformatics Conference, May 16-18, 2014, Cincinnati, Ohio.
J. Cavalcoli, L. Welch, B. Aronow, S. Draghici, & D. Kihara
Bioinformatics, 30: 148-149 (2014)
- [1] WWW Homepages for Biophysicists. Part 1-6.
Biophysics (Japan) (1996-1998)
(Short columns for bioinformatics tools)

Invited/Selected Oral Presentations

- [187] Computational protein structure modeling for medium to low resolution cryo-electron microscopy density maps, Dept. of Biochemistry, Purdue, Jan. 16, 2018
- [186] Structure modeling of disordered protein interactions, the 4th International conference on protein & RNA structure prediction, Montego Bay, Jamaica, Dec. 5-8, 2017
- [185] Modeling report at CryoEM Structure Challenges Workshop, Stanford Univ., CA, Oct 6-8, 2017
- [183-4] 25th Intelligent Systems for Molecular Biology (ISMB) 2017, Prague, Czech Republic, July 21-25, 2017
- 3DSIG, (Keynote): Protein bioinformatics of low-resolution structural data
 - DextMP: Deep dive into text for predicting moonlighting proteins, I. Khan, M. Bhuiyan, & D. Kihara
- [182] Computational modeling of various types of protein complexes, July 14, 2017, AIST, Tokyo, Japan
- [181] In silico screening of biomolecules, July 12, 2017, Ono Pharmaceutical, Kyoto, Japan

- [180] Molecular surface-based in silico screening of biomolecules, July 10, 2017, Teijin-Pharma, Tokyo, Japan
- [179] Global analysis of native protein complexes in *Cyanothecosp. ATCC 51142* using label-free quantitative proteomic profiling, U. Aryal, V. Hedrick, T. Sobreira, C. Ferreira, Z. Ding, D. Kihara, L. Sherman, Annual Conference of American Soc. for Mass Spectrometry, Indianapolis, IN, June 4-8, 2017
- [178] Computational modeling of flexible protein-protein and protein-drug interactions, Computational Biophysics to Systems Biology (CBSB2017), Cincinnati, Ohio, May 18-20, 2017
- [174-7] Great Lakes Bioinformatics Conference (GLBIO) 2017, The Univ. Illinois at Chicago, Chicago, IL, May 15-17, 2017
- Phylo-PFP: Highly accurate phylogenomics-based protein function prediction method, A. Jain & D. Kihara
 - Variability of protein structure models from electron microscopy, L. Monroe, G. Terashi, & D. Kihara
 - Molecular surface-based screening methods for repurposing drugs: application to find novel NAD binders in the *E. coli* proteome, W. H. Shin, L. Zhang, X. Zhu, S. H. Park, C. Park, W. A. Tao, & D. Kihara
 - MAINMAST: Building main-chain models for medium resolution electron microscopy maps, G. Terashi & D. Kihara
- [172-3] Hitchhikers' Guide to the Biomolecular Galaxy, Purdue University, May 10-11, 2017
- Phylo-PFP: Highly accurate phylogenomics-based protein function prediction method, A. Jain & D. Kihara
 - Variability of protein structure models from electron microscopy, L. Monroe, G. Terashi, & D. Kihara
- [171] Structure of the catalytic domain of a plant CesaA, P. S. Rushton, C. Rayon, A. T. Olek, L. Makowski, H. Kim, J. Badger, D. Kihara, C. N. Steussy, C. Stauffacher, & N. Carpita, 253rd ACS National Meeting, April 2-6, 2017
- [170] In silico screening and modeling of protein-drug and protein-protein interactions, Albert Einstein College of Medicine, New York, NY, Jan. 24, 2017
- [169] 12th Critical Assessment of Techniques for Protein Structure Prediction (CASP12) Evaluation meeting, CAPRI docking & Quality assessment round table Gaeta, Italy, December 10-13, 2016
- [168] In silico screening and modeling of protein-drug and protein-protein interactions, Biomedical Informatics Speaker Series, Cincinnati Children's Hospital & University of Cincinnati, Nov. 18, 2016
- [167] In silico screening and modeling of protein-drug and protein-protein interactions, Purdue University Center for Cancer Research Seminar Series, Purdue Institute for drug discovery, November 17, 2016
- [166] Predicting gene functions: Departing from single gene-single function paradigm, Bioinformatics seminar, Purdue University, Oct. 25, 2016
- [165] Genome-wide discovery of protein-ligand interactions by a combined computational and energy-based approach, International Conference on Computational Genomics and Proteomics, Guanacaste, Costa Rica, Oct. 18-22, 2016
- [164] The Boltzmann Sequence-Structure Channel" by A. Magner, D. Kihara, & W. Szpankowski, IEEE International Symposium in Information Theory, Barcelona, Spain, July 10-15, 2016
- [163] Considering chain flexibility in protein structure evaluation, 3D-SIG, Orlando Florida, July 8-9, 2016
- [162] Genome-scale prediction of moonlighting proteins using diverse protein association information, I. K. Khan & D. Kihara, Function-SIG at ISMB, Orlando Florida, July 9, 2016
- [161] PL-PatchSurfer: Molecular surface-based virtual screening program", National Institute of Advanced Industrial and Science, Tokyo Japan, June 17, 2016

