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<https://www.cs.purdue.edu/people/faculty/dkihara/>  
<http://kiharalab.org> (Lab)

**Education**

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

**Positions held**

2019.3-present	<b>Full member, Purdue University Center for Cancer Research</b>
2014.8-present	<b>Full Professor</b>
2018.3-present	<b>Adjunct Professor</b> , University of Cincinnati, Department of Pediatrics
2015.1-2015.8	<b>Visiting Scientist</b> , Eli Lilly, Indianapolis
2009.8-2014.8	<b>Associate professor</b>
2003.8-2009.8	<b>tenure-track Assistant professor</b> Purdue University, West Lafayette, Indiana Department of Biological Sciences/Computer Sciences (joint appointment)
2002.9-2003.7	<b>Senior Postdoctoral Research Associate</b> Advisor: Jeffrey Skolnick Buffalo Center of Excellence in Bioinformatics, Buffalo, NY, USA
1999-2002.9	<b>Postdoctoral Research Associate</b> Advisor: Jeffrey Skolnick Donald Danforth Plant Science Center, St. Louis, MO, USA
1998-1999	<b>Research Assistant</b> Advisor: Minoru Kanehisa Bioinformatics Center, Institute for Chem. Research, Kyoto University, Japan

**Awards & Recognitions**

- American Institute for Medical and Biological Engineering (AIMBE) Fellow, 2021
- 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, 2017

- 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 21<sup>st</sup> International Conference on Genome Informatics (GIW2010), December, 2010

## Publications

- [192] Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge.  
C.L. Lawson, ,,, D. Kihara, ,,, D. Sarkar, ,,, G. Terashi, H.M. Berman, & W. Chiu. (54 authors) *Nature Methods*. 18: 156-164. (2021)
- [191] Genotype & Phenotype in Lowe Syndrome: Specific OCRL1 patient mutations differentially impact cellular phenotypes.  
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- [190] EnAET: A self-trained framework for semi-supervised learning with ensemble transformations.  
X. Wang, D. Kihara, J. Luo, & G.-J. Qi, *IEEE Trans Image Process.*, 30: 1639-1647 (2021)
- [189] Current progress and future perspective of polypharmacology: From the view of non-small cell lung cancer.  
R. Karuppasamy, S. Veerappapillai, S. Maiti, W.H. Shin, & D. Kihara, *Seminars in Cancer Biology*, 68: 84-91, (2021)
- [188] SHREC2020: Classification in cryo-electron tomograms.  
I. Gubins, M.L. Chaillet, G.v.d. Schot, R.C. Veltkamp, F. Foerster, Y. Hao, X. Wan, X. Cui, F. Zhang, E. Moebel, Xiao Wang, Daisuke Kihara, X. Zeng, M. Xu, N.P. Nguyen, T. White, & F. Bunyak, *Computers & Graphics*, 91: 279-289 (2020)
- [187] SHREC2020: Multi-domain protein shape retrieval challenge.  
F. Langenfeld, Y. Peng, Y.-K. Lai, P.L. Rosin, Tunde Aderinwale, Genki Terashi, Charles Christoffer, Daisuke Kihara, H. Benhabiles, K. Hammoudi, A. Cabani, F. Windal, M. Melkemi, A. Giachetti, S. Mylonas, A. Axenopoulos, P. Daras, E. Otu, R. Zwiggelaar, D. Hunter, Y. Liu, & M. Montes, *Computers & Graphics*, 91: 189-198 (2020)
- [186] LZerD: Software for protein-protein docking modeling.  
D. Kihara, C. Christoffer, S. Chen, V. Bharadwaj, T. & Aderinwale. *Jikken Igaku (Experimental Medicine)*, 38: 3271-3276. (in Japanese). (2020)
- [185] Current Challenges and Opportunities in Designing Protein-Protein Interaction Targeted Drugs.  
W.H. Shin, K. Kumazawa, K. Imai, T. Hirokawa, & Kihara D. *Adv Appl Bioinform Chem*. 13: 11-25 (2020).
- [184] Computational structure modeling for diverse categories of macromolecular interactions.  
T. Aderinwale, C.W. Christoffer, D. Sarkar, E. Alnabati, & D. Kihara. *Curr. Opin. Str. Biol.* 64: 1-8. (2020).
- [183] Protein structure modeling from cryo-EM map using MAINMAST and MAINMAST-GUI plugin.  
G. Terashi, Y. Zha, & D. Kihara. *Methods Mol Biol*. 2165: 317-336. (2020)
- [182] IDP-LZerD: Software for Modeling Disordered Protein Interactions.  
C. Christoffer & D. Kihara. *Methods Mol Biol*. 2165: 231-244. (2020)

- [181] Phage G Structure at 6.1 Å Resolution, Condensed DNA, and Host Identity Revision to a *Lysinibacillus*.  
B. González, L. Monroe, K. Li, R. Yan, E. Wright, T. Walter, D. Kihara, S.T. Weintraub, J. A. Thomas, P. Serwer & W. Jiang.  
*J Mol Biol.* doi: 10.1016/j.jmb.2020.05.016. (2020).
- [180] MAINMASTseg: Automated Map Segmentation Method for Cryo-EM Density Maps with Symmetry.  
G. Terashi, Y. Kagaya, & D. Kihara.  
*J Chem Inf Model.* 60:2634-2643 (2020)
- [179] Trends in software developments of biomolecular structural modeling and prediction.  
D. Kihara,  
*Jikken Igaku (Experimental Medicine)*, 38: 866-871, (in Japanese) (2020)
- [178] A simple but effective BERT model for dialog state tracking on resource-limited systems.  
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*International Conference on Acoustics, Speech, and Signal Processing (ICASSP)* (2020)
- [177] Path-LZerD: Predicting assembly order of multimeric protein complexes.  
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*Methods in Mol. Biol.*, 2074: 95-112, (2020)
- [176] Protein secondary structure detection in intermediate-resolution cryo-EM maps using deep learning.  
G. Terashi, S.R.M.V. Subramaniya & D. Kihara,  
*Jikken Igaku (Experimental Medicine)*, 38: 82-86, (in Japanese) (2020)
- [175] 2DKD: A toolkit for content-based local image search.  
J.S. Deville, D. Kihara, & A. Sit,  
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- [174] Protein docking model evaluation by 3D convolutional neural networks.  
X. Wang, G. Terashi, C. Christoffer, M. Zhu, & D. Kihara,  
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- [173] Performance and enhancement of the LZerD protein assembly pipeline in CAPRI 38-46.  
C. Christoffer, G. Terashi, W.H. Shin, T. Aderinwale, S.R.M.V. Subramaniya, L. Peterson, J. Verburgt, & D. Kihara,  
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- [172] Advances in structure modeling methods in cryo-electron microscopy maps.  
E. Alnabati & D. Kihara,  
*Molecules*, 25: 82, (2019)
- [171] Matching of EM map segments to structurally-relevant Bio-molecular regions.  
M. Zumbado-Corrales, L. Castillo-Valverde, J. Salas-Bonilla, J. Viquez-Murillo, D. Kihara, & Juan Esquivel-Rodriguez,  
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- [170] A prospective compound screening contest identified broader inhibitors for Sirtuin 1.  
S. Chiba, , W.H. Shin, D. Kihara, , & M. Sekijima. (53 authors).  
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- [169] NNTox: Gene ontology-based protein toxicity prediction using neural network.  
A. Jain & D. Kihara,  
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- [168] Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment.  
M.F. Lensink, , C. Christoffer, G. Terashi, W.H. Shin, T. Aderinwale, S.R.M.V. Subramaniya, D. Kihara , , & S. J. Wodak, (105 authors)  
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- [167] The CAFA challenge reports improved protein function prediction and new functional annotations for hundreds of genes through experimental screens.  
N. Zhou, , A. Jain, , , D. Kihara, , , P. Radivojac, & I. Friedberg (167 authors),

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Z. Ding & D. Kihara,  
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- [161] Three-dimensional Krawtchouk descriptors for protein local surface shape comparison. A. Sit, W.S. Shin, & D. Kihara,  
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- [160] SHREC'19 Classification in cryo-electron tomograms.  
I. Gubins, G. van der Shot, R. C. Veltkamp, F. Foerster, X. Du, X. Zeng, Z. zhu, L. Chang, M. Xu, E. Moebel, T. M. Lai, X. Han, G. Terashi, D. Kihara, B. A. Himes, X. Wan, J. Zhang, S. Gao, Y. Hao, Z. Lv, X. Wan, Z. Yang, Z. Ding, X. Cui, & F. Zhang,  
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F. Langenfeld, A. Axenopoulos, H. Benhabiles, P. Daras, A. Giachetti, X. Han, K. Hammoudi, D. Kihara, T. M. Lai, M. Melkemi, S. K. Mylonas, G. Terashi, Y. Wang, F. Windal, & M. Montes,  
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X. Han, A. Sit, C. Christoffer, S. Chen, & D. Kihara  
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- [156] The balancing act of intrinsically disordered proteins: enabling functional diversity while minimizing promiscuity  
Mauricio Macossay-Casillo, Giulio Marvelli, Mainak Guharoy, Aashish Jain, Daisuke Kihara, Peter Tompa, & Shoshana Wodak,  
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- [154] Modeling protein-protein interactions with intrinsically disordered proteins.  
C. Christoffer, & D. Kihara  
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- [153] Study of the variability of the native protein structure.  
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I.K. Khan, A. Jain, R. Rawi, H. Bensmail, & D. Kihara  
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G. Terashi & D. Kihara  
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A. Jain, H. Gali, & D. Kihara  
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G. Terashi & D. Kihara  
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G. Terashi & D. Kihara  
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Z. Ding, Q. Wei, & D. Kihara  
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W. H. Shin & D. Kihara  
*Methods in Mol. Biol.*, 1762: 105-121 (2018)
- [142] Recent computational methods for predicting protein-protein interactions using various protein features.  
Z. Ding & D. Kihara.  
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- [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  
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L. X. Peterson, W. H. Shin, H. Kim, & D. Kihara  
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- [139] Protein structure model refinement in CASP12 using short and long molecular dynamics simulations in implicit solvent.  
G. Terashi & D. Kihara  
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S. Yerneni, I. K. Khan, Q. Wei & D. Kihara  
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- [137] Protein 3D structure and electron microscopy map retrieval using 3D-SURFER2.0 and EM\_SURFER.  
X. Han, Q. Wei, & D. Kihara  
*Current Protoc Bioinformatics*, 60: 3.14.1-3.14.15 (2017)
- [136] 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  
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W. H. Shin, C. Christoffer, & D. Kihara  
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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)
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Q. Wei, J. McGraw, I. Khan, & D. Kihara.  
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- [4] Protein structure prediction (4th Edition), *Methods in Molecular Biology*, D. Kihara (ed.)  
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### Miscellaneous Publications:

