

JIE LIANG

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Education

UNIVERSITY OF ILLINOIS Urbana, IL
Ph.D. in Biophysics. May 1994.
M.C.S. (Computer Science). January 1995.

FUDAN UNIVERSITY Shanghai, China
B.S. in Biophysics. July 1986.

Permanent Positions

DEPTS. OF BIOENGINEERING, AND COMPUTER SCIENCE (COURTESY)
UNIVERSITY OF ILLINOIS AT CHICAGO Chicago, IL
2007-present. Professor
2003-2007. Associate Professor with tenure.
1999-2003. Assistant Professor.

DEPT. OF CHEMINFORMATICS
SMITHKLINE BEECHAM PHARMACEUTICALS King of Prussia, PA
1997-1999. Investigator.

Other Positions

INSTITUTE OF SYSTEMS BIOMEDICINE,
SHANGHAI JIAOTONG UNIVERSITY Shanghai, China
2006. Visiting Professor

DEPT. OF BIOCHEMISTRY, UNIVERSITY OF MINNESOTA Minneapolis, MN
1997. Research Associate with Dr. Woodward.

INSTITUTE OF MATHEMATICS AND ITS APPLICATIONS
UNIVERSITY OF MINNESOTA Minneapolis, MN
1996-1997. Visiting Fellow.

BECKMAN INSTITUTE, NATIONAL CENTER FOR SUPERCOMPUTING APPLICA-
TIONS AND DEPT. OF COMPUTER SCIENCE, UNIVERSITY OF ILLINOIS

Urbana, IL
1994–1996. Research Associate with Drs. Edelsbrunner & Subramaniam

DEPT. OF BIOPHYSICS, UNIVERSITY OF ILLINOIS Urbana, IL
1987–1994. Teaching and Research Assistant. Graduate Studies with Dr. Ebrey

PLANT PATHOLOGY, SOUTHWEST AG. UNIVERSITY Chongqing, China
1986–1987. Assistant Instructor.

Awards/Distinctions

Elected Fellow, American Institute of Medical and Biological Engineering. 2008.

Faculty Research Silver Award, College of Engineering, University of Illinois at Chicago. 2006.

Faculty Research Award, College of Engineering, University of Illinois at Chicago. 2004.

NSF Faculty Early Career Development Award. 2002.

NSF Institute of Mathematics and its Applications: Research awarded for the special year of Mathematics in High Performance Computing. 1996–1997.

NSF Postdoctoral Research Associate Fellowship (Computer and Information Science and Engineering Division). 1994–1996.

Best Paper Award. Hawaii International Conference on System Sciences. Biotechnology Computing. (With H. Edelsbrunner, M. Facello and P. Fu). 1995.

Advisor to 1st Place Student Poster Award, Chicago Proteomics Symposium, 2004. (Authors: Xiang Li, Brian Kay, and Jie Liang).

Advisor to 2nd Place Postdoctoral Researcher Poster Award, Chicago Proteomics Symposium, 2004. (Authors: Larisa Adamian and Jie Liang).

Editorial Work

Associate Editor, Conference Editorial Board, IEEE Engineering in Medicine and Biology Society (EMBS), 2008.

Guest co-editor (with Gerald Sidel) for a special issue of *Annals of Biomedical Engineering* on Systems Biology and Bioinformatics, 2007.

Guest co-editor (with Bahskar DasGupta and Piotr Berman) for special issue of *Algorithmica*, 2007.

Co-Editor (with Dong Xu) for special issue of *International Journal of Bioinformatics Research and Applications (IJBRA)*, 2005.

Founding Editorial Board member, *International Journal of Bioinformatics Research and Applications (IJBRA)*, 2004–present.

Editorial Board member *Advances in Bioinformatics*, 2007–present.

Book Editor (with Ying Xu and Dong Xu), *Computational Methods for Protein Structure Prediction and Modeling*. Volume 1: Basic characterization, Springer, 2007.