- [160] Computational modeling of various types of protein complexes, Molecular modeling of energy storage devices & Biomolecular complexes, CERM 2016 47th Central Region Meeting of American Chemical Society, May 19, 2016
- [159] Ensemble-based evaluation for protein structure models, The 3rd International Conference on Mathematical & Computational Medicine May 16-18, 2016
- [157-8] The Hitchhiker's guide to the biomolecular galaxy, Purdue University, May 11-12, 2016:
- "IDR-LZerD: structure prediction of disordered protein interactions", Lenna Peterson
 - "An automated Calpha tracing from cryo-EM map", Genki Terashi
- [156] Human and server prediction using LZerD with combined scoring functions", 6th CPARI protein docking prediction evaluation meeting, April 17-19 2016, Tel Aviv, Israel
- [155] Computational docking of multifarious protein complexes, Dept. of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, Feb. 29, 2016
- [154] PL-PatchSurfer: A fast surface-patch-based virtual screening program using three dimensional Zernike descriptors, 60th Biophysical Society meeting, Los Angeles, Feb. 27- March 2, 2016
- [153] Computational docking of multifarious protein complexes, Dept. of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, Feb. 29, 2016
- [152] Protein structure prediction using residue- and fragment-environment potential in CASP11, 3rd International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, Dec. 14-18, 2015
- [151] Unified biomolecular 3D surface matching for big data in structural and chemical biology, Workshop on Big Data and Computational Sciences, University of Kansas, Lawrence, Kansas, Nov. 21, 2015
- [150] Patch-Surfer and PL-PatchSurfer: Predicting binding ligands for target proteins by molecular surface similarity and complementarity, University of Kansas, Lawrence, Kansas, Nov. 20, 2015
- [149] Protein structure prediction using residue- and fragment-environment potential in CASP11, KIAS Workshop, Korea Institute for Advanced Study, Seoul, Korea, September 17-19, 2015
- [148] Origin of protein superfamilies and superfolds" (oral presentation), 3D-SIG 2015, Dublin, Ireland, July 10-11, 2015. Received the Best Oral Presentation Award
- [147] Gene function prediction in biological contexts, Hokkaido University, Sapporo, Japan, July 2 , 2015
- [146] On the origin of protein superfamilies and superfolds. 4th SNU Bioinformatics Workshop, Seoul National University, Seoul, Korea, June 29-30, 2015.
- [145] Genome-scale identification and characterization of moonlighting proteins. The 15th Annual Meeting of the Protein Science Society of Japan. Tokushima, Japan, June 24-26, 2015
- [144] Surface structure-based ligand prediction for target proteins and application for drug development", D. Kihara, Workshop on "Drug development based on predicted structure and function of target proteins", Tokyo University of Pharmacy and Life Sciences, Hachioji, Tokyo, Japan, June 23, 2015
- [143] Comparison and fitting of molecular shapes for low-resolution structural data, RIKEN, Yokohama, Japan, June 19, 2015
- [141-2] Great Lakes Bioinformatics Conference (GLBIO 2015), Purdue University, IN, May 18-20, 2015
- (talk) IAS: Interaction specific GO term associations for predicting protein-protein interaction networks. Satwica Yerneni, Ishita K. Khan, Qing Wei & D. Kihara
 - (talk) Residue environment score for selecting protein structure models and protein-protein docking models. Hyung-Rae Kim & D. Kihara
- [140] PL-PatchSurfer: surface-patch-based virtual screening program using three dimensional Zernike descriptors. Purdue Mini-Symposium on Integrated Structure, Function, and Interactions of Protein Universe. Purdue University, May 13-14, 2015.
- [139] EM-Surfer: real-time electron microscopy map database search. Purdue Mini-Symposium on Integrated Structure, Function, and Interactions of Protein Universe. Purdue University, May 13-14, 2015.

- [138] Selecting protein structure models with a residue environment score that recognizes multi-residue interactions. The Chem-Bio Informatics Society, Tokyo Institute of Technology, Tokyo, Japan, June 22, 2015.
- [137] Detecting local residue environment similarity for recognizing near-native protein structure models. From Computational Biophysics to Systems Biology (CBSB2015), The University of Oklahoma, Oklahoma, May 17-19, 2015.
- [136] Fast shape-based global and local electron density map search. J. Esquivel-Rodriguez, X. Han, C. Christoffer, X. Kang, L. Monroe, & D. Kihara, the 59th Biophysical Society Annual Meeting, Baltimore, MA, Feb. 7-11, 2015.
- [135] Phase transition in a sequence-structure channel. A. Magner, D. Kihara & W. Szpankowski. Information Theory and Applications, Scripps Seaside Forum, La Jolla, CA, Feb. 1-3, 2015.
- [134] Local image comparison using Krawtchouk moment invariants. A. Sit & D. Kihara, 2015 Joint Mathematics Meetings, San Antonio, Jan. 12, 2015
- [133] Invited talk at Free Modeling category, 11th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP11), Riviera Maya, Mexico, Dec. 7-10, 2014
- [132] Exploring Protein-Ligand Interactions Using Molecular Local Surface Comparison Methods. Department of Chemistry, Purdue University, Dec. 5, 2014
- [131] Detecting local residue environment similarity for recognizing near-native structure models. Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO, Aug 4-8, 2014
- [130] A proteomic strategy for global analysis of protein complex composition and localization in Arabidopsis leaves. Aryal Uma, Jun Xie, Daisuke Kihara, Mark Hall, Dan Szymanski, 25th International Conference on Arabidopsis Research (ICAR), University of British Columbia, Vancouver, Canada, July 28-Aug. 1, 2014
- [129] Genome-scale Identification and Characterization of Moonlighting Proteins, The Biological and Biomedical Consequences of Protein Moonlighting , London, UK, 29-30 July 2014
- [128] Comparison and fitting of molecular shapes and low-resolution structural data, EBI, Hinxton, UK, July 28, 2014.
- [127] Why Protein Folds and Superfamilies have Skewed Distributions?, Zing Conference on Protein Folding, Punta Cana, Dominican Republic, July 16-19, 2014
- [126] Small-angle x-ray scattering reveals the structure of the catalytic domain of a plant cellulose synthase and its assembly into dimers. P.S. Rushton, N. Carpita A.T. Olek, C.V. Stauffacher, C. Rayon, L. Makowski, H.R. Kim, P. Ciesielski, J. Badger, L.N. Paul, D. Kihara, M. Crowley, & M. E. Himmel, Plant Biology 2014, Portland, Oregon, Jul 12-16, 2014.
- [125] PFP: Protein function prediction using distantly related sequences and function association, Automatic Function Prediction Meeting (AFP-SIG), Boston, July 11-12, 2014
- [124] Genome-scale identification and characterization of moonlighting proteins, I. Khan & D. Kihara, Automatic Function Prediction Meeting (AFP-SIG), Boston, July 11-12, 2014
- [123] Predicting protein complex assembly pathway using multiple-protein docking algorithm, Yoichiro Togawa, Juan Esquivel-Rodriguez, Amit Roy, & D. Kihara, 3D-SIG, Boston, July 11-12, 2014
- [122] Navigating 3D Electron Microscopy Density Maps and Protein Shapes with EM-SURFER and 3D-SURFER 2.0, Juan Esquivel-Rodriguez, Yi Xiong, Juan Esquivel-Rodriguez, Xusi Han, Shuomeng Guang, and Daisuke Kihara, Great Lakes Bioinformatics Conference (GLBIO 2014), Cincinnati, OH, May 16-18, 2014
- [121] Unified biomolecular 3D surface matching for proteins, ligands, and interactions. Iowa State University, Apr 10, 2014.
- [120] Evaluating protein structure models considering local structure contexts, 2nd Zing Protein and RNA Structure Prediction Conference, Cancun, Mexico, Dec. 1-5, 2013
- [119] Prediction of macromolecular structures of protein interactions, Beckman Institute, Univ. Illinois at Urbana-Champaign, Oct 28, 2013

