Curriculum Vitae

Sheng Wang, Ph.D.

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Research Scientist

King Abdullah University of Science and Technology

Thuwal, Saudi Arabia

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Education

09/2005-06/2010: *Ph.D*:

Institute of Theoretical Physics, **Chinese Academy of Sciences**, Beijing, China

Supervisor: Prof. Wei-Mou Zheng

Dissertation: “CLEPAPS: Conformational Letter based Pairwise Alignment of Protein Structure”

09/2001-06/2005: *Bachelor of Sciences*:

School of Life Sciences and Biotechnology, **Shanghai Jiao Tong University**, Shanghai, China

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Research Interest

Theoretical and Algorithmic:

Machine Learning: deep learning, graphical model, big data learning, class imbalance data learning.

Computational Biology: protein structure prediction, protein structure alignment, sequence analysis.

Applications in Biological Problems:

Protein Science: membrane protein prediction, disordered protein prediction, protein-protein interaction.

Sequencing: RNA-seq analysis, Nanopore sequencing analysis, transcriptome assembly.

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Research Experience

03/2017-now: *Research Scientist*:

King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Advisor: Prof. Xin Gao

Programs: Apply contact-assisted protein folding for membrane protein structure prediction.
Develop a Wavelet-based Dynamic Time Warping approach for signal alignment.
Design a new Deep Learning model to handle ultra-long sequence for Nanopore base-calling.

10/2014-02/2017: *Research Professional*:
Department of Human Genetics, **University of Chicago**, Chicago, IL, USA.
Advisor: Prof. Natalia Maltsev
Programs: Develop a systematic and analytical platform for integrative medicine.
Design a novel Machine Learning algorithm for sequence labeling of class imbalanced data.
Develop an Ultra-Deep Learning model for protein contact prediction.

11/2010-09/2014: *Postdoctoral Research Fellow*:
Toyota Technological Institute at Chicago, Chicago, IL, USA.
Advisor: Prof. Jinbo Xu
Programs: Design a Graphical Model method for protein homology detection.
Design a Machine Learning method for protein template-based modeling.
Develop a comprehensive protein structure prediction server RaptorX.

08/2010-10/2010: *Postdoctoral Research Associate*:
Institute of Computing Technology, **Chinese Academy of Sciences**, Beijing, China
Advisor: Prof. Dong-Bo Bu
Programs: Develop a new approach to incorporate ab initio energy for protein template-based modeling.

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Academic Awards

2018:

- **Best Paper Award** in **APCB 2018** for our team work *RaptorX-Angle: real-value and confidence prediction of protein backbone dihedral angles through a hybrid method of clustering and deep learning.*

- **Breakthrough in Advance Award** of the **PLoS Computational Biology Research Prize 2018** for my work *Accurate De Novo Prediction of Protein Contact Map by Ultra-Deep Learning Model.*

- **Highly Cited Paper Award** by **WEB OF SCIENCE** for my work *Accurate De Novo Prediction of Protein Contact Map by Ultra-Deep Learning Model.*

2017:

- **Top10 reviewers** for the journal *Molecular BioSystems*.

2016:

- **First rank** in contact prediction in **CASP (Critical Assessment of protein Structure Prediction) XII** for our team *RaptorX-Contact*.

- **Best Poster Award** in **IJCAI BOOM 2016** for my work *AUC-maximized Deep Convolutional Neural Fields for Protein Sequence Labeling*.

2014:

- **Warren DeLano Award** for Structural Bioinformatics and Computational Biophysics in **ISMB 3DSIG 2014** for our team work *Protein Homology Detection Through Alignment of Markov Random Fields: Using MRFalign.*

- **Best Paper Award** in **RECOMB 2014** for our team work *MRFalign: Protein Homology Detection through Alignment of Markov Random Fields*.

2012:

- **Warren DeLano Award** for Structural Bioinformatics and Computational Biophysics in **ISMB 3DSIG 2012** for my work *DeepAlign: Protein Structure Alignment beyond Spatial Proximity*.