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### Invited Talks/Selected Oral Presentations in Conferences

- [217] Protein 3D structure modeling for medium-resolution cryo-EM density maps, Online Seminar at the Carnegie Mellon University-Pitt CPCB Seminar series, October 30, 2020
- [216] Deep learning for detecting 3D structures of biomolecules, Data Science and Machine Learning seminar series, Purdue Fort Wayne, October 6th, 2020
- [213-5] Oral (video) presentations at ISMB 2020, July 13-16, 2020
- EM map segmentation and de novo protein structure modeling for multiple chain complexes with MAINMAST. Genki Terashi, Y. Kagaya, & D. Kihara
  - Protein contact map denoising using generative adversarial networks. Sai Raghavendra Maddhuri Venkata Subramaniya, A. Jain, Y. Kagaya, & D. Kihara
  - ContactPFP: Protein function prediction using predicted contact information. Yuki Kagaya, S. Flannery, A. Jain, & D. Kihara
- [212] "Protein 3D structure modeling from cryo-EM density maps", The 5th International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, December 2-6, 2019
- [211] "Deep neural network-assisted protein structure modeling for drug development from low resolution 3D cryo-EM maps", Annual Symposium of Purdue Institute of Drug Discovery, October 14, 2019
- [210] "Computational protein tertiary structure modeling from cryo-EM maps of intermediate resolution", D. Kihara, The Frontiers in Biophysics Seminar, Dept. of Physics, Purdue University, Sep 10, 2019
- [209] "Computational protein 3D structure modeling from cryo-electron microscopy density maps". Latin American High Performance Computing Conference (CARLA) 2019, University of Costa Rica, Sept 25-27, 2019
- [208] "Protein structure modeling for structure-based drug design", Symposium on Studies and development of treatment for rare disease, Ritsumeikan University, Shiga, Japan, Aug 30 2019
- [207] "Computational protein tertiary structure modeling from cryo-EM maps of intermediate resolution", Workshop on Mathematics and Computer Science in Modeling and Understanding of Structure and Dynamics of Biomolecules, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Banff, Alberta, Canada, August 9-11, 2019
- [206] "Enhancement for MAINMAST, de novo main-chain tracing method:symmetric multi-chain modeling, local refinement, and graphical user interface", Genki Terashi, Yuhong Zha, & D. Kihara M&M 2019 Microscopy & Microanalysis , Portland OR, August 4-8, 2019
- [205] "Defining the critical amino acids in the plant-conserved region and class-specific regions of cellulose synthase catalytic domains", Philip Rushton, Anna T. Olek, Lee Makowski, John Badger, C. Nicklaus Steussy, Cynthia Stauffacher, Daisuke Kihara, Maureen C. McCann, Nicholas Carpita, XV Cell Wall Meeting, July 7-12 , 2019, Cambridge UK
- [204] "Computational protein tertiary structure modeling from cryo-EM maps, protein docking, and protein 3D shape analysis", AIST, Tokyo, Japan, July 11, 2019
- [203] "Computational protein tertiary structure modeling from cryo-EM maps of intermediate resolution", RIKEN, Waco, Japan, July 8, 2019
- [202] "Computational protein tertiary structure modeling from cryo-EM maps of intermediate resolution", Tohoku University, Dept. of Computer Science, Sendai, Japan, July 5, 2019
- [201] Lactose derivatives as potential inhibitors of pectin methyltransferases, Melanie L'Enfant, Pricillia Kutudila, Catherine Rayon, Jean-Marc Domon, Woong-Hee Shin, Daisuke Kihara, Anne Wadouachi, Jerome Pelloux, Gwladys Pouceau, Corinne Pau-Roblot, Reseau francais des parois, May 13-16, 2019, Roscoff, France
- [200] 2019 Purdue Hitchhiker's Guide to the Biomolecular Galaxy Symposium , May 8-9 , 2019



- LZerD pipeline for template-based and ab initio protein-protein interaction modeling (oral), C. Christoffer, D. Kihara
- [199] Human and LZerD server pipeline for template-based and ab initio protein-protein interaction modeling. 7th CAPRI Evaluation meeting, April 3-5, 2019, Hinxton, UK.
- [198] Computational protein structure modeling for medium to low resolution cryo-electron microscopy, 16th Annual Conference of the Midsouth Computational Biology & Bioinformatics Society (MCBIOS '19), March 28-30, 2019
- [198] Computational prediction of protein toxicity from sequence using gene ontology terms(oral), A. Jain & D. Kihara, 2019 ASM Biothreats, Jan 29-31, 2019
- [197] CASP13 evaluation meeting, Round table discussion on CAPRI protein docking session, Cancun, Mexico, Dec. 1-4, 2018
- [196] Computational modeling of protein-protein interactions, Indiana University, Dept. of Chemistry, Bloomington, Oct 16 (Tue), 2018
- [195] Computational protein structure modeling for high to medium resolution cryo-electron microscopy density maps, University of Illinois, Urbana-Champaign, 2269 Beckman Institute, Sept. 24, 2018, 3pm
- [194] Computational prediction and modeling for protein-drug and protein-protein interactions, The University of Alabama at Birmingham, Sept. 14, 2018
- [193] De novo protein structure modeling for cryo-EM maps, Coarse-grained modeling of structure and dynamics of biomacromolecules, Telluride, CO, July 23-27, 2018
- [191-2] 3D-SIG at ISMB, Chicago, IL
- Predicting the assembly order of multimeric heteroprotein complexes, LX Peterson, Y. Togawa, J. Esquivel-Rodriguez, G. Terashi, C. Christoffer, A. Roy, W.H Shin, D. Kihara
  - MAINMAST: De novo main-chain modeling for EM maps using tree-graph optimization, G. Terashi, D. Kihara
- [190] Computational protein structure modeling for medium to low resolution cryo-EM density maps, National Institutes for Quantum and Radiological Science and Technology, Kizu, Nara, Japan, July 4, 2018
- [189] Computational protein structure modeling for medium to low resolution cryo-EM density maps, AIST, Tokyo, June 25, 2018
- [188] Algorithm and Chimera plugin of MAINMAST, de novo main-chain tracing method for EM Maps (talk and poster), Genki Terashi and Yuhong Zha, & D. Kihara, Hitchhiker's Guide to the Biomolecular Galaxy, May 9-10, 2018, Purdue University
- [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 *Cyanothece* sp. 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 Alpha 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. 4<sup>th</sup> SNU Bioinformatics Workshop, Seoul National University, Seoul, Korea, June 29-30, 2015.
- [145] Genome-scale identification and characterization of moonlighting proteins. The 15<sup>th</sup> 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 59<sup>th</sup> 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, 11<sup>th</sup> 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, 25<sup>th</sup> 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, 5<sup>th</sup> 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 4<sup>th</sup> IEEE International Conference on e-Science, IUPUI, Indianapolis, Dec. 12, 2008
- [51] Informatics approaches for studying protein sequence, structure, and function in omics era.  
Dept. of Biological Sciences, Purdue University, October 15, 2008
- [50] Quality assessment of template-based protein structure prediction.  
University of Illinois at Chicago, Department of Bioengineering, Chicago, IL, February 26, 2008
- [49] Computational protein structure and function prediction.  
Chung-Ang University, Statistics Department, Seoul, Korea, December 27, 2007
- [48] Template-based protein structure prediction and beyond.  
Korea Institute for Advanced Study (KIAS), Daejeon, Korea., December 26, 2007
- [47] Protein function prediction for proteomics era.  
7th KIAS-Soongsil Conference, Soongsil Univ., Seoul, Korea., October 4-6, 2007
- [46] A fast method for high throughput comparison of tertiary structure and physicochemical properties. (Session chair)  
Biomedical Engineering Society Annual Meeting, Los Angeles, CA, September 26-29, 2007
- [45] Surface shape-based protein structure classification and search.  
Interface 2007: the 39th Symposium on the interface of statistics, computing science, and applications, Doubletree Hotel, Philadelphia, May 23-26, 2007
- [44] Protein function and structure prediction for proteomics analyses.  
Indiana University, Dept. of Informatics, Bloomington, IN, May 3, 2007.
- [43] Advanced techniques for protein function prediction and protein tertiary structure search for proteomics analyses.  
Nara Institute of Science and Technology, Nara, Japan, December 28, 2006
- [42] Bioinformatics: Introduction and advanced topics.  
Graduate program, Kansai Medical University, Osaka, Japan, December 25, 2006
- [41] Advanced techniques for protein function prediction and protein tertiary structure search for proteomics analyses.  
Ajinomoto Life Science Institute, Kawasaki, Japan, December 22, 2006
- [40] Round table discussion on function prediction at Critical Assessment of Techniques for Protein Structure Prediction (CASP7) Asilomar Conference Center, CA, November 26-30, 2006
- [39] Enhanced protein function prediction for proteomics analysis.  
Daisuke Kihara & Troy Hawkins, Biomedical Engineering Society Annual Meeting 2006, Systems Biology and Bioinformatics track, Hyatt Regency Chicago, IL. IUPUI, Indianapolis, IN, October 12, 2006.
- [38] Protein function prediction from sequence and structure.  
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: 10<sup>th</sup> Anniversary of KEGG. PALULU Plaza, Kyoto, Japan, December 15-16, 2005
- [32] Protein Function Prediction in the Proteomics Era.  
International Symposium on Frontiers of Computational Science 2005  
Noyori Conference Hall, Nagoya University, Japan, December 12-13, 2005
- [31] Protein function prediction methods beyond BLAST search.  
Structural Biology Seminar Series, Dept. of Biological Sciences, Purdue University, November 16, 2005
- [30] Protein function prediction in structural genomics era.  
Computing Research Institute, CS&E Seminar Series, Purdue University, October 19, 2005
- [29] Protein function prediction from sequence and structure.  
Mini-Workshop on Computational Studies on Proteins, Children's Hospital Research Foundation, Cincinnati, Ohio, Sep. 8, 2005
- [28] The use of context-based functional association in automated protein function prediction methods.  
Automated Function Prediction – Special Interest Group, (AFP-SIG), ISMB (International Conference on Intelligent Systems for Molecular Biology), Detroit, Michigan, 24, June, 2005.
- [27] Voxelized Protein Model for Fast Protein Docking and Function Prediction.  
Midwest Computational Structural Biology Workshop Brook Lodge,  
Michigan State University, Augusta, Michigan, April 30 – May 1, 2005
- [26] Toward a better template-based protein structure prediction.  
Dept. of Chemistry, Biochemistry Division seminar, Purdue University, 1 April, 2005
- [25] Conserved Small RNA Families in Gamma-Proteobacteria.  
Computational Biology Research Center, Tokyo, Japan, 28 December 2004.
- [24] Computational sequence and structure analyses.  
Biological Sciences Faculty Research Presentations, Dept. of Biological Sciences, Purdue University, 9 December, 2004
- [23] Comparative genomics study of non-coding RNA in Gamma-proteobacteria  
Ecolunch, Dept. of Biological Sciences, Purdue University, 17 November, 2004
- [22] Genome-scale Protein Structure Assignment to Microbial Genome Sequences.  
Ninth Annual Purdue University Biophysics Symposium, 25 October 2003
- [21] PDB is a Covering Set of Small Protein Structures.  
Bioinformatics Center, Kyoto University, Japan, 20 October 2003.
- [20] Genome-scale protein structure assignment to microbial genomes.  
International Workshop for Escherichia coli towards New Biology in the 21<sup>st</sup> Century.  
Awaji-shima, Japan, 15-17 October, 2003
- [19] Revisiting protein Structure Space – PDB is a Covering Set of Small Protein Structures.  
Computational Biology Research Center, Tokyo, Japan, 14 October 2003.
- [18] Revisiting Protein Structure Space for Prediction – PDB is a Covering Set of Small Protein Structures.  
Bioinformatics Seminar Series, Purdue University, 9 September 2003.
- [17] Protein Structure/Function Prediction on a Genome Scale.  
The Whitney Laboratory/Dept. of Computer Science, University of Florida, Gainesville, Florida, 7-8 April, 2003.
- [16] Genome Scale Protein Structure Prediction.  
Computer Science Dept., Virginia Polytechnic Institute and State University, Blacksburg, Virginia, 3 April, 2003.
- [15] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biology, The University of Nebraska at Omaha, Omaha, Nebraska, 1 April, 2003.