- [118] Prediction of macromolecular structures of protein interactions. *Frontiers in Bioinformatics and Computational Biology*, Cold Spring Harbor Conferences Asia, Suzhou, China, Sept. 23-27, 2013.
- [117] Computational prediction of protein function and protein-protein docking. University College London, Sep. 13, 2013
- [116] Predicting gene function in biological contexts , 2nd ACSL International Summer School, Imperial College London, Sep 8-14, 2013
- [115] Unified biomolecular 3D surface matching for proteins, ligands, and interactions, Eli Lilly, Lilly Grand Rounds, Eli Lilly, Indianapolis, Aug 14, 2013
- [114] Machine learning approach for protein structure modeling, Telluride Workshop on Modeling Biomolecular Structures, Interactions, and Functions, Telluride, CO, July 1-5, 2013.
- [113] Structure prediction of protein interactions, Seoul National University, Dept. of Chemistry, Seoul, Korea, June 27, 2013
- [112] Information flow in biological systems, Chung-Ang University, 4th International Conference of Biostatistics and Bioinformatics, Seoul, Korea, June 25, 2013
- [111] Predicting gene function in biological contexts, Seoul National University, Computer Science and Engineering, Seoul, Korea, June 24, 2013.
- [110] Information flow in biological systems, Tokyo Institute of Technology, June 21, 2013
- [109] Predictions of structures of protein interactions. Univ. Chicago Computation Institute, Chicago, IL, May 20, 2013
- [108] Macromolecular structure modeling and EM fitting. D. Kihara & J. Esquivel-Rodriguez, 5th CAPRI (Critical Assessment of Predicted Interactions), Utrecht, the Netherlands, April 17-19, 2013.
- [107] Predictions of Protein Function, Structures, Dynamics, and Interactions. *Bioinformatics and Machine Learning Roundtable*, Qatar Computing Res. Institute, Doha, Qatar, March 19-20, 2013.
- [106] Macromolecular Structure Modeling and Electron Microscopy Fitting Using 3D Zernike Descriptors. Highlights Track, ISCB-Asia/SCCG 2012, Shenzhen, China, Dec. 17-19, 2012.
- [105] Binding ligand prediction by comparing local surface patches of potential pocket regions. Zing conference, Mathematical and Computational Medicine, Xcaret, Cancun, Mexico, Dec. 1-15, 2012.
- [104] Predictions of structures of protein interactions. International Summer School of Life & Health Science, Education Academy of Computational Life Sciences, Tokyo Institute of Technology, Shonan, Kanagawa, Sept. 3-5, 2012
- [103] Suboptimal alignments & 3D Zernike descriptors for structure prediction and docking. Workshop on Coarse-grained modeling of structure and dynamics of biomacromolecules, Telluride, CO, July 23-27, 2012.
- [102] A "catalytic dimer" hypothesis for the synthesis of cellulose and other (1,4)-beta-glycans Nicholas C. Carpita, Anna T. Olek, Catherine J. Rayon, Lee Makowski, Shi-you Ding , Peter Ciesielski, Lake Paul, Subhangi Ghosh, Daisuke Kihara, Michael Crowley, Michael Himmel, Jeffrey Bolin, The 23rd International Conference on Arabidopsis Research (ICAR), Vienna, Austria, July 3-7, 2012
- [101] Predictions of structures of protein interactions. Telluride Meeting on Protein folding and Dynamics: From experiment to theory, Telluride, Colorado, June 17-21, 2012
- [100] Predicting binding ligand and protein docking using surface shape". D. Kihara, Graduate School of Information Science, Tohoku University, Sendai, Japan. May 30, 2012
- [99] Predictions of structures of protein interactions. Bioinformatics Seminar series at Institute of Chemical Research, Kyoto University, Uji, Kyoto, Japan. May 28, 2012
- [98] Structural features that predict real-value fluctuations of globular proteins, M. Jamroz, A. Kolinski & D. Kihara, at Special Session, " Proteins in motion: Computational studies in protein flexibility and dynamics" co-organized by D. Kihara & L. Kurgan, Great Lakes Bioinformatics Conference (GLBIO) 2012, May 15-17, 2012, Ann Arbor, MI.
- [97] Computational characterization of moonlighting proteins using Gene Ontology annotations (selected talk), by I. Khan, M. Chitale, & D. Kihara, Great Lakes Bioinformatics Conference (GLBIO) 2012, May 15-17, 2012, Ann Arbor, MI.

- [96] Macromolecular structure modeling and electron microscopy fitting using 3D Zernike descriptors (selected talk), J. Esquivel-Rodriguez, & D. Kihara, Great Lakes Bioinformatics Conference (GLBIO) 2012, May 15-17, 2012, Ann Arbor, MI.
- [95] Sequence- and structure-based protein function prediction. The Research Institute at Nationwide Children's hospital, The Ohio State University, March, 22, 2012.
- [94] Functional coherence assessment for protein groups and its application to pathway assignment, Zing conference, IECA (International E. coli Alliance) 2011, Cancun, Mexico, Dec. 5-9, 2011
- [93] Unified Molecular Representation for Protein Shape Comparison and Interaction, Zing conference on Protein and RNA Structure Prediction", Cancun, Mexico, Dec. 3-7, 2011
- [92] Next generation structural bioinformatics and gene function prediction
Biological Sciences Research Retreat, Swan Lake resort, Plymouth IN, Nov. 5, 2011
- [91] Next generation protein 3D structure analysis: Rapid global/local surface comparison, docking, and low-resolution data. D. Kihara, Dept. of Biological Sciences Faculty Research Presentations, Purdue University, Oct. 27, 2011
- [90] Protein surface representation for ligand binding site screening, Eli Lilly, Indianapolis, October 3, 2011
- [89] Next Generation Protein 3D Structure Analysis: Rapid Global/Local Surface Comparison, Docking and Low-Resolution Data, University of Alberta, Edmonton, Canada, September 16, 2011
- [88] Binding ligand prediction by comparing local surface patches of potential pocket regions. Computational Biology Research Center, Tokyo, Japan, September 2, 2011
- [87] Next generation protein structure analysis for structure comparison and interaction prediction. Fukushima Medical University, Fukushima, Japan, September 1, 2011.
- [86] Binding ligand prediction by comparing local surface patches of potential pocket regions. RIKEN, Yokohama, Japan, August 30, 2011
- [85] 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
- [84] 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
- [83] 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
- [82] 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.
- [78-81] 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
- [77] Surface Representation for Molecular Global and Local Shape Comparison and Docking. International Institute of Molecular and Cell Biology, Warsaw, Poland, May 25, 2011
- [71-76] 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.
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.
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, 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 Status 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 (Total 183, Listing from 2016)