2007:

- **Hilary Booth Prize** for Best talk in **BioInfoSummer07** for my work *CLEPAPS: Protein Structure Alignment based on Conformational Letters.*

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Academic Fundings

- **KAUST URF/1/3007-01** (main participant): 11/1/12018-10/31/2021
  - *Novel Computational Approaches for Long-read Single-molecule Sequencing Technologies*

- **NIH-R01GM08973** (main participant): 5/1/2010-8/31/2019
  - *New Computational Methods for Data-driven Protein Structure Prediction*

- **NSF-DBI0960390** (main participant): 7/1/2010-6/30/2013
  - *Algorithm and Web Server for Low-homology Protein Threading*

- **NSF-DBI1262603** (main participant): 7/1/2013-6/30/2016
  - *Continued Development of RaptorX Server for Protein Structure and Functional Prediction*

- **NSF-CCF1149811** (participant): 7/1/2012-6/30/2017
  - *Exact and Approximate Algorithms for 3D Structure Modeling of Protein-Protein Interactions*

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Publications

(†= corresponding author, *= contribute equally)

Works in Progress

- **Sheng Wang**†*, Shiyang Fei*, Zongan Wang*, Yu Li, Jinbo Xu, Feng Zhao†, Xin Gao†. *PredMP: a web server for de novo prediction of membrane protein.* (submitted)

- Renmin Han, Xiaohua Wan, Lun Li, Albert Lawrence, Peng Yang, Yu Li, **Sheng Wang**, Fei Sun, Zhiyong Liu, Xin Gao†, Fa Zhang†. *AuTom-dualx: a toolkit for fully automatic alignment of dual-axis tilt series with simultaneous reconstruction*. (submitted)
- Renmin Han, Yu Li, Xin Gao†, **Sheng Wang†**. *An accurate and rapid continuous wavelet dynamic time warping algorithm for unbalanced global mapping in nanopore sequencing.* **bioRxiv**
- **Sheng Wang†**, Yu Li, Renming Han, Minh-Duc Cao, Xin Gao†. *Learning Context-dependent Pore Model for Nanopore Sequencing via BiLSTM-extended Deep Canonical Time Warping.* (in preparation)

Journal Publications

2018:

- **Sheng Wang†***, Zhen Li*, Yizhou Yu, Xin Gao†. *WaveNano: a signal-level nanopore base-caller via simultaneous prediction of nucleotide labels and move labels through bi-directional WaveNets.* **Quantitative Biology**, 2018.
- Hong Zeng*, **Sheng Wang***, Tianming Zhou*, Feifeng Zhao, Xiufeng Li, Qing Wu†, Jinbo Xu†. *ComplexContact: a web server for inter-protein contact prediction using deep learning*. **Nucleic Acids Research**, 2018.
- Haotian Teng†*, Minh Duc Cao*, Michael B Hall, Tania Duarte, **Sheng Wang**, Lachlan J M Coin†. *Chiron: Translating nanopore raw signal directly into nucleotide sequence using deep learning*. **GigaScience**, 2018.
- Yu Li, Renmin Han, Chongwei Bi, Mo Li, **Sheng Wang†**, Xin Gao†. *DeepSimulator: a deep simulator for Nanopore sequencing*. **Bioinformatics**, 2018.
- Jianwei Zhu, **Sheng Wang**, Dongbo Bu†, Jinbo Xu†. *Protein threading using residue co-variation and deep learning*. **Bioinformatics**, 2018.
- Dinanath Sulakhe*†, Mark D'Souza*, **Sheng Wang**, Sandhya Balasubramanian, Prashanth Athri, Bingqing Xie, Stefan Canzar, Gady Agam, T. Conrad Gilliam, Natalia Maltsev†. *Exploring the functional impact of alternative splicing on human protein isoforms using available annotation sources*. **Briefings in Bioinformatics**, 2018.
- John J. Skinner*, **Sheng Wang***, Ji-Young Lee, Colin Ong, Ruth F Sommese, Sivaraj Sivaramakrishnan, Wolfgang Koelmel, Maria Hirschbeck, Hermann Schindelin, Caroline Kisker, Kristina Lorenz, Tobin R. Sosnick†, Marsha R Rosner†. *A conserved salt bridge theft triggered by phosphorylation regulates the protein interactome*. **Proceedings of the National Academy of Sciences of USA**, 2018.
- Yujuan Gao, **Sheng Wang**, Minghua Deng†, Jinbo Xu†. *RaptorXAngle: real-value and confidence prediction of protein backbone dihedral angles through a hybrid method of clustering and deep learning.* **BMC Bioinformatics**, 2018.
- Yu Li, **Sheng Wang**, Ramzan Umarov, Bingqing Xie, Xin Gao†. *DEEPre: sequence-based enzyme EC number prediction by deep learning.* **Bioinformatics**, 2018.