- [14] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biological Sciences, Purdue University, West Lafayette, Indiana, 25 March, 2003.
- [13] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Informatics, Indiana University, Bloomington, Indiana, 6 March, 2003.
- [12] Protein Structure/Function Prediction on a Genome Scale.  
Dept. of Biology, University of Kentucky, Lexington, Kentucky, 4 February, 2003.
- [11] Protein Structure/Function Prediction on a Genome Scale.  
Donald Danforth Plant Science Center, St. Louis, Missouri, 28 October, 2002.
- [10] Ab initio Protein Structure Prediction Method on a Genome Scale.  
Computational Biology Research Center, Tokyo, Japan, 12 October, 2001
- [9] An Ab initio Protein Structure Method Using a Lattice Model.  
Structural Bioinformatics Division Seminar, Yokohama City University, Japan, 11 October, 2001
- [8] A Lattice Model Based Protein Structure Prediction which Does Not Use  
Template Structures of Homologous Proteins.  
Biophysics Department Seminar, Nagoya University, Japan, 10 October, 2001
- [7] TOUCHSTONE: Ab initio Structure Prediction Method Using Restraints  
Derived from Threading.  
Research Society of Computational Genomics, the Biophysical Society of Japan  
Institute for Protein Research, Osaka University, Japan, 9 October, 2001
- [6] Ab initio Protein Structure Prediction Using Restraints Derived from Threading.  
Department of Biochemistry, Cambridge University, UK, 9 September, 2001
- [5] Toward Genome Scale Ab initio Protein Folding Prediction.  
Conference on “Experimental & Theoretical Approach for Protein Folding”,  
sponsored by Mirai Kaitaku Kenkyukai (Frontier Research Society)  
Okazaki Conference Center, Institute for Molecular Science, Okazaki, Japan, 10-12 January, 2001
- [4] Prediction of Protein Structure and Function on a Genome Scale.  
Jeffrey Skolnick, Andrzej Kolinski, Daisuke Kihara and Piotr Rotkiewicz.  
23<sup>rd</sup> Annual Meeting of Molecular Biology Society of Japan, Kobe, Japan, 15 December, 2000
- [3] Generalized Comparative Modeling of Protein Structures.  
Electrotechnical Laboratory, National Inst. of Advanced Industrial Science,  
Tsukuba, Japan, 18 September, 2000
- [2] Analyses of Genome Sequences through Internet.  
Kansai Medical University, Japan, 24 March, 1998
- [1] Current 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

- [206-8] 3 online poster presentation at Frontiers in Cryo-Electron Microscopy, Keystone Symposia, Feb. 3-4, 2021
- Super resolution cryo-EM maps with 3D generative adversarial networks. Sai Raghavendra Maddhuri Venkata Supramaniya, Genki Terashi, & D. Kihara
  - VESPER: Global and local cryo-EM map alignment and database search using local density vectors. Genki Terashi, Xusi Han, Siyang Chen, & D. Kihara
  - Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning. Xiao Wang, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, & D. Kihara
- [204-5] 2 poster presentations at 5th Annual Southern California Cryo-EM Symposium, Oct 30, 2020

- Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning. Xiao Wang, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, & D. Kihara
  - De novo protein structure modeling tool MAINMAST for multiple chain complexes, bound ligands in EM maps and map alignment. Genki Terashi, Xusi Han, Siyang Chen, Yuki Kagaya, & D. Kihara
- [203] (invited online forum) Pandemic Supermind, MIT Center for Collective Intelligence, May-June 2020
- [202] “Protein secondary structure detection in intermediate resolution cryo-EM maps using deep learning” S.R.M.V. Subramanya, G. Terashi, D. Kihara, 2020 Midwest Consortium for High-resolution cryo-EM, March 5, 2020.
- [201] "Ema2sec: Protein secondary structure detection in intermediate resolution cryo-EM maps using deep learning", Sai Raghavendra Maddhuri Venkata Subramanya, Genki Terashi, D. Kihara, Workshop on "Learning Meaningful Representations of Life", 33rd Conference on Neural Information Processing Systems (NeurIPS), Vancouver, Canada, December 13, 2019
- [200] Improved de novo main-chain tracing method MAINMAST for multi-chain modeling, local refinement, and graphical user interface (poster), Genki Terashi, Yuhong Zha, & D. Kihara, Missouri Symposium in Molecular Biophysics, Structural Electron Microscopy, April 25-26, 2019
- [199] Extending computational protein complex modeling: Disordered protein interactions & Assembly order of multimeric protein complexes (poster), 7th CAPRI Evaluation meeting, April 3-5, 2019, Hinxton, UK
- [197-8] 2019 Annual Biophysical Society Meeting, Baltimore, MD, March 2-6, 2019
- (poster) Improved de novo main-chain tracing method MAINMAST for multi-chain modeling, local refinement, and graphical user interface (poster), Genki Terashi, Yuhong Zha, & D. Kihara
  - (poster) Modeling the assembly order of multimeric heteroprotein complexes (poster), Lenna X. Peterson et al.
- [193-6] Sigma Xi Purdue Chapter poster competition, Stewart Center, Purdue, Feb. 20, 2019.
- "De novo main-chain modeling for EM maps using MAINMAST", Genki Terashi
  - "Accelerating protein function discovery using computational tools", Aashish Jain
  - "Emap2sec: protein secondary structure detection in intermediate resolution cryo-EM maps using deep learning", Sai Raghavendra Maddhuri Venkata Subraman
  - "PL-Patchsurfer: a virtual screening program for template-based modeling structure using molecular surfaces", Woong-Hee Shin
- [192] Purdue Institute for Drug Discovery, 5th Annual Symposium, Sep. 28 (Fri), Stewart Center, Purdue University 2018
- Research project presentation D. Kihara
  - (poster) "PL-PatchSurfer2: A virtual screening method tolerant to receptor structure variation using surface patch matching", Woong-Hee Shin & D. Kihara
- [191] Detecting multifunctional proteins by applying deep learning to academic literature", Hareesh Gali, Purdue Undergraduate Research Poster Symposium, Apr 10 (Tue), 2018, PMU Ballrooms, Purdue University
- [189-90] 62nd Biophysical Society Annual Meeting, San Francisco, CA, February 17-21, 2018
- (poster) Reliability of electron microscopy atomic model refinement, Lyman Monroe, G. Terashi, & D. Kihara
  - (poster) Structure modeling of disordered protein interactions, L.X. Peterson, A. Roy, C. Christoffer, G. Terashi, & D. Kihara
- [184-8] Sigma Xi Research Award Poster Competition, Stewart 218A-D, Purdue University, Feb. 21 (Wed), 2018
- Computational methods for predicting protein-protein interactions in plants, Ziyun Ding, D. Kihara

- Structure Fitting for low-resolution EM maps, Eman Alnabati, Juan Esquivel-Rodriguez, D. Kihara
  - Local structure detection in cryo-EM maps, Sai Raghavendra Madduhuri, Genki Terashi, D. Kihara
  - PL-PatchSurfer2: a virtual screening method tolerant to receptor structure variation using surface-patch matching, Woong-Hee Shin, D. Kihara
  - Elastic network models for flexible protein-protein docking, Charles Christoffer, D. Kihara
- [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] Three 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] Five poster 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
- [167-170] Great Lakes Bioinformatics Conference (GLBIO 2015), Purdue University, IN, May 18-20, 2015
- (poster) Protein side-chain conformation prediction methods are accurate in different residue environments. Lenna Peterson, X. Kang, & D. Kihara
  - (poster) PL-PatchSurfer2.0: A fast virtual screening program using surface patch based on 3DZernike Descriptors. Woong-Hee Shin & D. Kihara
  - (poster) Genome-scale identification and characterization of moonlighting proteins. Ishita Khan & D. Kihara
  - (poster) Fitting of multiple protein chains by iterative manipulation of cryo-EM maps. Lyman Monroe & D. Kihara
- [165-6] Undergraduate Research Poster Symposium, Purdue University, April 14, 2015
- Distributed heterogeneous cluster computing with computational proteomics, Aditya Vaidyam, & D. Kihara