- [183] Using deep learning to predict binding ligands and drugs to protein targets, C. Belth, M. Zhu, R. Chikhi, D. Kihara, 2017 Undergraduate Research and Poster Symposium, Purdue University, April 11, 2017

- [180-2] Multiple poster presentations at Tessman Symposium, Purdue University, May 1, 2017
- Variability of protein structure models from electron microscopy, L. Monroe, G. Terashi, & D. Kihara
 - MAINMAST: Building main-chain models for medium resolution electron microscopy maps, G. Terashi & D. Kihara
 - Computational methods for predicting protein-protein interactions in plants, Z. Ding & D. Kihara
- [175-9] Multiple presentations at 'The Hitchhikers' Guide to the Biomolecular Galaxy, Purdue University, May 10-11, 2017
- MAINMAST: Building main-chain models for medium resolution electron microscopy maps, G. Terashi & D. Kihara
 - Computational methods for predicting protein-protein interactions in plants, Z. Ding & D. Kihara
 - Navigating 3D electron microscopy density maps and protein shapes with EM-SURFER and 3D-SURFER2.0, X. Han & D. Kihara
 - Structure detection in cryo-EM maps, S. R. M. Venkatraman, G. Terashi & D. Kihara
 - Efficient computational framework for biological 3D image data retrieval, M. Zhu & D. Kihara
- [174] Efficient computational framework for biological 3D image data retrieval, M. Zhu, C. Belth, A. Sit, & D. Kihara, NSF SI2 PI Meeting, Arlington, VA, Feb. 21-22, 2017
- [172-3] The Hitchhiker's guide to the biomolecular galaxy, Purdue University, May 11-12, 2016:
- Identification of protein-protein interactions in *Arabidopsis thaliana* using mass spectrometry and computational methods, Ziyun Ding, & D. Kihara
 - Navigating 3D Electron Microscopy Density Maps and Protein Shapes with EM-SURFER and 3D-SURFER 2.0, Xusi Han, & D. Kihara
- [171] Significance of amino acid entropy and mutual information in multiple sequence alignments, Josh McGraw & D. Kihara, Undergraduate Research Poster Symposium, April 12, 2016, Purdue University

Research Support

Current:

Structural Modeling of Multifarious Protein Complexes
(NIH, R01, \$1,216,750 total, 6/1/2017-5/31/2021) Role: PI

An integrated experimental and computational strategy for identification of genome-wide protein-protein interactions in plants.

(PRF, 1 grad RA, 6/1/2017 – 5/31/2018) Role: PI

Collaborative Research: Efficient mathematical and computational framework for biological 3D image data retrieval

(NSF, Mathematical Biology, \$542,383 total, 6/1/2016-5/31/2019) Role: PI

Integrative genomics approach to computational assessment of threats (IGACAT)

(IARPA, Virginia Tech, \$94, 500 total, 6/16/2017-11/30/2018) Role: co-PI (PI: Ron Kenyon)

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

(NSF, IOS, 10/01/2011-09/30/2015 no cost extension until Nov. 2017, \$1,709,230 total) Role: co-PI (PI: D. Szymanski)

Deep learning for 3D protein target – drug interaction

(NVIDIA Academic Hardware Grant, one Tesla K40 GPU, ~\$3200 value) Role: PI

Past

ABI Innovation: Protein functional site identification using sequence variation.
(NSF, ABI, 06/01/2013-05/31/2016, \$480,195) Role: PI

III: Small: Rapid screening of interacting ligands and proteins.
(NSF, \$492,509 total, 8/1/2013-7/31/2016) Role: PI

Identification of protein-metabolite interactome.
(NIH, R01, 9/1/2011-05/31/2016, \$1,118,554, total), PI

Designing new ligands for new targets through novel computational methods for binding site characterization.
(Eli Lilly, \$244,969 total, 3/1/2013-4/12/2016) Role: PI

Research Support.
(Eli Lilly, \$42,643 total, 1/1/2015-5/31/2015) Role: PI

Information Transfer in Biological Systems.
(NSF, DMS, 06/01/2008-05/31/2014, \$480,000) Role: co-PI, (PI: Wojciech Szpankowski)

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, 300 million KRW total) Role: co-PI (PI: C. Park)

Template-based protein structure prediction beyond sequence homology.
(NSF, ABI, \$716,001, 06/01/2009-05/31/2013) Role: PI

Surface shape based screening of large protein databases.
(Agency: NIH, R01, Total: \$1,408,659 direct cost, 09/01/2005-08/31/2012, no-cost extension to 2012)
Role: PI

III: Small: Quality assessment of computational protein models.
(NSF, IIS, \$327,606, 09/01/2009 – 08/31/2012) Role: PI

Elucidating genetic pathways for curing retinal degeneration
(Showalter Trust, \$75,000, 6/1/2010-5/31/2012) Role: co-PI, (PI: Yuk Fai Leung)

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)

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

Current

Woong-Hee Shin (PhD in Chemistry), August 2014 – current

Genki Terashi (PhD in Pharmaceutical Sciences) April 2017 - current

Former postdocs

Hyungrae Kim (PhD in physics), September 2011 – August 2016

Jian James Zhang (PhD in Chem. Engineering), August 2014 – May 2015, Zymoworks Inc.