2017:

- **Sheng Wang**, Siqi Sun, Jinbo Xu†. *Analysis of deep learning methods for blind protein contact prediction in CASP12.* **Proteins**, 2017.

- **Sheng Wang***, Zhen Li*, Yizhou Yu, Jinbo Xu†. *Folding membrane proteins by deep transfer learning.* **Cell Systems**, 2017.

- Mingfu Shao*†, Jianzhu Ma*, **Sheng Wang***†. *DeepBound: Accurate Identification of Transcript Boundaries via Deep Convolutional Neural Fields.* **Bioinformatics**, 2017.

- Adriana Manas, **Sheng Wang**, Adam Nelson, Jiajun Li, Yu Zhao, Huaiyuan Zhang, Aislinn Davis, Bingqing Xie, Natalia Maltsev, Jialing Xiang†. *The functional domain for BaxΔ2 aggregate-mediated caspase 8-dependent cell death*. **Experimental Cell Research**, 2017.

- Natasha Barteneva†, Yeldar Baiken, Elizaveta Fasler-Kan, Kennet Alibek, **Sheng Wang**, Natalia Maltsev, Eugene Ponomarev, Zarina Sautbayeva, Sholpan Kauanova, Anna Moore, Christoph Beglinger, Ivan Vorobjev. *Extracellular vesicles in gastrointestinal cancer in conjunction with microbiota: on the border of Kingdoms.* **BBA Reviews on Cancer**, 2017.

- Mark D'Souza†, Dinanath Sulakhe, **Sheng Wang**, Bingqing Xie, Somaye Hashemifar, Andrew Taylor, Inna Dubchak, T Conrad Gilliam, Natalia Maltsev†. *Strategic Integration of Multiple Bioinformatics Resources for System Level Analysis of Biological Networks.* **Biological Networks and Pathway Analysis**, 2017.

- **Sheng Wang***, Siqi Sun*, Zhen Li, Renyu Zhang, Jinbo Xu†. *Accurate De Novo Prediction of Protein Contact Map by Ultra-Deep Learning Model.* **PLoS Computational Biology**, 2017.

2016:

- **Sheng Wang**, Siqi Sun, Jinbo Xu†. *AUC-maximized Deep Convolutional Neural Fields for Protein Sequence Labeling.* **Lecture Notes in Computer Science**, 2016.

- **Sheng Wang**†, Jianzhu Ma, Jinbo Xu†. *AUCpreD: Proteome-level Protein Disorder Prediction by AUC-maximized Deep Convolutional Neural Fields.* **Bioinformatics**, 2016.

- **Sheng Wang**†*, Wei Li*, Renyu Zhang, Shiwang Liu, Jinbo Xu†. *CoinFold: a web server for protein contact prediction and contact-assisted protein folding.* **Nucleic Acids Research,** 2016.

- **Sheng Wang**†*, Wei Li*, Shiwang Liu, Jinbo Xu†. *RaptorX-Property: a web server for protein structure property prediction.* **Nucleic Acids Research,** 2016.

- Xuefeng Cui, Zhiwu Lu, **Sheng Wang**, Jim Jing-Yan Wang, Xin Gao†. *CMsearch: simultaneous exploration of protein sequence space and structure space improves not only protein homology detection but also protein structure prediction.* **Bioinformatics,** 2016.

- **Sheng Wang**†, Jian Peng, Jianzhu Ma, Jinbo Xu†. *Protein Secondary Structure Prediction using Deep Convolutional Neural Fields.* **Scientific Reports**, 2016.

- Dinanath Sulakhe†, Bingqing Xie, Andrew Taylor, Mark D'Souza, Sandhya Balasubramanian, Somaye Hashemifar, Steven White, Utpal J. Dave, Gady Agam, Jinbo Xu, **Sheng Wang**, T. Conrad Gilliam, Natalia Maltsev†. *Lynx: A Knowledge Base and an Analytical Workbench for Integrative Medicine.* **Nucleic Acids Research**, 2016.