Book Editor (with Ying Xu and Dong Xu), *Computational Methods for Protein Structure Prediction and Modeling*. Volume 2: Structure prediction, Springer, 2007.

Steering committee member, *IEEE-ACM Transaction in Computational Biology and Bioinformatics*.

Member, publications committee, IEEE-Engineering in Medicine and Biology Society (EMBS).

Member, Council of Biometrics Society, IEEE, 2007–2008.

Professional Service

Bioinformatics and Computational Biology Journals and Conferences

Program committee, Intelligent Systems for Molecular Biology (ISMB), Vienna, 2007; Toronto, 2008.

Theme co-chair, *Bioinformatics and Computational Biology; Systems Biology; Modeling Methodologies*, 30th IEEE Engineering in Medicine and Biology Society (EMBS), Annual International Conference, Vancouver, Canada, August 20– August 24, 2008.

Track co-chair (with Gerald Saidel, 9 sessions), “*Systems Biology and Bioinformatics*”, *The 2006 Annual Meeting of the Biomedical Engineering Society (BMES)*, Chicago, USA, October 12– October 14, 2006.

Technical Program Committee, and Theme chair, *Bioinformatics and Computational Biology*, *28th IEEE Engineering in Medicine and Biology Society (EMBS)*, 8 sessions, Annual International Conference, New York, USA, August 31– September 3, 2006.

Program Committee, *The 5-th Computational Systems Bioinformatics Conference (CSB2006)*, Stanford, CA, USA, August 2006.

Chair, Organizing Committee, *The 27th IEEE Engineering in Medicine and Biology Society (EMBS) Satellite Symposium on Bioinformatics and Computational Biology*. Jiaotong University, Shanghai, China. August 30, 2005

Technical Program Committee, and Theme co-chair, *Bioinformatics and Computational Biology, 27th IEEE Engineering in Medicine and Biology Society (EMBS)*, Annual International Conference, Shanghai, China, September 1– September 4, 2005.

Co-organizer (with Bhaskar DasGupta), NSF Center for Discrete Mathematics & Theoretical Computer Science (DIMACS) Workshop: *Information processing by protein structures in molecular recognition*. DIMACS/BioMaPS/MB Center Special Focus on Information Processing in Biology. Rutgers University, June 13– June 14, 2005

Program committee, Intelligent Systems for Molecular Biology (ISMB), 2005.

Program committee, *International Conference on Bioinformatics and its Applications (ICBA '04)*, 2004, Ft Lauderdale, FA.

Technical Program Committee, and Theme co-chair, *Bioinformatics and Computational Biology, 26th IEEE Engineering in Medicine and Biology Society (EMBS)*, Annual International Conference, San Francisco, U.S.A., 2004.

Session Chair. *The Second Workshop on Monte Carlo Methods*. Harvard University, Boston, MA. August 28, 2004.

Chair, Organizing Committee, *Symposium on Computational Science of Biomolecules: Applications in Medicine and Therapeutics*. The University of Illinois at Chicago. October 8, 2004.

Organizing Committee member, *UIC-UIUC Symposium on Bioinformatics in Medicine and Biology*, April 13, 2002. Chicago, IL.

Session Chair. *Monte Carlo methods in bioinformatics*. ICSA 2001 Applied Statistics Symposium, June 7-9, 2001, Chicago.

platform session co-chair. *Session AR: Membrane Proteins and Transmembrane Helical proteins*. Biophysical Society Meeting, 2001, Boston.

Interuniversity Advisory Board Member, University of Illinois at Chicago-University of Chicago-Northwestern University Chicago Biomedical Consortium Proteomics and Informatics Scientific Board.