Amit Roy (PhD in physics), December 2013 – December 2015, computational structure biologist, NIH Rocky Mountain Laboratories

Atila Sit (PhD in Appl. Math) Sept. 2012 – July 2014, assistant professor, Eastern Kentucky University, Department of Mathematics

Xiaolei Zhu (PhD in Chem. Engineering), July 2012 – June 2014, assistant professor, Anhui University, China

Bingjie Hu (PhD in Pharmacy), Sept. 2013- May 2014, research scientist at Merck

Yi Xiong (PhD in CS), January 2012 – December 2013, assistant professor, Shanghai Jiaotong University, Shanghai, China

Choi Youn Im (PhD in Statistics), March 2012 – March 2013, research scientist at the Department of Statistics, Chung-Ang University, Seoul, Korea

Sael Lee (PhD in CS, Purdue) August 2010 – July 2011, moved on to researcher at Samsung, Korea, currently assistant professor at CS, SUNY Korea

Mateusz Kurcinski (PhD in Chemistry) March 2010 – March 2011, postdoc at Warsaw University, Chemistry

Vishwesh Venkatraman (PhD in Comp. Chemistry) September 2007 – July 2009, moved onto research scientist at LORIA, France, currently postdoctoral fellow at Dept. of Chemistry, Norwegian Univ. of Sci & Tech, Norway

Jianjun Hu (PhD in CS) Sept. 2004 – August 2005 Currently associate professor in Dept. of Computer Science and Engineering, University of South Carolina

Past Visiting Scholar

Genki Terashi, Junior Associate Professor, School of Pharmacy, Kitasato University, Tokyo, Japan, April 2015 – March 2017 (continuing as a postdoc)

Xinyuan Zhou, Assistant Professor, Dept. of Comp. Science & Technology, Changsha University, China March-December 2015

Catherine Rayon, Professor, Dept. of Biology, Universite de Picardie Jules Verne, France January – May 2012

Uttamkumar Samanta, October 2012 – May 2013

Hangchang Lee, Associate Professor, Dept. of Multi-media Engineering, Hangeung University, Seoul, Korea, Jan. 1. 2009 – May 2009
Changsoon Park, Full Professor at Statistics Dept., Chung-Ang University, Seoul, Korea, Jan 3, 2008 – Feb 28 2008

Supervised programmer

Michael Gillogly: August 2009 – April 2010
Stan Luban: January 2006 – June 2006
Yen Hock Tan: June - August 2004

Supervised Students

Graduated with Ph.D.

Lenna X. Peterson (Biol, Spring 2017) currently at Schrodinger Inc.
Ishita K. Khan (CS, Summer 2016) currently at Ebay
Juan Esquivel-Rodriguez (CS, Summer 2014), currently at Google
Meghana Chitale (CS, Spring 2013), currently software engineer at Epic
David La (Biol, Fall 2011) currently postdoc at David Baker lab, Univ. Washington, Seattle
Bin Li (CS, Fall 2011), currently postdoc at La Jolla Institute for Allergy & Immunology
Sael Lee (CS, July 2010) continued as postdoc, currently assistant professor at SUNY Korea, Dept. of CS
Hao Chen (Biol, May, 2010) currently bioinformatics programmer at Langone Medical Center, New York Univ.
Yifeng Yang (Biol, May 2010) currently senior quantitative analyst, Fifth Third Bank
Troy Hawkins, (Biol, October, 2008), currently research scientist at Eli Lilly, Indianapolis

Graduated with MS

Yoichiro Togawa (Biology, Spring 2014), currently at Self Defense Force, Japan
Chao Yuan (PULSe, Spring 2012), MS student in Rice University, Computer Science, currently at Amazon

Current Graduate Students:

Aashish Jain (Biol)
Xusi Han (PULSe)
Ziyun Ding (PULSe)
Lyman Monroe (Biol)
Mengmeng Zhu (PULSe)
Sai Subramaniya (CS)
Charles Christoffer (CS)
Eman Alnabati (CS)

Other Former Graduate Students in the Lab

Xuejiao Kang (CS), (8/12-5/15)	Shiqi Yang (Animal Science) Fall 2016
Kristen Johnson (CS) (8/13 – 5/14)	Xin Cheng (CS) (8/13-5/14)
Hongyun Gao, 8/12, (Math, Sci, Dalian U. Tech, China, visiting PhD Student)	Farrukh Arslan (ECE) (8/2009-5/2010)
Muyi Liu (PULSe) (4-8/2012)	Padmasini Chakravarthy (ECE) (2008-2009)
Kyle Krull (PULSe) (Spring 2004)	Mingjie Tang (CS) (8/10-8/11)
Mingwu Zhang (CS), (co-supervised with S. Prabhakar; 2004-2006)	Manish Agrawal (ME) (co-supervised with K. Ramani; 2004)
Srinivasan S. Turuvekere (ME) (co-supervised with K. Ramani; 2004)	Khurram Siddiqi (EE), (co-supervised with B.L. Wanner; Fall 2003)
Qing Wei (CS) MS, Spring 2017	Michal Jamroz (Warsaw U.) Oct 2010-May 2011
Keisuke Yanagisawa (ITTEch, Japan) Aug.-Nov. 2017	Israa Al-Qassem (CS) Jan.-Dec. 2017

Current Undergraduate Students

Caleb Belth (CS) Fall 2015-
Xi He (Bio) Fall 2017-
Yuhong Zha (CS) Fall 2017-
Dan Ntala (Bio) Spring 2017-
Max Shramuk Summer 2017-

Hareesh Gali (CS) Fall 2017-
Govind Girish (CS) Fall 2017-
Aditi Acharya (Eng) Fall 2017-
Kavya Nagalakunta (CS) Fall 2017-

Former Undergraduate Students

Long-Term Research Project (2+ Semesters)

Stan Luban (Bio/CS) (Spring2004-Spring2006)
Ei Ei Phyu (CS), Spring/Fall 2005
Yen Hock Tan (CS) 2004-2006
Jennifer S Reeve (CS) (Summer 2004, 2011)
Rupal Trivedi (Bio) Fall 2007-Spring2008,
Spring 2010
Devin Luckett (Bio) Fall 2008 – Spring 2010
Paul Tuck (CS) Summer 2009 – Spring 2010
Nickett Gupta (CS) Fall 2009-Spring 2010
Malvika Mathur (Bio) Fall 2008 – Spring 2010
Abram Magnier (CS/Math)Spring 09 – Spring 10
Matt Herron (Bio/CS) Summer 2008 – Spring 2010
Mi-Sun Kong (Bio) Fall 2010 - Fall 2011
William Hoffman (Biol) Spring 2010 –Spring 2011
Roshna Agrawal (CS) Spring 2010-Summer 2011
Su Lin Ooi (CS) Fall 2011- Summer 2012
Sam Yap (Biol) Spring 2012- Spring 2013
Chang Liu (Math, DUR) Fall 12-Spring 13
Guanqun Mao (CS, DUR) Fall 12-Spring 13
Xiaowei Hong (Biol) Summer 2012 – Spring 2013