2015:

- Jianzhu Ma*, **Sheng Wang***, Zhiyong Wang, Jinbo Xu†. *Protein contact prediction by integrating joint evolutionary coupling analysis and supervised learning.* **Bioinformatics**, 2015.
- **Sheng Wang**†*, Shunyan Weng*, Jianzhu Ma, Qingming Tang. *DeepCNF-D: Predicting Protein Order/Disorder Regions by Weighted Deep Convolutional Neural Fields.* **International Journal of Molecular Sciences** 2015.
- Jianzhu Ma, **Sheng Wang**†. *AcconPred: Predicting Solvent Accessibility and Contact Number Simultaneously by a Multitask Learning Framework under the Conditional Neural Fields Model.* **BioMed Research International**, 2015.

2014:

- Inna Dubchak†*, Sandhya Balasubramanian*, **Sheng Wang**, Cem Meyden, Dinanath Sulakhe, Alexander Poliakov, Daniela B?rnigen, Bingqing Xie, Andrew Taylor, Jianzhu Ma, Alex R Paciorkowski, Ghayda M Mirzaa, Paul Dave, Gady Agam, Jinbo Xu, Lihadh Al-Gazali, Christopher E Mason, M Elizabeth Ross, Natalia Maltsev†, T Conrad Gilliam. *An integrative computational approach for prioritization of genomic variants*. **PLOS One**, 2014.
- Jianzhu Ma, **Sheng Wang**†. *Algorithms, applications and challenges of protein structure alignment*. **Adv Protein Chem Struct Biol**, 2014.
- Jianzhu Ma, **Sheng Wang**, Zhiyong Wang, Jinbo Xu†. *MRFalign: protein homology detection through alignment of Markov Random Fields*. **PLoS Computational Biology**, 2014.
- Dinanath Sulakhe†, Sandhya Balasubramanian, Bingqing Xie, Bo Feng, Andrew Taylor, **Sheng Wang**, Eduardo Berrocal, Utpal Dave, Jinbo Xu, Daniela Börnigen, T. Conrad Gilliam, Natalia Maltsev†. *Lynx: a database and knowledge extraction engine for integrative medicine*. **Nucleic Acids Research**, 2014.

Before 2014:

- **Sheng Wang**, Jian Peng, Jianzhu Ma, Jinbo Xu†. *Protein structure alignment beyond spatial proximity.* **Scientific Reports**, 2013.
- Jianzhu Ma, **Sheng Wang**, Feng Zhao, Jinbo Xu†. *Protein threading using context-specific alignment potential*. **Bioinformatics**, 2013.
- Morten Källberg*, Haipeng Wang*, **Sheng Wang**, Jian Peng, Zhiyong Wang, Hui Lu, Jinbo Xu†. *Tmplate-based protein structure modeling using the RaptorX web server.* **Nature Protocols**, 2012.
- Jianzhu Ma*, Jian Peng*, **Sheng Wang,** Jinbo Xu†. *A Conditional Neural Fields model for protein threading.* **Bioinformatics**, 2012.
- **Sheng Wang**, Jian Peng, Jinbo Xu†. *Alignment of distantly-related protein structures: algorithm, bound and implications to homology modeling.* **Bioinformatics**, 2011.
- Mingfu Shao, **Sheng Wang**, Chao Wang, Xiongying Yuan, Shuai Cheng Li, Weimou Zheng†, Dongbo Bu†. *Incorporating Ab Initio energy into threading approaches for protein structure prediction.* **BMC Bioinformatics**, 2011.

- **Sheng Wang**, Wei-Mou Zheng†. *Fast multiple alignment of protein structures using conformational letter blocks.* **Open Bioinformatics Journal**, 2009.

- **Sheng Wang**, Wei-Mou Zheng†. *CLEPAPS: fast pair alignment of protein structures based on conformational letters.* **Journal of Bioinformatics and Computational Biology**, 2008.

Books / Book Chapters

- Jianzhu Ma, **Sheng Wang**, Jinbo Xu. *Protein homology detection through alignment of Markov Random Fields.* **SpringerBriefs in Computer Science**, 2015.