Journal Referees

Referee for *Biochemistry, Bioinformatics, Biophys. J., Biopolymers, BMC-Bioinformatics, FEBS Lett. EMBO Journal, IEEE Transactions on Information Technology in Biomedicine, J. of ACM, J. of American Chemical Society, Journal of Bioinformatics and Computational Biology, J. Chemical Information and Computer Sciences, J. of Comput. Chem., J. Computer-Aided Mol. Design, J. of Comput. Physics, J. Mol. Biol., Mol. Biol. Evol., Nucleic Acid Research, PLoS Computational Biology, Physical Review E., Physic. Rev. Lett., Proc. Natl. Acad. Sci. USA, Proteins, Protein Engineering, Protein Science, and Trends in Biochem. Sci.*

Grant Reviewers

Study section, permanent member, NIH, Biodata Management and Analysis (BDMA), 2004-Present.

Grant reviewer, Israel National Science Foundation, 2005, 2008.

Study section, NIH Computational Biophysics, Biophysical and Chemical Sciences (BPC-Q), 2005.

Special Emphasis Panel, P01 Program on *Membrane protein assembly*, Center for Scientific Review, NIH, 2004.

Special Emphasis Panel on Curriculum Development Award in Interdisciplinary Research grant in response to NIH Roadmap, NIGMS, 2004.

Special Emphasis Panel, NIH NCI, SBIR, Gene Expression in Cancer by Microarray Hybridization. 2001

Special Emphasis Panel, Biomedical Research and Research Training (BRT). 2001.

Study section, NIH NCI, Innovative Technologies for the Molecular Analysis of Cancer (IMAT). 2000 – 2002.

Special Emphasis Panel, Innovative Technology Programs, NCI, NIH, 2001

Review Panel, NSF ITR, 2001 – 2003.

Review Panel, NSF Division of Biological Infrastructure, 2001, 2002, 2004, and 2005.

Active Grants

“Collaborative Research: Monte Carlo Study of Pseudoknotted RNA Molecules: Motifs, Structure and Folding.” PI: Liang. NSF. (DMS-0800257). Period: June 1, 2008 - May 31, 2012.

“High-accuracy models of proteins from remote homology.” PI: Liang, co-PI: Xu. NIH/NIGMS. (R01-GM081682-01). Period: September 1, 2007-August 31, 2010

“Tools and databases for enzyme function prediction and active site identification: evolutionary matching of protein surfaces.” PI: Liang. NSF. (DB&I-0646035). Period: August 1, 2007-July 31, 2008.

“Computational assembly of beta-barrel membrane proteins”. Principal Investigator: Jie Liang, Co-Principal Investigator: Linda Kenney. NIH/NIGMS. (R01-GM079804). Period: March 1, 2007–February 28, 2012.

“Development of Nanoscale Neuromodulating Platform”. Principal Investigator: David Pepperberg, NIH/NEI (R01-EY016094-01A1). Period: Jan 1, 2007–Dec 31, 2011.

“Determination of nociceptive molecular effects in engineered tissues in response to active denial type 94-GHz irradiation”. Principle Investigator: Mike Cho. Agency: Office of Naval Research. Period: Nov 7, 2005 to September 30, 2008.

This project focus on developing 3D structural models of transient receptor potential (TRP) channel proteins, dynamic model of its conformational change and temperature effects, as well as identification of key residues important for stability and for agonist/antagonist binding.

“Constrained Sequential Monte Carlo and It’s Applications in Structural Bioinformatics.” Principle Investigator: Rong Chen (UIC), co-PI: Jie Liang (UIC)
Agency: NIGMS/NIH, R01- GM68958-01
Period: June 1, 2003 to May 30, 2008. Liang’s total cost: \$606,853.

This project focus on the following fundamental problems: (1) Identify functionally important surfaces on protein; (2) Identify significant similarity of protein surface patterns among proteins which may have different fold structures; (3) Effects of protein function on the folding and stability of proteins, namely, the inverse problem of the structure-function relationship, and (4) Relationship of geometric properties and the stability and functions of proteins.