- Analysis of bioinformartics databases, Weichuan Luo, Tiange Dong, Andrew Walden, Tianmu Hu, Ray Ji, Eric Petit, Tomii Lee, & D. Kihara
- [164] Fast large scale comparison and structure fitting for low-resolution electron microscopy maps (poster), Juan Esquivel-Rodriguez & D. Kihara, 3D-SIG, Boston, July 11-12, 2014
- [163] Towards Plant-specific protein gene function prediction (poster), Akshay Kumar, Ishita Khan, D. Kihara, Plant Biology 2014, Portland, Oregon, Jul 12-16, 2014
- [161] Exploring protein interfaces: Steered molecular dynamics and free energy calculations to rank protein-protein docking poses. L.J. Kingsley, J. Esquivel-Rodriguez, D. Kihara, M. Lill, Great Lakes Drug Metabolism & Disposition Group 2014 Meeting, Sheraton Indianapolis City Centre Hotel, Indianapolis, IN, May 15-16, 2014
- [159-160] Undergraduate Research Poster Symposium, Purdue University, April 8, 2014
  - Logic patterns for finding functionally related genes in Escherichia coli, Ishita Khan, Tiange Dong, Linzi Chen, Weichuan Luo, D. Kihara
  - Interactive visualization of Gene Ontology hierarchy, Qing Wei, I. Khan, D. Kihara
- [156-8] The Office of Interdisciplinary Graduate Programs, Spring Reception Poster Presentation, Purdue University, April 2, 2014
  - Assessing Protein Side - Chain Conformation Prediction Methods in Different Residue Environments, Lenna Peterson
  - Genome - scale Identification and Characterization of Moonlighting Proteins, Ishita Khan
  - Enhanced Electron Microscopy Fitting Using Markov Random Fields, Juan Esquivel-Rodriguez
- [155] 3D-SURFER 2.0: web platform for real-time comparison, visualization and characterization of protein surfaces" Y. Xiong, J. Esquivel-Rodriguez, L. Sael & D. Kihara, Annual Symposium of the Protein Society, Boston, MA, July 20-23, 2013
- [154] Biochemical characterization of an Arabidopsis pectin methylesterase AtPME3 and a pectin methylesterase inhibitor. F. Senechal, M. L'Enfant, JM Domon, E. Rosiau, P. Marcello, O. Surcouf, J. Esquivel-Rodriguez, A. Mareck, F. Guerineau, H-R. Kim, E. Bonnin, E. Jamet, J. Mravec, D. Kihara, M-C. Ralet, P. Lerouge, J. Pelloux, C. Rayon, The XI Cell Wall Meeting, Nantes, July 7-12, 2013
- [153] Characterization of cytosolic protein complexes in plants using multi-step chromatographic separation and quantitative mass spectrometry. U. Aryal1, Y. Xiong, E. Mallery, M. Hall, J. Xie, D. Kihara, D. Szymanski. American Soc. for Mass Spectrometry, June 9-13, 2013, Minneapolis, MN.
- [152] Protein docking prediction guided by predicted protein-protein interface. D. Kihara, B. Li, J. Esquivel-Rodriguez, & D. La, 5<sup>th</sup> CAPRI (Critical Assessment of Predicted Interactions), Utrecht, the Netherlands, April 17-19, 2013.
- [151] Development of computational method for visualizing disordered regions during protein docking. Arthi Anand & D. Kihara, Undergraduate Research Poster Symposium, Purdue University, March 26, 2013.
- [150] EM-LZerD: EM Map Fitting for Multimeric Protein Complexes Using Rotation Invariant Surface Representation. J E.-Rodriguez & D. Kihara Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Keystone Symposia, Lake Tahoe, Mar 3-7, 2013.
- [149] Computational function prediction for moonlighting proteins. I Khan, M. Chitale, C. Rayon, D. Kihara. Sigma Xi Graduate Student/Post Doc Poster Competition, Purdue Univ, Feb.13, 2013.
- [148] Macromolecular structure modeling and electron microscopy fitting using 3D Zernike descriptors. D. Kihara, J. Esquivel-Rodriguez. Biophysical Society 57<sup>th</sup> Annual Meeting, February 2-6, 2013, Philadelphia, PA.
- [147] Next generation molecular surface representation for rapid global/local protein shape comparison, docking, and low-resolution data. D. Kihara, National Centers for Biomedical Computing (NCBC) Showcase, Nov. 8-9, Natcher Conference Center, Bethesda, MD
- [146] Local Similarity Search of Physicochemical Properties in Protein-Ligand Binding Sites. Lee Sael & Daisuke Kihara  
Translational Bioinformatics Conference (TBC) 2012, Jeju Island, Korea, Oct 13-16, 2012

- [145] Novel quantitative proteomic methods to discover and localize protein complexes.  
U.K. Aryal, Y. Xiong, E. Mallery, M.C. Hall, J. Xie, D. Kihara, P.N. Baker, D. B. Szymanski  
2012 Plant Genome Awardee Meeting, National Science Foundation, Arlington, VA, Sep. 6-7, 2012.
- [144] Biochemical characterization of an Arabidopsis pectin methylesterase AtPME3 and a pectin methylesterase inhibitor.  
F. Senechal, J-M Domon, M. L'Enfant, D. Tall-Ndoye, J. Esquivel-Rodriguez, F. Guerineau, HR Kim, E. Jamet, E. Bonnin, D. Kihara, M-C Ralet, J. Pelloux, C. Rayon  
Gordon Conference on Plant Cell Wall, Colby College, Waterville, ME, August 5-10, 2012
- [143] Computational function prediction for moonlighting proteins.  
Ishita Khan, Meghana Chitale, Catherine Rayon, Daisuke Kihara  
Automatic Function Prediction-Special Interest Group (AFP-SIG), ISMB Satellite meeting, Long Beach, CA, July 13-14, 2012
- [141-2] 3DSIG 2012, Structural Bioinformatics and Computational Biophysics, ISMB Satellite meeting, Long Beach, CA, July 13-14, 2012
- Fitting multimeric protein complexes into electron microscopy maps using 3D Zernike descriptors, Juan Esquivel-Rodriguez, Daisuke Kihara
  - Prediction of real-value fluctuation of globular proteins, Michal Jamroz, Andrzej Kolinski, Daisuke Kihara
- [140] A 'catalytic dimer' hypothesis for the synthesis of cellulose and other (1,4)-beta-glycans  
Nicholas C. Carpita (oral presentation), Anna T. Olek, Catherine J. Rayon, Lee Makowski, Shiyou Ding, Peter Ciesielski, Lake Paul, Subhangi Ghosh, Daisuke Kihara, Michael Crowley, Michael Himmel, Jeffrey Bolin  
The 23<sup>rd</sup> International Conference on Arabidopsis Research (ICAR), Vienna, Austria, July 3-7, 2012
- [139] Logic Patterns of Homologous Genes Across Species. Lillian Liu, Huairuo Ren, Yu Leng, Meghana Chitale, Daisuke Kihara, 2012 Undergraduate Research and Poster Symposium, Purdue University, April 10 2012
- [138] Fitting multimeric protein complexes into electron microscopy maps using 3D Zernike descriptors.  
Juan Esquivel-Rodriguez, Daisuke Kihara  
6<sup>th</sup> International Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods. Lake Tahoe, CA, March 14-18, 2012
- [137] Computational methods for multiple protein docking for asymmetric complexes.  
J. Esquivel-Rodriguez, Daisuke Kihara  
Biophysical Society 56th Annual Meeting, San Diego, California, Feb. 25-29, 2012
- [135-6] Sigma Xi Graduate Student Research Award Competition, Purdue University, Feb. 15, 2012
- Macromolecular structure modeling and electron microscopy fitting using 3D Zernike descriptors, J. Esquivel-Rodriguez & D. Kihara
  - In-depth performance evaluation of PFP and ESG sequence-based function prediction methods in CAFA 2011 experiment, I. Khan, M. Chitale, & D. Kihara
- [133-4] Purdue University Nano-Bio Student Symposium, Purdue University, Sept. 1, 2011
- Protein Docking Prediction Using Predicted Protein-Protein Interface, B. Li & D. Kihara
  - Multi-LZERD: Multiple Protein Docking for Asymmetric Complexes, J. E. Rodriguez & Kihara
- [130-2] International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July 17-19, 2011
- Binding ligand prediction by comparing local surface patches of potential pocket regions, L. Sael & D. Kihara
  - MULTI-LZERD: Multiple protein docking for asymmetric complexes, J. Esquivel-Rodriguez & D. Kihara

- Functional coherence assessment for protein groups and its application to pathway assignment, M. Chitale, S. Palakodety & D. Kihara
- [127-9] 3D-SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July 15-16, 2011
- Binding ligand prediction by comparing local surface patches of potential pocket regions, L. Sael & D. Kihara
  - Rapid comparison and multimeric protein complex fitting for low-resolution electron microscopy data, D. Kihara, L. Sael & J. Esquivel-Rodriguez
  - MULTI-LZERD: Multiple protein docking for asymmetric complexes, J. Esquivel-Rodriguez & D. Kihara
- [126] Binding ligand prediction by comparing local surface patches of potential pocket regions. L. Sael & D. Kihara  
Automated Function Prediction (AFP) SIG, International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July 15-16, 2011
- [124-5] International Conference on Structural Genomics, May 10-14, 2011, Toronto, Canada.
- Rapid comparison and multimeric protein complex fitting for low-resolution electron microscopy data, J. Esquivel-Rodriguez, L. Sael & D. Kihara
  - Binding ligand prediction by comparing local surface patches of potential pocket regions, L. Sael & D. Kihara
- [121-3] 2011 Undergraduate Research and Poster Symposium, April 12 2011, North Ball Room, Purdue Memorial Union, Purdue University
- Fast identification of interacting proteins by considering shape and sequence features. Roshna Agarwal, Lee Sael, & D. Kihara.
  - SiteHunter: Interactive web application for determining protein ligand binding site location Yinlong Jin, R. Ren, K. Modi, S. Jain, D. La, & D. Kihara.
  - Mining association between gene ontology terms by using protein-protein interaction networks. Satwica Yersini, Meghana Chitale & D. Kihara.
- [120] General framework for multiple protein docking. Juan Esquivel-Rodriguez, D. Kihara  
Interdisciplinary Graduate Program Spring Reception, PMU, Purdue Univ., April 20, 2011
- [117-9] 3 poster presentations at Discovery Park Student Poster Session, April 6, 2011, Hall for Discovery and Learning Research (DLR), Purdue University
- Information theoretical approaches for protein sequences and structure. Yingfei Ma, & D. Kihara
  - SiteHunter: Interactive web application for determining protein ligand binding site location. Yinlong Jin, R. Ren, K. Modi, S. Jain, D. La, D. Kihara.
  - Docking low-resolution cryo-EM density maps aided by structural homology searching Wansuk Lim, L. Sael, D. Kihara.
- [115-6] Biophysical Society 55<sup>th</sup> Annual Meeting, Baltimore, Maryland, March 5-9, 2011.
- Novel methods for rapid comparison and multimeric protein complex fitting for low resolution electron microscopy data, Lee Sael, J. Esquivel-Rodriguez, D. Kihara
  - Local protein surface patch method for protein-ligand binding prediction, Lee Sael, J. Esquivel-Rodriguez, D. Kihara
- [111-4] The 21st International Conf. on Genome Informatics, Hangzhou, China, Dec. 16-18, 2010.
- Performance of SUPRB Threading Method in CASP9, M. Kurcinski, D. Kihara
  - Multiple Protein Docking for Asymmetric Hetero Oligomeric Complexes, J. Esquivel-Rodriguez, Y. Yang, D. Kihara
  - Functional coherence for protein groups by considering associations between gene ontology terms. Meghana Chitale, Shriphani Palakodety, D. Kihara
  - Protein Docking Prediction Using Predicted Protein-Protein Interface, B. Li, D. Kihara
- [110] A novel method for protein-protein interaction site prediction with phylogenetic substitution models.