- Morten Källberg, Gohar Margaryan, **Sheng Wang**, Jianzhu Ma, Jinbo Xu. *RaptorX Server: a resource for template-based protein structure modeling.* **Methods in Molecular Biology**, 2013.

Conferences Presentations

2018:

- Jianwei Zhu, **Sheng Wang**, Dongbo Bu†, Jinbo Xu†. *Protein threading using residue co-variation and deep learning*. **ISMB** 2018.

- Yujuan Gao, **Sheng Wang**, Minghua Deng, Jinbo Xu†. *RaptorXAngle: real-value and confidence prediction of protein backbone dihedral angles through a hybrid method of clustering and deep learning.* **APBC** 2018.

- **Sheng Wang**†*, Shiyang Fei*, Zongan Wang*, Yu Li, Jinbo Xu, Feng Zhao†, Xin Gao†. *PredMP: a web server for de novo prediction of membrane protein.* **Biophysical Society 62nd Annual Meeting** 2018.

- Tianming Zhou*, **Sheng Wang***†, Jinbo Xu†. *Deep learning reveals many more inter-protein residue-residue contacts than direct coupling analysis.* **RECOMB** 2018.

2017:

- Mingfu Shao*†, Jianzhu Ma*, **Sheng Wang***†. *DeepBound: Accurate Identification of Transcript Boundaries via Deep Convolutional Neural Fields.* **ISMB** 2017.

- **Sheng Wang**, Siqi Sun, Zhen Li, Renyu Zhang, Jinbo Xu†. *Folding Large Proteins by Ultra-Deep Learning.* **RECOMB** 2017.

- Zhen Li*, **Sheng Wang***, Yizhou Yu, Jinbo Xu†. *Predicting membrane protein contacts from non-membrane proteins by deep transfer learning.* **RECOMB** 2017.

- **Sheng Wang***, Zongan Wang*, John Jumper, Karl F Freed, Tobin R Sosnick, Jinbo Xu†. *Folding Membrane Proteins by Contacts Inferred from Non-membrane Proteins and Near-atomic Level Refinement.* **Biophysical Society 61st Annual Meeting** 2017.

- Tobin R Sosnick, John J Skinner, **Sheng Wang**, Jiyoung Lee, Ruth Sommese, Sivaraj Sivaramakrishnan, Wolfgang Kölmel, Maria Hirschbeck, Hermann Schindelin, Caroline Kisker, Kristina Lorenz, Marsha R Rosner†. *A Phospho-Induced Theft of a Salt Bridge in RKIP Links Map Kinase and G Protein-Mediated*

Signaling. **Biophysical Society 61st Annual Meeting** 2017.

2016:

- **Sheng Wang**, Jinbo Xu†. *De novo protein structure prediction by big data and deep learning.* **Rocky** 2016.
- **Sheng Wang**, Siqi Sun, Jinbo Xu†. *AUC-maximized Deep Convolutional Neural Fields for Protein Sequence Labeling.* **ECML** 2016.
- **Sheng Wang**†, Jianzhu Ma, Jinbo Xu†. *AUCpreD: Proteome-level Protein Disorder Prediction by AUC-maximized Deep Convolutional Neural Fields.* **ECCB** 2016.
- Xuefeng Cui, Zhiwu Lu, **Sheng Wang**, Jim Jing-Yan Wang, Xin Gao†. *CMsearch: simultaneous exploration of protein sequence space and structure space improves not only protein homology detection but also protein structure prediction.* **ISMB** 2016.

2015:

- Qingming Tang, **Sheng Wang**, Jian Peng, Jianzhu Ma, Jinbo Xu†. *Bermuda: de novo assembly of transcripts with new insights for handling uneven coverage.* **ACM-BCB** 2015.
- Siqi Sun, Jianzhu Ma, **Sheng Wang**, Jinbo Xu†. *Predicting diverse M-best protein contact maps.* **BIBM** 2015.
- Jianzhu Ma, Qingming Tang, **Sheng Wang**, Jinbo Xu†. *Structure Learning Constrained by Node-Specific Degree Distribution.* **UAI** 2015.
- Jianzhu Ma, **Sheng Wang**, Zhiyong Wang, Jinbo Xu†. *Protein Contact Prediction by Integrating Joint Evolutionary Coupling Analysis and Supervised Learning.* **RECOMB** 2015.