Rodney Weaver (CS) (Spring /Fall 2004)
Jairav Desai (CS, DUR*), 2005-2006
Steve Krawczyk (Bio), Fall 2006, Spring 2007
Preston Spratt (Bio), Fall 2006 – Spring 2008
Steven Ahrendt (Bio/CS) Fall 2008-
Spring 2009
Gregg Thomas (Bio) Summer 2008 – Fall 2009
Priyanka Surana (Bio) Fall 2007 – Spring 2010
Sangwook Lee (Bio) Fall 2009 – Spring 2010
Kunal Modi (CS) Fall 2009 – Fall 2010
Sajat Jain (CS) Fall 2009 – Fall 2010
Shriphani Palakodety (CS) Fall 2009 - Spring 2010
Sanmeet Kanhere (CS) Summer 2010 - Spring 2011
Xin Lu Tan (Stat) Fall 2010-Spring 2011
Benjamin Bastnagel (Bio) Spring 2011- Spring 2012
Yingfei Ma (Stat) Spring 2011-Spring 2012
Vianney Gonzalez (Math, DUR) Fall2012-Sprng 2013
Linsheng Shen (Bio, DUR) Fall 12-Spring 13
Yanan Tao (Biol) Fall 2012- Spring 2013
Minxian Li (CS, Beijing U of Chem Tech,
China) Fall 2012 – Spring 2013
Arthi Anand (Biol) Spring-Fall 2013
Fangyuan Hou (CS) Summer-Fall 2013
Qing Xu (Stat) Summer-Fall 2014
Qing Wei (CS), Spring 2014-Fall 2014
Ray Ji (Biol) Fall 2014-Fall 2015
Yue Wang (Stat) Spring 2014-Summer 2015
Tianzhao Wu (Biol) Fall 2014-Fall 2015
Hayley Chan (MCMP) Fall 2015-Spring 2017
Brian Lembong (Bio) Summer 2016-Spring 2017
Aditya Vaidyam (CS) Spring 2015-Spring 2017

Lillian Liu (CS) Spring 2012-Spring 14
Linzi Chen (Biol/Stat, HHMI) Spring'13-Spring 2014
Andrew Walden (Biol/CS) Fall 2014-Fall 2015
Weichuan Luo (Biol), Fall 2013-Spring 2015
Tiange Dong (Biol) Spring 2013-Fall 2015
Charles Christoffer (math/CS) Sprg14-Smr 15
Eric Petit (Biol) Fall 2014-Fall 2015
Josh McGraw (Biol) Summer 2015-Smr 2016
Andrew Walden (Bio) Summer 2016-Spring 2017
Sarah Rodenbeck (Biol) Spring 2016-Spring 2017
Siddharth Prabhu (BME), Fall 2016-Spring 2017

1 (One) Semester Research Project

Jason Pardieck (CS), Spring 2004
Danny Varghese (CS), Spring 2004
Jasmine Williams (MARC/AIM*), Sum.2004
Antonius Sardjito (CS) Summer 2004
Jonathan Williford (CS), Fall 2004
Yuhao Lin (Comp. Engng), Spring 2005
Jiyoung Lee (Bio) Fall 2005

Brian Seckinger (CS), Spring 2004
C. Sujjapong (Comp. Eng) (Summer 2004)
Irvan Sutiono (CS), Summer, 2004
Joel Hayburst (CS), Fall 2004
Brian Trisler (CS), Spring 2005
Luis Avila (MARC/AIM), Summer 2005
Howard Chang (CS), Summer 2006

Robert Helms (Bio), Fall 2006
 De'Rael Darling (Marc/Aim) Summer 2007
 Sparsh Shekhar (CS) Summer 2008
 Emily Flynn (Bio) Fall 2008
 Shen Liang (CS) Summer 2009
 Roy Ren (CS) Fall 2009
 Gabriel Martinez (CS) Spring 2010
 Shuai Liu (CS) Fall 2010
 Satwica Yerneni (Vellore I. Tech, India)Spg11
 Liyun Fan (Biol) Spring 2011
 Qiting Wu (Bio) Spring 2011
 Daniel Lee (BME) Fall 2011
 Shing Jay Ong (CS) Fall 2011
 Yang Shen (Bio) Spring 2012
 Kara Kahue (CS, SROP), Summer 2012
 Alex Gao (Stat) Fall 2012
 Shawn Deboth (Biol) Spring 2013
 Yuqian Chen (Biochem, DURl) Spring 2013
 Grant Gumina (CS, DURl) Spring 2013
 Tommy Lee (Spring 2015)
 Hanfu Zhang (Tsinghua U, Summer 2015)
 Alexander Engstrom (Biol) Spring 2016
 Alexandre Dias (Fed U Lavras, Brazil) Smr2016
 Natalie Oda (Bio) Spring 2017
 Hannah Zentner (CS) Fall 2017
 Simeng Liao (Nankai U.) Summer 2017
 Hao Zhu (Beijing U. Posts & Tel) Summer 2017

Rex Chang (CS), Spring 2007
 Stephen Ueng (CS) Fall 2007
 Jared Bannister (CS/Math) Fall 2008
 Subhash Atluri (CS) Summer 2009
 En-hsun Liu (CS) Summer 2009
 Gunjan Raghav (CS) Spring 2010
 Yidi Wang (Bio) Fall 2010
 Wei-Chia Sun (CS) Fall 10
 Yilong Jin (CS) Spring 2011
 Hayun Lee (Biol) Spring 2011
 Gaonan Zhang (Bio) Spring 2011
 Shucong Zhang (CS) Fall 2011
 Zilong Zhou (Math) Fall 2011
 Danny Antakli (Bio, HHMI) Summer 2012
 Liuning Wang (Stat, DURl) Fall 2012
 Wuwei Zhang (CS, DURl), Spring 2013
 Aanchal Kanodia (VNIT-Nagpur, India) Sum13
 Joel Crist (Biol) Summer 2013
 Wen Sun (Biol) Fall 2013
 Karan Dua (IIT Roorkee), Summer 2014
 Ryan Hancock (Industr. Engng), Summer 2015
 Morgan Farrell (Biol) Summer 2016
 Shan Lu (BME) Fall 2016
 Matthew Muhoberac (CS) Spring 2017
 Varun Gupta (CS) Fall 2017
 Xiao Wang (Xi'an Jiaotong U.) Summer 2017
 Kevin Shim (Bio) Spring 2017