- David La, D. Kihara  
The 24th Annual Symposium of the Protein Society, San Diego, CA, USA. August 1-5, 2010
- [109] Multiple protein docking prediction based on genetic algorithms and physics based scoring.  
Juan Esquivel-Rodriguez, D. Kihara  
18th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB),  
Boston, MA, July 11-13, 2010
- [108] Multiple Protein Docking Prediction Method Which Can Handle Asymmetric Hetero Oligomeric  
Complexes.  
J. Esquivel-Rodriguez, Y. Yang, D. Kihara  
3D-SIG, ISMB 2010, Boston, MA, July 9-10, 2010
- [107] Fitting Multimeric Complexes into Cryo-EM Maps Using Protein Docking Procedure and 3D  
Zernike Descriptors  
D. Kihara, J. Esquivel-Rodriguez, L. Sael  
3D-SIG, ISMB 2010, Boston, MA, July 9-10, 2010
- [102-6] 2010 Undergraduate Research Poster Symposium, Purdue University, Apr 7, 2010
- Why is there a limited number of protein fold in nature?, A. Magner, Y. D. Yang, & D. Kihara
  - Classification of local surface shape of ligand binding pockets, G. Martinez, Sael L. & Kihara
  - Structure-basis for protein-DNA interaction, William Hoffmann, & D. Kihara
  - Detecting surface shape complementarity for quick identification of interacting proteins, Paul Justin Tack, Roshna Agarwal, Sael Lee, D. Kihara
  - Conservation of sequence and atomic interactions in ligand binding sites of proteins, Sang Wook Lee, Sael Lee, D. Kihara
- [101] Comparative study of protein structure prediction methods  
Priyanka Surana, D. Kihara  
18th Undergraduate Research Day, Dept. of Biological Sciences, Purdue Univ. Apr. 3, 2010
- [100] A unified protein docking procedure with a shape complementarity screening using 3D Zernike  
descriptors  
D. Kihara, V. Venkatraman, YD Yang, L. Sael  
Biophysical Society meeting, San Francisco, CA, Feb 20-24, 2010
- [99] A unified protein docking procedure with a shape complementarity screening using 3D Zernike  
descriptors and ranking by physics-based scoring.  
D. Kihara, J. Esquivel-Rodriguez, V. Venkatraman, D. La, Y.D. Yang, L. Sael, B. Li, S. Ueng, S.  
Ahrendt.  
CAPRI Critical Assessment of Predicted Interactions 4th Evaluation Meeting, Barcelona, Spain,  
Dec 9-11, 2009
- [98] www.EcoliHub.org: An information resource for experimentation and modeling of E. coli K-12  
BL Wanner, WG Aref, T. Conway, KA Datsenko, SC Ess, MR Gribskov, JC Hu, D Kihara, H  
Mori, D Siegle, DR Whitaker  
American Society for Microbiology, May 17-21, 2009, Philadelphia, PA
- [97] N terminal Gly224-Gly411 domain in Listeria adhesion protein (LAP) interacts with receptor  
Hsp60  
B. Jagadessan, D La, D Kihara, AK. Bhunia  
American Society for Microbiology, May 17-21, 2009, Philadelphia, PA
- [96-99] The 21st Undergraduate Research Conference at Butler University, Butler University, Indianapolis,  
IN, April 17, 2009
- Computational protein function prediction, Gregg Thomas & D. Kihara
  - Protein Tertiary Structure Universe Viewed from the Perspective of Surface Shape, Matt Herron  
& D. Kihara
  - Comparative study of tertiary structure prediction methods, Priyanka Surana & D. Kihara
- [94-95] Biophysical Society Meeting, March 4, 2009, Boston MA.



- Local surface-based protein function prediction using Zernike descriptors. D. Kihara, Sael Lee, Rayan Chikhi
  - Threading without optimizing weighting factors for scoring function. Yifeng D Yang, C. Park, D. Kihara.
- [90-93] Sigma-Xi Graduate Student poster presentation, Stewart Center, Purdue Univ., Feb 18, 2009.
- Threading without optimizing weighting factors for scoring function. Yifeng D Yang, C. Park, D. Kihara.
  - Improvement of template-based protein structure prediction by suboptimal alignments. Hao Chen, D. Kihara.
  - ESG: Extended similarity group method for automated protein function prediction. Meghana Chitale, C. Park, D. Kihara.
  - Protein Representation for Efficient Comparison of Surface Properties. Sael Lee, Bin Li, David La, Raif Rustamov, D. Kihara.
- [89] EcoliHub: An information resource for experimentalists and modelers.  
D.R. Whitaker, W. G. Aref, K.A. Datsenko, S. Ess, M.R. Gribskov, D. Kihara, S. Kim, H. Mori, A. Roumani, B.L. Wanner  
Intelligent Systems for Molecular Biology (ISMB) 2008, July 19-23, 2008, Toronto, Canada
- [88] ESG: Extended Similarity Group Method for improved automated protein function prediction.  
M. Chitale, T. Hawkins, C. Park, D. Kihara  
Invited oral presentation at Automated function prediction special Interest Group at ISMB 2008 (AFP/Biosapiens 2008), July 18-19, Toronto, Canada
- [87] Automated protein function prediction using Extended Similarity Group (ESG) of sequences.  
M. Chitale, T. Hawkins, C. Park & D. Kihara  
Intelligent Systems for Molecular Biology (ISMB) 2008, July 19-23, 2008, Toronto, Canada
- [86] Ecolihub: Development of the [www.ecolicommunity.org](http://www.ecolicommunity.org) Information resource. B.L. Wanner, W.G. Aref, K. Datsenko, S. Ess, M.R. Gribskov, D. Kihara, S. Kim, H. Mori, D. R. Whitaker  
American Society for Microbiology, 108<sup>th</sup> General Meeting, Boston  
June 1-5, 2008
- [85] A fast methodology for high throughput comparison of tertiary structure and physicochemical properties  
Sael Lee, Bin Li, David La, Raif Rustamov, Daisuke Kihara  
The Computer Research Institute Poster Session, Purdue-Industry High Performance Computing Workshop, Purdue Memorial Union, Purdue Univ., April 6, 2008.
- [84] Disorder region prediction of E. coli proteins.  
Rupal Trivedi, Yifeng Yang, D. Kihara.  
Undergraduate Research and Poster Symposium, College of Science, Purdue University, Purdue Memorial Union, March 31, 2008.
- [83] Computational modeling of ABC transporters.  
Priyanka Surana, Yifeng Yang, D. Kihara.  
Undergraduate Research and Poster Symposium, College of Science, Purdue University, Purdue Memorial Union, March 31, 2008.
- [82] A fast methodology for high throughput comparison of tertiary structure and physicochemical properties.  
D. Kihara, Sael Lee, Bin Li, David La & Raif Rustamov  
Meeting of the Biophysical Society 52<sup>nd</sup> Annual Meeting and 16<sup>th</sup> International Biophysics Congress, Long Beach, CA  
February 2-6, 2008.
- [81] Predicting the error of template-based protein structure modeling by suboptimal alignment stability.  
Hao Chen & D. Kihara

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

- Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [70] Function prediction for proteomics datasets using PFP.  
Troy Hawkins, Meghana Chitale, & Daisuke Kihara.  
Indy'07: Indy Regional Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 31-June 2, 2007.
- [69] Structure modeling of E. coli proteome: Quality evaluation.  
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.  
The Computer Research Institute Poster Presentation, Atrium of MSEE building, Purdue University.  
April 5, 2007
- [68] Benchmark of new amino acid similarity matrices on recognition of distant protein structures.  
Yu-Hsuan Rex Cheng, Hao Chen & Daisuke Kihara.  
2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.  
April 4, 2007.
- [67] Structure modeling of E. coli proteome: Quality evaluation.  
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.  
2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.  
April 4, 2007.
- [66] Structure modeling of E. coli proteome: Homology models.  
Steve Krawczyk, Preston Spratt, Yifeng Yang & D. Kihara  
2007 Undergraduate Research and Poster Symposium, College of Science, Agriculture, Engineering, and Technology, Purdue University.  
April 4, 2007.
- [65] Structure modeling of E. coli proteome: Quality Evaluation  
Preston Spratt, Steve Krawczyk, Yifeng Yang & Daisuke Kihara.  
Dept. of Biological Science Undergraduate Research Presentation, Purdue University,  
March 31, 2007.
- [64] PFP: Sequence-based annotation of sequences and local sequence motifs with contextual GO term association  
Troy Hawkins, Stan Luban, David La & Daisuke Kihara  
Automated Function Prediction meeting, 2006, UC San Diego, San Diego, CA.  
Aug 30 – Sep 1, 2006.
- [63] EMD: an ensemble DNA regulatory motif discovery algorithm for Grid computing.  
Yifeng D. Yang, Jianjun Hu & Daisuke Kihara.  
TeraGrid '06, Indianapolis University Purdue University Indianapolis, Indianapolis, IN,  
June 12-15, 2006.
- [62] Template-based protein structure prediction with a reliability measure for structural genomics era.  
Hao Chen, Yen Hock Tan, & Daisuke Kihara.  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [61] Ligand binding site prediction with the visibility criteria.  
Bin Li, S. Thruvekere, M. Agrawal, K. Ramani & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [60] Multi-resolution protein representation for fast protein structure searching.