Completed Grants

“CAREER: A Database for Modeling Protein Spatial Geometry - Discovering Protein Functions”. PI: Jie Liang, Co-PI: None
Agency: National Science Foundation, DBI-0133856, Period: Sept 1, 2002 to August 30, 2007

The goal of this project is three-folds: (1) to develop informatics tools to identify similar surface pockets on different proteins, (2) to construct a database of libraries of spatial surface motifs from all known protein structures, and (3) to enhance bioinformatics education by integrating proposed research with curriculum development, classroom teaching, and student mentoring.

“Carolina exploratory center for cheminformatics research”. NIH/National Human Genome Research Institute. (P20 HG003898-01, Subcontract) Period: Sept 23, 2005–July 31/2006

“Computational tools for discovery of diagnostics and therapeutics of pleural metastases of breast cancer”. Principle Investigator: Jie Liang. Agency: Whitaker Foundation (TF-04-0023). Period: March 1, 2005 to February 28, 2006.

This project focus on developing computational tools for diagnosis and treatment of pleural metastatic breast cancer.

“MURI: Integrated approaches to determine molecular and subcellular effects in response to non-lethal EM radiation exposure.” Principle Investigator: Michael

Cho (UIC), co-PI: Jie Liang (UIC), Susan McCormick (UIC), E. Moros (Wash U), Michale Picard (Wash U), H. Thatte (Harvard)

Agency: ONR/DOD N000140310329

Period: Oct. 1, 2002 to Sept. 30, 2005

This project combines molecular, cellular, and imaging techniques to investigate the interactions between non-lethal electromagnetic (EM) radiation and brain cell lines and neurons from gene expression to intracellular and cell surface processes.

“Geometric tools for drug discovery”. Principal Investigator: Jie Liang. Agency: Eli Lilly Foundation. Period: Jan 1, 2004 – Dec 31, 2004

The purpose of this project is to develop protein structure based molecular descriptor for rapid compound screening.

“Microcirculation of Uveal Melanoma”. PI: Robert Folberg, co-PI: Jie Liang, and others. NIH/NEI, R01 EY010457-09. 04/01/03–03/31/08

The purpose of this project is to identify genes important for microcirculation of uveal melanoma.

“A database of protein topographic surfaces from computational geometry”. Principal Investigator: Jie Liang, Co-PI: None.

Agency: National Science Foundation. Type: Biological Databases and Informatics DBI-0078270, Period: Oct. 1, 2000 to Oct 31, 2003.

The purpose of this project is to develop informatics tools based on computational geometry to characterize protein surfaces, and to construct a database of protein surface maps for all known protein structures. The goal is to provide a resource for structural genomics, drug development, and the engineering of novel proteins.

“Research Experience for Teachers (RES Supplement to existing NSF CAREER grant”. Principal Investigator: Jie Liang, Agency: National Science Foundation. Period: June 1, 2002 – May 31, 2003.

“Intelligent computational genomic analysis”. Principal Investigator: Simon Kasif (Boston U). Co-PI: Robert Grossman (UIC), Jie Liang (UIC), Steven Salzberg (TIGR)

Agency: National Science Foundation. Type: Knowledge and Distributed Intelligence MCB998008, Period: Sept. 15, 1999 to August 31, 2002.

The goal is to develop novel computer systems to support scientific discovery in large-scale whole genomic sequence databases. These systems will make sophisticated computational analysis an integral part of the process of developing, integrating and disseminating new scientific knowledge.

“Modeling nonspecific effects of organic molecules on heteropolymers in solutions”.

Principal Investigator: Jie Liang, Co-PI: None.

Agency: American Chemical Society.

Type: G (PRF#35616-G7), Period: Sept. 1, 2000 to August 31, 2002.

The purpose of this project is to extend the transfer free energy model by incorporating details of the molecule shapes to develop a more realistic and accurate model of the cosolvent-heteropolymer interactions. The goal is to predict and rationalize how the effects of a cosolvent changes in different protein solutions.

“Rational Design of cDNA Array for Breast Cancer Prognosis and Diagnosis”.