Before 2015:

- Jianzhu Ma, **Sheng Wang**, Zhiyong Wang, Jinbo Xu†. *MRFalign: protein homology detection through alignment of Markov Random Fields.* **RECOMB** 2014.
- Jianzhu Ma*, Jian Peng*, **Sheng Wang***, Jinbo Xu†. *Estimating the partition function of graphical models using Langevin importance sampling.* **AISTATS** 2013.
- Jianzhu Ma, **Sheng Wang**, Feng Zhao, Jinbo Xu†. *Protein threading using context-specific alignment potential.* **ISMB** 2013.
- Jianzhu Ma, Jian Peng, **Sheng Wang,** Jinbo Xu†. *A Conditional Neural Fields model for protein threading.* **ISMB** 2012.

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Servers and Softwares

(†= corresponding author, *=main contributor)

Servers

- **PredMP** *†: a web resource for computationally predicted membrane proteins via Deep Learning (http://predmp.com:3001/#/home).
- **RaptorX** *: predict tertiary structure of a protein sequence using templates. (http://raptorx.uchicago.edu/)
- **RaptorX-Property** *†: predict structure properties of a protein sequence without using templates, including 3-/8-state secondary structure, solvent accessibility, and disordered regions. (http://raptorx2.uchicago.edu/StructurePropertyPred/predict/)
- **RaptorX-Contact Predict** *†: predict contact map of a protein sequence and tertiary structure guided by predicted contacts, but without using any templates. (http://raptorx2.uchicago.edu/ContactMap/)
- **RaptorX-Complex Contact** *: predict the interfacial contacts between two potentially interacting protein sequences using co-evolution and deep learning techniques. (http://raptorx2.uchicago.edu/ComplexContact/)
- **RaptorX-Structure Alignment** *†: a comprehensive structure alignment server with combined pairwise and multiple proteins as inputs. (http://raptorx.uchicago.edu/DeepAlign/submit/)
- **RaptorX-Binding** *†: model-assisted binding site prediction for a protein sequence. (http://raptorx.uchicago.edu/BindingSite/)
- **LynX** : a knowledge extraction engine for integrative medicine. (http://lynx.ci.uchicago.edu/)

Softwares

- **cwDTW** *†: Continuous Wavelet Dynamic Time Warping for unbalanced global mapping of two signals. (https://github.com/realbigws/cwDTW)
- **cwDTW_nano** *†: global mapping in nanopore sequencing analysis using cwDTW. (https://github.com/realbigws/cwDTW_nano)
- **cwDTW_genome** *†: whole genome alignment based on cwDTW. (https://github.com/realbigws/cwDTW_genome)
- **DeepBound** *†: Predict the boundary of transcript start and end from RNA-seq reads alignment, via Deep Convolutional Neural Field model. (https://github.com/realbigws/DeepBound)
- **DeepCNF** *†: Deep Convolutional Neural Field model, with three training methods for maximization: (1) log probability, (2) posterior probability, or (3) AUC value. (https://github.com/realbigws/DeepCNF_AUC)
- **DeepCNF_D** *†: a program for predicting protein disorder regions via DeepCNF model. (http://ttic.uchicago.edu/~wangsheng/DeepCNF_D_package_v1.00.tar.gz)
- **AcconPred** *†: a program for predicting protein solvent accessibility and contact number simultaneously by a multi-task learning framework under the Conditional Neural Fields (CNF) model. (http://ttic.uchicago.edu/~majianzhu/AcconPred_package_v1.00.tar.gz)
- **DeepAlign** *†: a program for pairwise protein structure alignment that incorporates evolutionary information

and beta strand orientation in addition to geometric similarity. (https://github.com/realbigws/DeepAlign)