- Sael Lee, Bin Li, David La, Raif Rustamov, & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [59] On the effect of long-range interactions on the secondary structure formation of proteins.  
Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [58] Coiled-coil structures in E. coli interactome.  
Stan Luban, Akiyasu Yoshizawa & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [57] Neural network based protein domain prediction.  
Yen Hock Tan, Otoniel Venezuela, Evans A. Tapia & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006.
- [56] Statistical potential-based amino acid similarity matrices for aligning distantly related protein sequences.  
Yen Hock Tan, He Huang & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [55] Accounting for natural flexibility in protein structure prediction comparisons.  
Jairav Desai & Daisuke Kihara  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [54] EcoliPredict: bioinformatics prediction resource for EcoliHub.  
Barry Wanner, Daisuke Kihara, Troy Hawkins & Yifeng D. Yang  
The Third Annual Indiana Bioinformatics Conference, Center for Computational Biology and Bioinformatics, Indiana Univ. School of Medicine.  
May 19-20, 2006
- [53] EcoliPredict: bioinformatics prediction resource for EcoliHub  
Barry Wanner, Daisuke Kihara, Troy Hawkins and Yifeng D. Yang  
American Society for Microbiology ASM-FEMS Conference on Protein Traffic in Prokaryotes, Crete, Greece  
May 6-10, 2006
- [52] Using Neural Network in Protein Domain Prediction.  
Yen Hock Tan and Daisuke Kihara  
Undergraduate Research & Poster Symposium, College of Science, Purdue University  
April 11, 2006
- [51] Using Neural Network in Protein Domain Prediction.  
Yen Hock Tan and Daisuke Kihara  
14<sup>th</sup> Annual Undergraduate Research Day, Dept. of Biological Sciences, College of Science, Purdue University  
April 1, 2006
- [50] Including natural protein flexibility in predicted protein structure comparisons.  
Jairav Desai and Daisuke Kihara  
14<sup>th</sup> Annual Undergraduate Research Day, Dept. of Biological Sciences,

- College of Science, Purdue University  
April 1, 2006
- [49] Protein structure-sequence alignment with a reliability measure.  
Hao Chen and Daisuke Kihara  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006
- [48] A New Perspective on an Old Tool: Extending the Coverage of Sequence  
Similarity-Based Function Prediction with PFP.  
Troy Hawkins, Stan Luban and Daisuke Kihara  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006
- [47] Bridging geometric protein surface features and phylogenetic information for rapid identification  
of protein-protein interaction interfaces.  
David La, Denis Liversay and Daisuke Kihara  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006
- [46] Multi-resolution protein representation.  
Sael Lee, Bin Li, David La, Raif Rustamov and Daisuke Kihara  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006.
- [45] Ligand Binding Sites Prediction with the Visibility Criteria.  
Bin Li, Srinivasan Turuvekere, Manish Agrawal, Karthik Ramani and  
Daisuke Kihara.  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006
- [44] EMD: An ensemble algorithm for discovering regulatory motifs in DNA sequences.  
Yifeng D. Yang, Jianjun Hu, and Daisuke Kihara.  
Sigma Xi Graduate Student Research Poster Presentation, Purdue University  
February 14, 2006
- [43] A New Perspective on an Old Tool: Extending the Coverage of Sequence  
Similarity-Based Function Prediction with PFP.  
Troy Hawkins, Stan Luban and Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [42] Ligand Binding Sites Prediction with the Visibility Criteria.  
Bin Li, Srinivasan Turuvekere, Manish Agrawal, Karthik Ramani and  
Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [41] Protein-Protein Docking Algorithm Using Preidentified Binding Site Patches.  
Daisuke Kihara, Sael Lee, Karthik Ramani, Srinivasan Turuvekere, Manish Agrawal,  
And Bin Li  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [40] Dependence of the Accuracy of Protein Secondary Structure Prediction on  
Long-Range Interactions.  
Daisuke Kihara  
16th International Conference on Genome Informatics, Yokohama, Japan  
December 19-21, 2005
- [39] Evaluation and development of protein function prediction.  
Stan Luban, Troy Hawkins and Daisuke Kihara (Oral presentation)

- 16th Annual Argonne Symposium for Undergraduates in Science, Engineering and Mathematics,  
Argonne National Laboratory, Argonne, Illinois  
November 4th, 2005
- [38] Using neural network in protein domain prediction.  
Yen Hock Tan, Adolfo Tapia, Otoniel Venezuela, and Daisuke Kihara (Oral presentation)  
16th Annual Argonne Symposium for Undergraduates in Science, Engineering and Mathematics,  
Argonne National Laboratory, Argonne, Illinois  
November 4th, 2005
- [37] BioQ: A 3D Querying Engine for Proteins.  
Athurva Gore, Bin Li, Karthik Ramani & Daisuke Kihara  
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering,  
College of Science, Purdue University.  
August 2, 2005
- [36] Protein-protein Interaction Data Assessment.  
Ei Ei Phyu & Daisuke Kihara  
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering,  
College of Science, Purdue University.  
August 2, 2005
- [35] Comparison of distantly related protein sequence alignments with multiple amino acid similarity  
matrices.  
Yen Hock Tan & Daisuke Kihara  
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering,  
College of Science, Purdue University.  
August 2, 2005
- [34] Comparative study of small RNAs and small peptides in complete genome sequences.  
Stan Luban & Daisuke Kihara  
Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering,  
College of Science, Purdue University.  
August 2, 2005.
- [33] Protein Structure Prediction with ZDock 2.3.  
Luis Avila, Bin Li & Daisuke Kihara  
Marc/Aim Research Presentation, Burton Morgan Center for Entrepreneurship, Purdue  
University.  
July 28, 2005
- [32] PFP: Automatic annotation of protein function by relative GO association in multiple function  
prediction methods.  
Troy Hawkins & Daisuke Kihara  
ISMB, Detroit, Michigan, June 25 – 29, 2005.
- [31] Protein Structure-Sequence Alignment with a Reliability Measure.  
Hao Chen, Yen Hock Tan & Daisuke Kihara.  
Midwest Computational Structural Biology Workshop, Brook Lodge,  
Michigan State University, Augusta, Michigan  
April 30 – May 1, 2005
- [30] Comparing Tertiary Structures of Protein Active Sites.  
Yuhao Lin and Daisuke Kihara.  
Undergraduate Research Day, College of Science & College of Agriculture, Purdue University.  
April 11, 2005
- [29] Comparative Study of Small RNA and Small Peptides in Complete Genome Sequences.  
Stan Luban and Daisuke Kihara.  
Undergraduate Research Day, College of Science & College of Agriculture, Purdue University.  
April 11, 2005.
- [28] Computer Graphics Program in Foreign Language Instruction.

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

- First Annual Indiana Bioinformatics Conference.  
IUPUI, Indianapolis, 27 May, 2004.
- [15] Real-Time Manipulation of Keyframe Animation.  
Brian Seckinger, Rodney Weaver and Daisuke Kihara  
School of Science Undergraduate Research Day, Purdue University  
Purdue University, 17 April, 2004.
- [14] A Web-Interface for a Database of Microbial Intergenic Sequences.  
Jason Pardieck and Daisuke Kihara  
School of Science Undergraduate Research Day, Purdue University  
Purdue University, 17 April, 2004.
- [13] Comparative Study of Structural Non-Coding RNAs  
Stanislav Luban and Daisuke Kihara  
School of Science Undergraduate Research Day, Purdue University  
Purdue University, 17 April, 2004.
- [12] Computational prediction and experimental validation of iron and phosphate gene regulatory sites in the *Escherichia coli* K-12 and *Pseudomonas aeruginosa* PA01 genomes.  
Sam-Il Jung, Kaushik M. Setty, Khurram Siddiqi, Lu Zhou, Barry L. Wanner and Daisuke Kihara  
International Workshop for *Escherichia coli* Towards New Biology in the 21<sup>st</sup> Century.  
Awaji-shima, Japan, 15-17 October, 2003.
- [11] All-against-all protein structure comparison reveals the current database (PDB) is a covering set of small protein structures.  
Daisuke Kihara and Jeffrey Skolnick  
Corporate Partner Faculty Poster Session, Department of Computer Sciences, Purdue University.  
the Buchanan Club at Ross-Ade Stadium, Purdue University, 15 September, 2003.
- [10] PDB is a covering set of a single-domain protein structures.  
Daisuke Kihara and Jeffrey Skolnick  
Frontiers in Bioinformatics Symposium, Buffalo NY  
5-8 June, 2003
- [9] Classification and Analysis of Eukaryotic ABC Transporters in Complete Eukarya Genomes.  
Yoshinobu Igarashi, Daisuke Kihara and Minoru Kanehisa  
Genome Informatics 11: pp .274-275, Universal Academy Press, Tokyo (2000)
- [8] Classification and Analysis of Eukaryotic ABC Transporters in Complete Eukarya Genomes.  
Yoshinobu Igarashi, Daisuke Kihara and Minoru Kanehisa  
The Cold Spring Harbor Laboratory Meeting (New York, May 2000)
- [7] Detection of Membrane Proteins in the Whole Genome Sequences.  
Daisuke Kihara and Minoru Kanehisa  
Genome Informatics 1997, pp.300-301, Universal Academy Press, Tokyo (1997)
- [6] Systematic Analysis of Enzyme Structures and Metabolic Pathways.  
Daisuke Kihara and Minoru Kanehisa  
18<sup>th</sup> Annual Meeting of Molecular Biology Society of Japan (1997)
- [5] Prediction Method of Transmembrane Segments in Proteins Using Multiple Discrimination Functions.  
Daisuke Kihara and Minoru Kanehisa  
35<sup>th</sup> Annual Meeting of the Biophysical Society of Japan. P.172 (1997)
- [4] A Prediction Method for Transmembrane Segments in Proteins Utilizing Multiple Discrimination Functions.  
Daisuke Kihara, Toshio Shimizu and Minoru Kanehisa  
Genome Informatics 1996, pp.244-245, Universal Academy Press, Tokyo (1996)
- [3] Prediction of Transmembrane Segments in Proteins Using Characteristics by their Numbers and Positions.



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

## Research Support

### Current:

Building protein structure models for intermediate resolution cryo-electron microscopy maps.  
(NIH, \$1,200,000 total, 9/20/2020-7/31/2024) Role: PI

Modeling of Solution and SQ Behavior of Highly Concentrated IgG Based on Amino Acid Sequence  
(Eli Lilly, \$454,544 total, 2019-2021) Role: Multi-PI (with Michael Ladisch)

IIBR Informatics: Development of multimodal approaches for protein function prediction.  
(NSF BIO, \$427,507 total, 2020-2023) Role: PI

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

Revolutionizing the development and manufacturing of next-generation biologics  
(Discovery Park: Big Idea Challenge 2.0, \$300,000 total, 2019-2020) Role: co-PI (PI: R. Fischer)

Nanomanufacturing of protein macromolecular frameworks through integrated bioengineering and  
computational approaches  
(NSF, \$120,000 total, 2019-2022). Role: co-PI (PI: Masaki Uchida, Indiana University)

Collaborative Research: RoL: Nonlinear biochemistry of transcriptional activation domains  
(NSF, BIO, \$226,230 total, 09/01/2019-08/31/2022) Role: Multi-PI

Gift fund  
(Adobe, \$7,000, 8/1/2019 - ) Role: PI

### Completed

Deep neural network-assisted protein structure modeling for drug development for low-resolution 3D  
cryo-electron microscopy maps.  
(Purdue Institute of Drug Discovery, Purdue, \$150,000, 1/1/2019-12/31/2020) Role: PI

Collaborative Research: Efficient mathematical and computational framework for biological 3D image  
data retrieval  
(NSF, Mathematical Biology, \$542,383 total, 6/1/2016-7/31/2020) Role: PI

Purdue University Molecular Biophysics Training program. Trainee (1 year RA, 2019-2020) Charles  
Christoffer