Principal Investigator: Jie Liang. Co-PI: Carol Westbrook (UIC)

Agency: Whitaker Foundation . Period: Jan 1, 2001 to Dec. 31, 2003.

The goal is to computationally design a cDNA chip based on data from breast cancer cell lines, and the output is the diagnosis and classification of breast cancer metastasis and invasiveness based on hybridization results using the designed chip.

“Affymetrix Technology Platform for the Genomic Analysis of Women’s Neoplasms”.

Principle Investigator: Carol Westbrook (UIC), Co-PI: Zarema Abbieva (UIC), Mark Band (UIUC), Serdar Bulun (UIC), Benita Katzenellenbogen (UIUC), Harris Lewin (UIC), Jie Liang (UIC), Lei Liu (UIUC), Rajeshwari R. Mehta (UIC).

Agency: Intercampus Research Initiative in Biotechnology, University of Illinois.

Period: March 1, 2001 to Feb. 29, 2004.

This is an equipment grant for accessing affymetrix oligo array technology for microarray studies.

Teaching

Host to Visiting Professor:

Jian Zhang (Associate Professor, Center for Biophysics, Dept of Physics, Nanjing University, China). 2007 – Present.

Advisor to Postdoctoral Research Associates:

Chih-Hao Lu (Ph.D.: Natioanl Chiao-Tong Unviersity, Taiwan). 2008 – Present.

Larisa Adamian (Ph.D.: U Texas HSC at Galveston, B.S.: Moscow State, Biochemistry). 2000 – Present. Current appointment: Research Assistant Professor at UIC;

Changyu Hu (Ph.D.: Chinese Academy of Science, B.S.: Xuzhou University, Chemistry). 2001 – 2005. Current position: Senior research scientist, Michigan Technology University.

Arun Setty (Ph.D.: U Minnesota, Condensed matter physics). 2004 – 2005.

Thesis advisor to 7 Ph. D. students who have graduated:

Yaron Turpaz, May, 2004. (Ph. D. B.S.: Tel Aviv U, Biology). Current position: Director, Integrative Computational Sciences (ICS), Eli Lilly Singapore Centre for Drug Discovery.

Andrew Binkowski, June, 2004. (Ph. D. B.S.: University of Illinois at Urbana-Champaign, Mechanical Engineering). Current position: Principle Investigator (equivalent to Assistant Professor), Structural Genomics Center, Argonne National lab.

Nathan Stitzel, August, 2004. (M.D./Ph. D., B.S.: Washington University, Mathematics). Current position: Physician, University of Chicago.

Jinfeng Zhang, Oct., 2004. (Ph. D. B.S.: Beijing U, MCS: UIC, Chemistry and Computer Science). Current position: Assistant Professor, Florida State University.

Jeffrey Tseng, June, 2006. (Ph. D. M.D.: Yangming Medical University, Medicine, Taiwan). “Evolutionary matching of protein local surfaces for predicting and characterizing biochemical functions”. Current position: Postdoctoral research associate with Prof. Wen-Hsiung Li at University of Chicago.

Ronald Jackups, Jr, Jan, 2007. “Prediction of transmembrane β -barrel protein structures”. (M.D./Ph. D., B.S.: Washington University, statistics). Current position: Pathology Resident, Washington University.

Xiang Li, Jan, 2007. “Protein structure and stability: Geometric analysis and applications”. (Ph. D., B.S.: Nankai University, M.S.: Chinese Academy of Medical Sciences). Current position: Postdoctoral research associate with Prof. Shankar Subramaniam at UCSD.

Thesis advisor to 6 current Ph. D. students:

Seman Kachalo (B.S.: Moscow State U, Physics). Prelim exam passed.

Hsiao-Mei Lu (B.S.: Chiao-Tong U, Graduate training: Taiwan U, Statistics). Qualification exam passed.

Joseph Dundas (B.S.: UIC, Bioengineering). Qualification exam passed.