- **3DCOMB** *†: a program for multiple protein structure alignment. (https://github.com/realbigws/DeepAlign)
- **CNFpred** *: a standalone threading software that could perform low homology template-based protein structure prediction. (http://raptorx.uchicago.edu/download/)
- **MRFalign** *: a standalone homology detection software through alignment of Markov Random Fields (MRF). (http://raptorx.uchicago.edu/download/)
- **CLEPAPS** *: a fast pairwise alignment of protein structures based on conformational letters. (http://weblab.cbi.pku.edu.cn/programdoc/html/clepaps/CLePAPS.html)
- **BLOMAPS** *: a fast multiple alignment of protein structures using conformational letter blocks. (http://www.itp.ac.cn/~zheng/blomaps.rar)
- **PDB_Tools** *†: an integrated software for handling PDB file that could parse the coordinate, do SEQRES-ATOM mapping, calculate secondary structure as well as solvent accessibility, compute conformational letter, reconstruct missing residues. (https://github.com/realbigws/PDB_Tool)
- **Complex_Tools** *†: an integrated software for handling monomer and complex structures in PDB, which could be applied to extract contact/distance map of the complex. (https://github.com/realbigws/Complex_Tool)

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Academic Service

Scientific Memberships

- International Society for Computational Biology (ISCB) Member
- Biophysical Society (BPS) Member
- Institute of Electrical and Electronics Engineers (IEEE) Member

Journal Reviewing Activities

- Nucleic Acid Research
- Bioinformatics
- Briefings in Bioinformatics
- Proteins: Structure, Function, and Bioinformatics
- BMC Bioinformatics
- Journal of Molecular Biology
- Scientific Reports
- PLoS ONE
- Oncotarget
- Molecular BioSystems **[Top 10 reviewers]**
- Journal of Computer-Aided Molecular Design (JCAM)
- Advances in Protein Chemistry & Structural Biology (APCSB)

- Statistical Methods in Medical Research (SMM)
- Protein Peptide Letters (PPL)
- Journal of Bioinformatics and Computational Biology (JBCB)
- IEEE Transactions on Computational Biology and Bioinformatics (IEEE-TCBB)
- IEEE Transactions on Nano Biosience
- BioData Mining
- Acta Biomaterialia
- Neurocomputing
- Experimental Parasitology
- Genomics Proteomics and Bioinformatics
- Computers in Biology and Medicine

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Invited Talks

- *PredMP: A De Novo Membrane Protein Prediction Pipeline*. **Jiangnan University**, China, 2018.
- *Big Data and Deep Learning in Protein Structure Prediction*. **Zhejiang University**, China, 2018.
- *Machine Learning in Structure Prediction and Sequence Labeling of Proteins*. **Peking University**, China, 2018.
- *Machine Learning in Protein Structure Prediction*. **University of Science and Technology of China**, China, 2017.
- *De Novo Protein Structure Prediction by Big Data and Deep Learning*. **The Westin Snowmass Resort**, Rocky2016, USA, 2016.
- *Proteome-level protein disorder prediction by AUC-maximized Deep Convolutional Neural Fields*. **World Forum Convention Center**, ECCB, Netherlands, 2016
- *Protein Structure Prediction through Machine Learning.* **Chinese Academy of Agricultural Sciences**, China, 2015.
- *Protein Order/Disorder Prediction through Machine Learning*. **Institute of Computing Technology, Chinese Academy of Sciences**, China, 2015.
- *Protein threading using context-specific alignment potential.* **The International's Congress Centrum Berlin,** ISMB, Germany, 2013
- *RaptorX: a protein structure and function prediction server.* Shanghai Institutes of Life Sciences, Key Lab of System Biology, **Chinese Academy of Sciences**, China, 2013
- *Protein structure analysis tools: homology detection, structure alignment and protein prediction.* Department of Computer Sciences, Key Lab of Intelligent Information Processing, **Fudan University**, China, 2013
- *Estimating the partition function of graphical models using Langevin importance sampling.* Department of Physics, **Jilin University**, China, 2013

- *Protein structure prediction through template-based threading.* Institute of Theoretical Physics, **Chinese Academy of Sciences**, China, 2013
- *Protein structure analysis tools: from structure-structure to sequence-structure alignment.* Center for Systems Biomedicine, **Shanghai Jiao Tong University**, China, 2013
- *Protein structure alignment beyond spatial proximity*. **Long Beach Convention Center**, ISMB/3DSIG, USA, 2012
- *Conformational letter and its applications in protein structure analysis.* **RIKEN**, Japan, 2010
- *Conformational letter based multiple alignment of protein structure.* **Fudan University**, Chinese Conference on Bioinformatics & Systems Biology, China, 2008
- *Conformational letter based pairwise alignment of protein structure.* **Australian National University**, BioInfoSummer07, Australia, 2007

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