Integrative genomics approach to computational assessment of threats (IGACAT)  
(IARPA, Virginia Tech, \$94, 500 total, 6/16/2017-5/31/2020) Role: co-PI (PI: Ron Kenyon)

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

Deep learning for 3D protein target – drug interaction  
(NVIDIA Academic Hardware Grant, one Tesla K40 GPU, ~\$3200 value) Role: PI

Novel quantitative proteomic methods to discover and localize endogenous protein complexes.  
(NSF, IOS, 10/01/2011-09/30/2015, \$1,709,230 total) Role: co-PI (PI: D. Szymanski)

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](http://www.EcoliCommunity.org) Information Resource.  
(NIH, 4/1/09 – 6/30/09, \$410,000 direct) Role: co-PI, (PI: Barry Wanner)

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

Bayesian models and Monte Carlo strategies in identifying protein or DNA sequence motifs.  
(Agency, NSF, Dev. of Math. Sci, \$ 160,246, 7/1/2006-6/30/2009, PI: Jun Xie) Role: co-PI

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

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

Development of a Protein sequence-structure alignment method for distantly related proteins. (PRF Summer Faculty Grant, Total \$7,000 direct cost, 06/01/2005-08/31/2005) Role: PI

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

## **Supervised Postdocs**

### Current

Daipayan Sarkar (PhD in Mechanical Engineering), July 2019 – current  
Genki Terashi (PhD in Pharmaceutical Sciences) April 2017 - current

### Former postdocs

Woong-Hee Shin (PhD in Chemistry), August 2014 – March 2019, assistant professor, Suncheon National University, Korea

Hyunrae Kim (PhD in physics), September 2011 – August 2016, assistant professor, Kyonggi University, Korea

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 assistant professor 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

### **Current Visiting Professors/Scholars**

None

### **Past Visiting Professors**

Saeed Salem, Associate Professor, Department of Computer Science, North Dakota State University, August 2018-December 2018  
Kujin Kim, Associate professor, School of Computer Science and Engineering, Kyungpook National University, South Korea, August 2018-December 2018  
K. Ramanathan, Associate Professor, Department of Biotechnology, VIT University, Vellore, India, January 2019-June 2019  
Genki Terashi, Junior Associate Professor, School of Pharmacy, Kitasato University, Tokyo, Japan, April 2015 – March 2017 (continuing as a postdoc)  
Xinyuan Zhou, Assistant Professor, Department of Computer Science & Technology, Changsha University, China March-December 2015  
Catherine Rayon, Professor, Dept. of Biology, Universite de Picardie Jules Verne, France January – May 2012  
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

### **Past Visiting Scholars**

Manuel Zumbaro Corrales, MS student, Costa Rica Institute of Technology, January 15 – Feb. 14, 2020  
Zhiqiang Jackie Huang, Huazhong Agricultural University, China, August 2017-May 2018  
Uttamkumar Samanta, West Bengal State University, India, October 2012 – May 2013, May-June 2018

### **Supervised programmers**

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

### **Supervised Students**

#### **Current Graduate Students:**

Aashish Jain (Biol/CS)  
Lyman Monroe (Biol)  
Sai Subramaniya (CS)  
Charles Christoffer (CS)  
Eman Alnabati (CS)  
Tunde Adrinwale (CS)  
Xiao Wang (CS)  
Jacob Verburgt (Biol)

#### **Graduated with Ph.D.**

Xusi Han (PULSe, Spring 2020), currently Well Fargo

Ziyun Ding (PULSe, Fall 2019) currently Convergent Genomics Inc.  
 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, Amazon > currently Google

### Other Former Supervised Graduate Students

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 (TTTech, Japan) Aug.-Nov. 2017	Israa Al-Qassem (CS) Jan.-Dec. 2017
Mengmeng Zhu (PULSe) 2015-2018	Yuki Kagaya (CS, Tohoku U., Japan) Sep 2019-Mar 2020

### Current Undergraduate Students

Pinaki Mohanty (CS) Spring 2020-	Vijay Bharadwaj (CS) Fall 2019-
Hao Wu (CS) Summer 2020-	Rohan Narasimha (CS) Summer 2020-
Hanwen Gu (CS) Summer 2020-	

### Former Undergraduate Students

#### Long-Term Research Project (2+ Semesters)

Stan Luban (Bio/CS) (Spring2004-Spring2006)	Rodney Weaver (CS) (Spring /Fall 2004)
Ei Ei Phyu (CS), Spring/Fall 2005	Jairav Desai (CS, DURl*), 2005-2006
Yen Hock Tan (CS) 2004-2006	Steve Krawczyk (Bio), Fall 2006, Spring 2007
Jennifer S Reeve (CS) (Summer 2004, 2011)	Preston Spratt (Bio), Fall 2006 – Spring 2008
Rupal Trivedi (Bio) Fall 2007-Spring2008, Spring 2010	Steven Ahrendt (Bio/CS) Fall 2008-Spring 2009
Devin Lockett (Bio) Fall 2008 – Spring 2010	Gregg Thomas (Bio) Summer 2008 – Fall 2009
Paul Tuck (CS) Summer 2009 – Spring 2010	Priyanka Surana (Bio) Fall 2007 – Spring 2010
Nicket Gupta (CS) Fall 2009-Spring 2010	Sangwook Lee (Bio) Fall 2009 – Spring 2010
Malvika Mathur (Bio) Fall 2008 – Spring 2010	Kunal Modi (CS) Fall 2009 – Fall 2010
Abram Magner (CS/Math)Spring 09 – Spring 10	Sajat Jain (CS) Fall 2009 – Fall 2010
Matt Herron (Bio/CS) Summer 2008 – Spring 2010	Shriphani Palakodety (CS) Fall 2009 - 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, DURl) Fall 12-Spring 13  
Guanqun Mao (CS, DURl) Fall 12-Spring 13  
Xiaowei Hong (Biol) Summer 2012 – Spring 2013  
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  
Xi He (Bio) Fall 2017-Spring 2018  
Yuhong Zha (CS) Fall 2017-Spring 2018  
Hareesh Gali (CS) Fall 2017-Spring 2019  
Max Shramuk (Biol) Summer 2017-Fall 2019  
Aung Myat (CS) Spring 2018-Fall 2018  
David Rivera (Biol) Fall 2019-Spring 2020  
Nirali Rai (CS) Spring 2019-Spring 2020

### 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  
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

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, DURl) Fall2012-Sprng 2013  
Linsheng Shen (Bio, DURl) 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  
Caleb Belth (CS) Fall 2015-Spring 2018  
Dan Ntala (Bio) Spring 2017-Fall2017  
Govind Girish (CS) Fall 2017-Fall 2018  
Aditi Acharya (Eng) Fall 2017-Spring 2019  
Qifen Chen (CS) Spring 2018-Fall 2018  
Sean Flannery (CS) Spring-Summer 2019  
Adrian Gerard Raj (CS) Spring 2019-Spring 2020

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  
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

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  
 Aishwara Mudgal (CS) Fall 2016  
 Kevin Shim (Bio) Spring 2017  
 Simeng Liao (Nankai U.) Summer 2017  
 Hao Zhu (Beijing U. Posts & Tel) Summer 2017  
 Varun Gupta (CS) Fall 2017  
 Yibin Wu (CS) Fall 2018  
 Nikita Rajaneesh (CS) Fall 2018  
 Vidhur Kumar (CS) Fall 2018  
 Adil Bozai (CS) Fall 2018  
 Yingfeng Lu (Shanghai Jiaotong U., CS) Sum. 19  
 Yilin He (Shandong U., CS) Summer 2019  
 Joseph Veltri (CS) Spring 2020  
 Jacob Moore (CS) Summer 2020-  
 Yifan Deng (CS, Wuhan U.) Summer 2020  
 Anurupa Karmakar (NIT Durgapur), Sum20

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  
 Natalie Oda (Bio) Spring 2017  
 Xiao Wang (Xi'an Jiaotong U.) Summer 2017  
 Hannah Zentner (CS) Fall 2017  
 Kavya Nagalakunta (CS) Fall 2017  
 Shohbit Makhija (CS) Fall 2018  
 Shantanu Nair (CS) Fall 2018  
 Matin Hormati (CS) Fall 2018  
 Rohith Ravindranath (CS) Spring 2019  
 Yiwei Zhang (Renesselaer Polytech, CS) Sum. 19  
 Manish Kannan (CS) Summer 2020  
 Abhinam Adari (CS) Summer 2020  
 David H. Kim (Biol) Summer 2020  
 Nguyen Do (CS) Spring 2020

### **K-12 Students**

Aditi Acharya (West Lafayette High), Summer 2014-Fall 2016  
 Katie Kranjak, Summer 2005 (high school student, Indiana Academy of Science)  
 Kashyap Akkinapally (Carmel High School, IN) Spring 2021-

### **Student Awards**

- Jacob Verburgt, Honorable Mention, NSF Graduate Research Fellowship application, April 2020.
- Sai Raghavendra Maddhuri Venkata Subramaniya, Travel Award, the Biophysical Society, for attending the 64<sup>th</sup> Annual Biophysical Society meeting, February 15-19, 2020.
- Sai Raghavendra Maddhuri Venkata Subramaniya, College of Science Travel Award, Purdue University, (for attending NeurIPS, “Learning Meaningful Representation of Life” workshop) , October 2019
- Lyman Monroe, The Teaching Academy 2018-2019 Graduate Teaching Award, Purdue University, April 9, 2019
- Lyman Monroe, Best TA Award, Department of Biological Sciences, Purdue University, March 29, 2019.
- Woong-Hee Shin, Poster Competition Award, Sigma Xi postdoc research poster competition, Purdue University, February 20, 2019
- Aashish Jain (CS), Poster Competition Award, Sigma Xi graduate student research poster competition, Purdue University, February 20, 2019
- 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 10<sup>th</sup> 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), 1<sup>st</sup> Place, Sigma Xi Graduate Poster Competition, February 14, 2006
- Yen Hock Tan (CS). Nominated for the Computing Research Association's (CRA) Outstanding Undergraduate Award for 2006 from Dept. of Computer Science
- Athurva Gore (ME) Top Poster Award at the Summer Undergraduate Research Fellowship (SURF) Poster Presentation, College of Engineering, College of Science, Purdue University, August 2, 2005
- Stan Luban (CS/Biol). Outstanding Research Award at the Undergraduate Research Day of College of Science & College of Agriculture, Purdue University. April 11, 2005.
- Otoniel Venezuela (CS). Graduate School Incentive Grant. School of Science, Purdue University. April 8, 2005.
- Yen Hock Tan (CS). Hewlett-Packard Fellowship. April, 2005.
- Ei Ei Phyu (CS). 2005 Howard Hughes Fellowship for Undergraduate Research in Bioinformatics.
- Stan Luban (CS/Biol). 2005 Summer Howard Hughes Undergraduate Research Internship.
- Yen Hock Tan (CS). 2005 Summer Howard Hughes Undergraduate Research Internship.
- Stan Luban (CS/Biol). Honorable Mention in the Computing Research Association's (CRA) Outstanding Undergraduate Award for 2005
- Stan Luban (CS/Biol). 2004 Summer Howard Hughes Undergraduate Research Internship.