Zheng Ouyang (B.S.: Beijing U, M.S.: Loyola University, Chemistry and Computer Science). Qualification exam passed.

Yun Xu (M.S.: Fudan University). Qualification exam passed.

David Morales-Jiminez (B.S.: University of Madrid). Qualification exam passed.

Hammad Naveed (B.S.: Pakistan). Fulbright scholar.

Thesis advisor to Master degree student:

Ying Wang (B.S.: Beijing Science and Technology University). 2007.

Ying Sun (B.S.: Nankai U, Chemistry). 2005. Current position: Graduate Student at U of Chicago.

Undergraduate students guided:

Shapor Naghibzadeh, 1999 – 2002; Patrick Freeman, 2002 – 2004; Tomasz Piotr Palarz, 2004 – 2005 (Currently CS PhD student at Carnegie-Mellon U); Matthew Dabrowski, 2005.

Thesis Committees

Preliminary Exam Committee: Dinakar Thirumalai, Ph.D. candidate, (Advisor: Mike Strosio), BioE. 2005; Yi Han, Jane Tseng, Ph.D candidate, (Advisor: Tony Hopfinger), Dept. of Medicinal Chemistry. UIC. 2001; Jie Lian. Ph.D Candidate, (Advisor: Bin He) Dept. of Bioengineering. UIC. 2001

Ph.D. Thesis Committee: Jie Lian, Ph.D. (Advisor: Bin He), Dept. of Bioengineering, UIC. 2002; Andrea Reaka, Ph.D. (Advisor: Tony Hopfinger), Dept. of Medicinal Chemistry. UIC. 2000; Jane Tseng, Ph.D. (Advisor: Tony Hopfinger), Dept. of Medicinal Chemistry. UIC. 2001; Han Yi, 2002.

M.S. Thesis Committee: Mingshu Wang (Thesis Advisor: Richard Magin, Bioengineering), May, 2000; Srikanth B Yellanki (Thesis Advisor: Bill O'Neil), Oct, 2002; Aparna Sapre (Thesis Advisor: Bill O'Neil), Oct, 2002; Mono Pirun, 2003.

Courses Developed

1. BioE 480. “*Introduction to Bioinformatics*”. Molecular biology concepts for non-biologists, sequence alignment, scoring method, database search methods, dynamic programming, Hidden Markov Model, functional motifs and profiles, protein folding problem, sequence-fold recognition, structure-based functional site analysis, genome-wise expression analysis, metabolism and pathways, computational and data mining methods for drug discovery.

2. BioE 580. “*Principle of Bioinformatics*”. Probabilistic and geometric modeling of biological sequences and structures. Distribution functions, Bayesian theorem. Conjugate distributions, Dirichlet mixture of chain models, Hidden Markov Models, expectation maximization, and bioinformatics applications (*e.g.* Coiled coil prediction, ME, gene prediction); Methods for supervised and unsupervised learning (discriminant analysis, *k*-nearest neighbor method and approximation, minimum spanning trees) and bioinformatics applications (*e.g.* protein function predictions, gene expression clustering). Computational structural bioinformatics.

3. BioE 594. “*Topics in Bioinformatics: Geometric Modeling of Molecules*” Topics include space filling model, solvent accessible surface, and molecular surface; Geometric structures of Voronoi diagram, Delaunay triangulation, alpha shape, and their computation; Connectivity by equivalence of spaces, homology groups, incremental algorithm, and matrix algorithm; Shape features of molecules in terms

of surface pockets, interior voids, and topological persistence; Shape matching and fitting: rigid motions, optimal motion, similarity, and complementarity, and shape space of proteins: native structures and decoy conformations, scoring functions, nonlinear parameterization of protein shape space.

4. Honors 200. “*Bioinformatics*” Flavor of computational studies in biology. This is an honor student class where I teach students the basic issues and future outlook of bioinformatics.