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
 Devin Luckett (Biol, graduated 2010) New York University
 Satwica Yersini (intern, Vellore Inst Tech, India, 2011) Indiana University
 Devin Luckett (Biol, graduated 2010) New York University
 Gregg Thomas (Biol, graduated 2011) Indiana University
 Minxian Li (intern, 9/2012-5/2013, Beijing U of Chem. Tech), Iowa State University

K-12 Students

Aditi Acharya (West Lafayette High), Summer 2014-Fall 2016
 Katie Kranjak, Summer 2005 (high school student, Indiana Academy of Science)

Student Awards

- Ishita Khan, Best presentation/poster award, Function-SIG, ISMB, Orlando, Florida, July 9, 2016
- Lenna Peterson, Bilsland Dissertation Fellowship from the Purdue Graduate School, April, 2016.
- Lenna Peterson, PULSe Outstanding Student Publication of the Year Award, Purdue University, April 2015
- Juan Esquivel-Rodriguez, Best Flash Talk, Great Lakes Bioinformatics (GLBIO), Cincinnati, May 16-18, 2014

- Juan Esquivel-Rodriguez, Excellence in Research Award in Poster presentation by Office of Interdisciplinary Grad Programs, Purdue University, April 9, 2014
- Hyung-Rae Kim, travel award for the 10th meeting of Critical Assessment of Techniques for Protein Structure Prediction (CASP10), Gaeta, Italy, December 9-12, 2012
- Lillian Liu (CS), Best Abstract Award, Undergraduate Research Poster Symposium, Purdue University, April 10, 2012
- Juan Esquivel-Rodriguez (CS), 1st Place Award, Sigma Xi graduate student research poster competition, Purdue University, February 15, 2012
- 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 from 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.
- Gregg Thomas (Biol), Sandy Ostroy Summer Internship Award, Purdue University, Summer 2009
- Yifeng Yang (Biol), Student Travel Grant to attend 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.
- 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
- 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 2011-2016)

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

CS497 honors research, coordinator (Fall 2010)

CS490B/Biol495S Introduction to Bioinformatics (Spring 2004, Spring & Fall 2005, Fall 2006-2008)

- 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

BIOL395 Genes + Proteins = Bing Data (Spring 2018)

BIOL563/(CS590B) Protein Bioinformatics (Spring 2006-2010, 2012-4, 2016)

BIOL696E Seminar Crystallography (Spring 2006)

Other Teaching Activities

- Short talk at Purdue Science Student Council meeting (Spring 2017)
- Guest lecture at BIOL197, Biology freshman honors seminar (Fall 2016)
- Guest lecture at CHEM599, Visualizing cells & molecules (Spring 2013)
- Guest lecture at CS397, honor research course (Fall 2012, Fall 2015)
- Guest lecture at CS591, honor research course (Fall 2011)
- Guest lecture at CS197, honor research course, (Spring 2009)
- 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
- 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 Janet Thornton, a renowned bioinformatics scientist (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

- BMC Bioinformatics (March 2016 – present)
- Scientific Reports (Nature journal) (May 2015 – present)
- Methods, guest editor (2015)
- Associate Editor, International Journal of Knowledge Discovery in Bioinformatics (IJKDB) (January 2009- present)

Review of Grants

Study Section/Panel

- National Institutes of Health (NIH), Biological Data Management and Analysis (BDMA) (Feb. 2015, Feb. 2017)
- NIH, STTR/SBIR (ZRG1) (March 2015, November 2015, March 2016, March 2017)

Ad hoc reviewer

Domestic:

- NIH P41 Research Resource (Feb. 2018)
- NIH Independence award (Dec. 2017)
- NIH, ZRG1, STTR/SBIR (June 2012, October 2012, March 2014)
- NIH, Challenge Grant, RC1 (June 2009)
- National Science Foundation (NSF), Division of Biological Infrastructure (DBI) (September 2006, October 2009, January 2015)
- NSF, Molecular Cellular Biosciences (MCB) (February 2009, September 2009, March 2011, April 2011, November 2011, February 2017)
- NSF, Chemistry (March 2007, September 2007, February, 2008)
- NSF, Mathematical Sciences (December 2017)
- Louisiana Board of Regents' Research Competitiveness Subprogram, EPSCoR-style grants program (November, 2009, 2011, 2012, 2013)

International

- National Science Centre, Polish Narodowe Centrum Nauki, Poland (August 2011, April/December 2017)
- Israeli Ministry of Science, Technology and Space (June 2017)
- AFM-TELETHON Scientific Council, France (January 2017)
- Biotechnology and Biological Science Research Council, (BBSRC), UK (July 2012, July 2017)
- Medical Research Council (MRC), UK (November 2016)
- European Research Council Executive Agency (September 2016)
- Qatar National Research Fund (2012, 2014, 2015)
- 2012 Edition of the Blue Sky program, French National Research Agency (March 2012)
- The Wellcome Trust, UK/Dept. of Biotechnology India Alliance, Intermediate fellowship (September 2011)
- Agency of Science, Research & Technology (A*STAR), Singapore (2010, 2011)
- 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)

PhD thesis external examiner:

- Department of Electrical and Computer Engineering, University of Alberta, Canada (September, 2011, January 2018)
- University of Zürich, Institute of Biochemistry, Switzerland (June 2013)
- Toyota Technological Institute at Chicago (May 2013)
- Department of Computer Science, National University of Singapore, Singapore (March 2012)

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

- Draft chapters of a new protein structure & dynamics textbook from Garland Science (March 2013)
- Proposal of a new bioinformatics textbook from Garland Science (July 2012)
- a draft manuscript of 3 chapters in Practical Bioinformatics to be published from Garland Science publishers (November 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