- Manish Agrawal and Srinivasan S. Turuvekere (Mechanical Engineering). 2<sup>nd</sup> place in 2004 Purdue University's Burton D. Morgan Entrepreneurship Competition

### **Courses Taught**

CS590 Computing for Life Sciences, core course in the Computing in Life Science CLS Specialization for graduate program (Fall 2011-2020)

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, 2018, 2020)

BIOL696E Seminar Crystallography (Spring 2006)

### **Other Teaching Activities**

- Organizing Online Bioinformatics & Computational Biology Seminar Series, (Fall 2020 - )
- 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, graduate research seminar (Fall 2011, Fall 2018, Fall 2020)
- 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

- Frontiers in Bioinformatics (May 2020-present)
- Biomolecules (June 2019 – present)
- BMC Bioinformatics (March 2016 – present)
- Scientific Reports (Nature journal) (May 2015 – present)
- Frontiers Molecular Biosciences, guest editor (2020)
- Molecules, guest editor (2020)
- Methods, guest editor (2015)
- Associate Editor, International Journal of Knowledge Discovery in Bioinformatics (IJKDB) (2009- 2018)

### Professional Society

International Society of Computational Biology (ISCB)

- Publications Committee (Fall 2020 – present)

### Review of Grants

Domestic:

- NIH ZRG1 F04B-T (Nov. 2020)
- NIH ZDA1 (Feb. 2020)
- NIH MSFD (Feb. 2020)
- NIH BDMA (Feb 2015, Feb 2017)
- NIH T32 Training Programs (Oct. 2018, Oct 2019)
- NIH P41 Research Resource (Feb. 2018)
- NIH Independence award (Dec. 2017)
- NIH, ZRG1, STTR/SBIR (June 2012, October 2012, March 2014, March 2015, November 2015, March 2016, March 2017)
- NIH, Challenge Grant, RC1 (June 2009)
- National Science Foundation (NSF), IIBR panel (October 2020)
- 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)
- C3.ai DTI COVID-19 (May 2020)

International:

EU: European Research Council (September 2016)

UK: The Royal Society (October 2019), Biotechnology and Biological Science Research Council (BBSRC) (July 2012, July 2017, July 2018, May 2019), Medical Research Council (MRC) (November 2016), The Wellcome Trust (September 2011)

France: French National Research Agency (March 2012; May 2019), AFM-TELETHON Scientific Council (January 2017)

Czech: Czech Science Foundation (July 2020)

Switzerland: Swiss National Science Foundation (June 2019)

Poland: Foundation for Polish Science (September 2018), Polish National Science Centre (August 2011, April 2017, December 2017)

Luxembourg: National Research Fund (FNR) (August 2010)

Netherlands: Netherlands Organization for Scientific Research (March, 2006)

Israel: Israeli Ministry of Science, Technology and Space (June 2017), US-Israel Binational Science Foundation (January 2018)

Qatar: Qatar National Research Fund (2012, 2014, 2015)

Singapore: Agency of Science, Research & Technology (A\*STAR) (2010, 2011)

Saudi Arabia: KAUST Competitive Research Funding program (August 2020)

External Review

MRC Laboratory of Molecular Biology (LMB), University of Cambridge (December 2020)

PhD thesis external examiner:

- School of Information and Communication Technology, Griffith University, Gold Coast, Australia (March 2018, April 2020)
- International Center for Chemical and Biological Sciences, University of Karachi, Pakistan (July 2019)
- School of Computer Science and Engineering, Nanyang Technological University, Singapore (February 2018, December 2019)
- 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 Journal Papers

Acta Crystallographica Section D  
Amino Acids  
Annals of Biomedical Engineering  
Bioinformatics  
Biophysical Journal  
Biophysics (Japan)  
Biopolymers  
BMC Bioinformatics  
BMC Structural Biology  
BMC Systems Biology  
Briefings in Bioinformatics  
Briefings in Functional Genomics and Proteomics  
Cancer Informatics  
Cell Research  
Communications Chemistry (Nature journal)  
Computational and Structural Biotechnology Journal  
Computational Biology and Chemistry  
Current Protein and Peptide Science  
DNA Research  
FEBS Letters  
Frontiers in Bioengineering  
Future Medicinal Chemistry  
IEEE Transactions on Information Technology in Biomedicine  
IEEE Transactions on Nanobioscience  
IEEE/ACM Transactions on Computational Biology and Bioinformatics  
International Journal of Data Mining and Bioinformatics (IJDMB)  
ISMB (International Conference on Intelligent Systems for Molecular Biology)  
Journal of Bioinformatics and Computational Biology (JBCB)  
Journal of Chemical Information and Modeling  
Journal of Chemical Theory and Computation  
Journal of Computer-Aided Molecular Design  
Journal of Computational Chemistry  
Journal of Medicinal Chemistry  
Journal of Structural Biology  
Journal of Theoretical Biology  
Methods

Nature Communications  
Nature Machine Learning  
Neural Computing & Applications  
Nucleic Acid Research  
Parallel Computing  
PLoS Computational Biology  
PLoS ONE  
Proceedings of the National Academy of Sciences of the USA  
Protein Science  
Proteins: Structure, Function, Bioinformatics  
Proteome Science  
Statistical applications in Genetics and Mol Biol.  
Structure

#### 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

- Book proposal on Methods in Molecular and Structural Biology (July 2020)
- 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 (98 total)

- Great Lakes Bioinformatics Conference (GLBIO) 2021 Virtual Conference, May 10-13, 2021
- Annual International Conference on Intelligent Systems for Molecular Biology (2021 ISMB/ECCB), Montreal, Canada, July 25-29, Lyon, France, 2021
- HiCOMB 2021 20th IEEE International Workshop on High Performance Computational Biology, Portland, Oregon, May 17, 2021
- Research in Computational Molecular Biology (RECOMB) 2021, Padua, Italy, April 18-21, 2021
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2020, virtual meeting, December 7-10, 2020
- The 11th International Conference on Computational Systems-Biology and Bioinformatics (CSBio 2020), Bangkok, Thailand, November 19-21, 2020
- 19<sup>th</sup> European Conference on Computational Biology (ECCB2020), Barcelona, Sept. 5-9 2020
- 11<sup>th</sup> International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD2020), Bratislava, Slovakia, September 14-17, 2020

- HiCOMB 2020 19th IEEE International Workshop on High Performance Computational Biology, New Orleans, Louisiana, May 28, 2020
- Annual International Conference on Intelligent Systems for Molecular Biology (2020 ISMB), Montreal, Canada, July 12-16, 2020
- 1st International Applied Bioinformatics Conference, Istanbul University, Turkey, Oct 1-3, 2020
- Research in Computational Molecular Biology (RECOMB) 2020, Padua, Italy, May 10-13, 2020
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2019, Vancouver, Canada, Aug 27-30 2019
- 15th BIOINFO, Annual conference of the Korean Society of Bioinformatics, Korea, August 22-23, 2019.
- Track chair, Annual International Conference on Intelligent Systems for Molecular Biology (2019 ISMB /ECCB), Basel, Switzerland on July 21-25, 2019
- 16<sup>th</sup> Annual Conference of Midsouth Computational Biology & Bioinformatics Society, (MCBIOS), Birmingham, Alabama, March 28-31, 2019
- Steering Committee, Great Lakes Bioinformatics Conference (GLBIO) 2019, Wisconsin-Madison, WI, May 19-22, 2019
- 10<sup>th</sup> International Workshop on Biological Knowledge Discovery and Data Mining (BIOKDD'19), Linz Austria, August 26-29, 2019
- The 9th International Conference on Computational Systems-Biology and Bioinformatics (CSBio 2018), Bangkok, Thailand, December 10-13, 2018
- International Symposium on Network Enabled Health Informatics, Biomedicine and Bioinformatics, HI-BI-BI 2018, Barcelona, Spain, Aug 28-31 2018
- Annual International Conference on Intelligent Systems for Molecular Biology (ISMB 2018), Chicago, IL, July 6-10, 2018
- 9<sup>th</sup> 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
- 8<sup>th</sup> 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
- 7<sup>th</sup> 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 13<sup>th</sup> 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
- 22<sup>nd</sup> 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
- 5<sup>th</sup> 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.
- 21<sup>st</sup> Annual International Conference on Intelligent Systems for Molecular Biology (2013 ISMB /ECCB), Berlin, July 19-23, 2013

- 4<sup>th</sup> 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.
- 3<sup>rd</sup> 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
- 11<sup>th</sup> 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 9<sup>th</sup> International Symposium on Bioinformatics & BioEngineering (BIBE09), Taichung, Taiwan, June 22-24, 2009

- Workshop organizer, 4<sup>th</sup> IEEE International Conference on e-Science, eBioinformatics, Indianapolis, Dec. 12, 2008
- GIW 2008: 19<sup>th</sup> International Conference on Genome Informatics, Brisbane, Australia, December 1-3, 2008
- Area chair, 2008 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, November 7-9, 2008
- BIBM Workshop on Data Mining in Functional Genomics (DMFG), 2008 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, November 5-7, 2008
- Program Committee and session co-chair, Biomedical Engineering Society Annual Meeting 2007, “Systems Biology and Bioinformatics” track, Los Angeles, CA, September 26-29, 2007.
- IEEE 7<sup>th</sup> International Symposium on Bioinformatics & BioEngineering (BIBE07), Boston, MA, October 14-17, 2007
- 7<sup>th</sup> International Workshop on Data Mining in Bioinformatics (BIOKDD '07), August 12th 2007, San Jose, CA, USA
- 2<sup>nd</sup> VLDB (Very Large DataBases) Workshop on Data Mining in Bioinformatics, September 23-28 2007, University of Vienna, Austria
- 15<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) & 6<sup>th</sup> 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 39<sup>th</sup> 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 18<sup>th</sup> International Conference on Systems Engineering 2005 (ICSEng'05). August 16-18 2005, Las Vegas, NV.

## Internal Services

### Department

#### Biological Sciences:

- Full Professor Career Development Planning, Spring 2021
- Data Science Faculty Search, Spring 2020
- Executive Committee, 2015-current
- Convener of Structural Biology and Computational Biology Area, 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, 2018
- PULSe Research Award review committee 2018
- 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, Discovery Park (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

- Data Science in Life Science Search Committee (2019-2020)
- 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) 2012

#### **Professional Societies**

The Biophysical Society

The Protein Society

The International Society of Computational Biology