- 9th International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD’18), Regensburg, Germany, September 3-6, 2018
- HiCOMB 2018 17th IEEE International Workshop on High Performance Computational Biology, Vancouver, British Columbia, Canada, May 21, 2018
- 4th International Conference on Biomedical and Bioinformatics Engineering (ICBBE 2017), Seoul, Korea, November 12-14, 2017
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2017, Sydney, Australia, July 31-Aug 3, 2017
- Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2017), Prague, Czech Republic, July 21-25, 2017
- 8th International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD’17), Lyon, France , August 28-31, 2017
- HiCOMB 2017 16th IEEE International Workshop on High Performance Computational Biology, Buena Vista Palace Hotel, Orlando, FL, California, May 29, 2017
- Steering committee, Great Lakes Bioinformatics Conference (GLBIO) 2017, Chicago, Illinois, May 15-17, 2017
- Symposium on Bioinformatics and Bioforensics (SBB’16), Jaipur, India, September 21-24, 2016.
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2016, UC Davis, CA, Aug 19-20, 2016
- 7th International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD’16), Porto, Portugal , September 5-8, 2016
- Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2016), Orlando, Florida, July 8-12, 2016
- Steering Committee, Great Lakes Bioinformatics (GLBIO)/Canadian Computational Biology Conference (CCBC), Toronto, Canada, May 16-19,2016
- X-meeting + BSB 2015 11th International Conference of the AB3C + Brazilian Symposium of Bioinformatics, Sao Paulo, Brazil, November 3-6, 2015
- Computational Systems-Biology and Bioinformatics 2015, Bangkok, Thailand, Nov. 22-25, 2015
- ICDM workshop on Biological Data Mining and its Applications in Healthcare, Atlantic City, New Jersey, Nov 13, 2015

- IEEE International Conference on Information Reuse and Integration) IRI 2015, San Francisco, CA, USA August 13-15, 2015
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2015, Paris, France, Aug 26-27, 2015
- International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD-DEXA'15), Valencia, Spain , September 1-5, 2015
- Program Chair, Great Lakes Bioinformatics (GLBIO) Conference, Purdue University, May, 2015
- The 5th International Conference on Computational Systems-Biology and Bioinformatics (CSBio 2014), Singapore, November 10-12, 2014
- Program Chair, ACLS Tokyo Institute of Technology – Purdue Summer School on Interdisciplinary Science, August 14-16, 2014, Purdue University
- Automatic Function Prediction/Critical Assessment of Automatic Function Assignment (AFP/CAFA) 2014, April 2014
- IEEE International Conference on Data Mining (ICDM 2014) BioDM workshop on "Biological Data Mining and its Applications in Healthcare", Shenzhen, China, Dec 14, 2014.
- The 13th Pacific Rim International Conference on Artificial Intelligence, Gold Coast, Australia, Dec. 1-5, 2014
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2014, Beijing, China, Aug 18-19, 2014
- 22nd Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2014), Boston, July 11-15, 2014
- International Workshop on Algorithms for Computational Biology (ACB-2014), September 24-27, 2014, Delhi, India
- 5th International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD-DEXA'14), Munich, Germany, September 1-5, 2014
- Program Chair, Great Lakes Bioinformatics (GLBIO) Conference, Cincinnati Children's Hospital Medical Center, May 16-18, 2014
- International Symposium on Network Analysis and Mining for Health Informatics, Biomedicine and Bioinformatics, Net-HI-BI-BI 2013, Shanghai, China Dec 18-21, 2013
- IEEE International Conference on Data Mining (ICDM 2013) BioDM workshop on "Biological Data Mining and its Applications in Healthcare", Dallas, Texas, Dec 8, 2013.
- Automatic Function Prediction/Critical Assessment of Automatic Function Assignment (AFP/CAFA) 2013, April 2013
- ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM-BCB) 2013, Washington DC, September 22-25, 2013
- 2013 ASE/IEEE International Conference on BioMedical Computing (BiomedCom2013), Washington DC, September 8-14, 2013
- International Symposium on Network Enabled Health Informatics, Bio-Medicine and Bioinformatics (HI-BI-BI 2013), Niagara Falls, Canada, August 26-27, 2013
- BIOTECHNO2013: The Fifth International Conference on Bioinformatics, Biocomputational Systems and Biotechnologies, Lisbon, Portugal, March 24-29, 2013.
- 21st Annual International Conference on Intelligent Systems for Molecular Biology (2013 ISMB /ECCB), Berlin, July 19-23, 2013
- 4th International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD'13) Prague, Czech Republic, August 26-30, 2013
- International Conference on Data Mining, (ICDM) 2012 workshop on "Biological Data Mining and its Applications in Healthcare", Brussels, Belgium, December 10, 2012
- ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM-BCB) 2012, Orlando, Florida, October 7-10, 2012

- 2012 ASE/IEEE International Conference on BioMedical Computing, Washington DC, December 14-16, 2012
- International Symposium on Network Enabled Health Informatics, Bio-Medicine and Bioinformatics (HI-BI-BI 2012), Istanbul, Turkey, August 27-28, 2012
- International Conference and Exhibition on Computer Aided Drug Design & QSAR, Double Tree by Hilton, Chicago, October 29-31, 2012
- "OMICS International Integrative Biology Summit" during 1-3 October 2012 at Chicago, USA.
- 3rd International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD'12) Vienna, Austria, Sept. 3-7, 2012
- Advisory Committee, Great Lakes Bioinformatics (GLBIO) 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.
- Automatic Function Prediction/Critical Assessment of Automatic Function Assignment (AFP/CAFA) 2011, February 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 (GLBIO) 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 2010 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:

- Executive Committee, 2015-current
- Convener of Structural Biology and Computational Biology 2016-current
- Convener of Molecular Science Cluster, 2015-2016
- Future of Department Discussion Committee 2014-2015
- International Program & Study Abroad Committee 2014-2015, 2016-2017
- Departmental representative for Computational Life Sciences (CLS) program (2010- on)
- Graduate and advanced studies committee, 2011-2014
- International Programs & Study Abroad, 2013-2014
- PRF/Bilsland fellowship review committee 2013, 2017
- Graduate School Admission Committee 2005-6, 2009-2010, 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

Computer Science:

- Graduate Study Committee 2007-9, 2012-2018
- Award Committee 2011-2012
- Undergraduate Committee 2009-2010
- Bioinformatics search committee 2004-5, 2005-6, 2006-7

Interdisciplinary

- Faculty Advisory Committee for Proteomics Profiling Facility (2017-on)

- Representative from Dept. of Biological Sciences for Computational Life Science (CLS) program at Purdue (2010- on)
- Review committee of RNA-Seq Illumina proposals (Bioinformatics Core, Discovery Park, Purdue)

College of Science

- College Grade Appeals Committee 2013-2015
- 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

University

- Search committee of Computational/Systems Biology Cluster (Chair: Rebecca Doerge) 2013-2014

Others

- Review committee of RNA-Seq Illumina proposals (Bioinformatics Core, Discovery Park, Purdue)

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