5. GCLS 504 Module V Graduate Education in Medical Sciences. “*Discovery bioinformatics and proteomics.*” This is a course for graduate students in Medical School. I organized this course, and co-taught with colleagues. This course covers bioinformatics and application tools in DNA and protein sequence analysis, microarray analysis, and protein structure analysis. The goal is to enable students to use bioinformatics tools and databases for their own research, and to develop essential sophistication in interpreting bioinformatics results.

Patent “**Molecular classification for property prediction**”. United States Patent, No. US6,182,016 B1, Jan. 30, 2001. (with H. Edelsbrunner).

Software and Webserver Release

1. castP: Computed Atlas of Surface Topography of proteins

CASTP provides computation of protein surfaces (<http://cast.engr.uic.edu/cast>). It is also listed in the Research Consortium of Structural Bioinformatics PDB website at San Diego Supercomputing Center (<http://www.rcsb.org/pdb/links.html>), which is the central portal of structural bioinformatics worldwide. We have provided about 50,000 computation since its launch. We estimate that the user community consists of 3,000-4,000 structural biologists and computational biologists.

T. Andrew Binkowski, Shapor Naghibzadeh, and Jie Liang. (2003). CASTp: computed atlas of surface topography of proteins. *Nucleic Acid Research*. 31(13):3352-3355

2. pvSOAR: pocket and void Surfaces Of Amino Acid Residues

This webserver provides detection of similar protein surfaces for discovering unrecognized or novel functional relationship between proteins. It has been used to predict biological functions of proteins in structural genomics. The pvSOAR webserver is available at <http://pvsoar.bioengr.uic.edu/>.

T. Andrew Binkowski, Patrick Freeman and Jie Liang (2004) pvSOAR: Detecting similar surface patterns of Pocket and Void Surfaces of Amino Acid Residues on proteins. *Nucleic Acid Research*. 32:W555-W558.

3. TopoSNP: A database of topographic mapping of single nucleotide polymorphism (SNPs) to protein structures.

This database provides structural and evolution information about currently known disease associated nonsynonymous SNPs (nsSNPs) derived from OMIM database,

and other nsSNPs derived from dbSNP. The URL is:
<http://gila.bioengr.uic.edu/snp/toposnp/>

Nathan O. Stitzel, T. Andrew Binkowski, Yan Yuan Tseng, Simon Kasif and Jie Liang (2004) topoSNP: A topographic database of non-synonymous single nucleotide polymorphisms with and without known disease association. *Nucleic Acid Research*. 32:D520-D522.

College and Campus Service

Member, UIC Cancer Center advisory committee,

Member, UIC NIH MD/PHD training program advisory committee,

Member, Executive Committee, Dept of Bioengineering. Current.

Member, Admissions Committee. Current.

Member, NIH Translational Research Center Grant Planning Committee. Current.

Member, Advisory Committee, UIC NIH MD/PHD Training Program, 2006-Present.

Fellow, Honors College, UIC. (2000–present)

Campus proteomics planning committee. (2005). I lead the efforts in providing the informatics component during the successful competition of the UIC Proteomics Platform from the Chicago Community Trust/Searle foundation. Working with Vice Provost Dr. Brenda Russell and others, I gave presentations on planned informatics activities, hosted tours of bioinformatics facilities, organized demos, and participated debates to convince multiple site-visiting teams that UIC possess the unique advantage of a strong bioinformatics group with strong faculty and students. I believe my contribution was essential for UIC to win the bid of the proteomics platform over Northwestern U and U of Chicago.

Campus bioinformatics task force. UIC. (2000–2001).

Advisory Committee of Research Resource Center Microarray Facility. UIC. (2001–2003)

Degree program development committee. Dept. of Bioengineering. (2000–present)
Developing and proposing of a Ph. D. program in Bioinformatics. In charge of curriculum development, determination and coordination of course sequences, and specification of degree requirement.

Recruiting Committee, National Center of Datamining. UIC. (1999–2000)

Faculty member. High school summer camp “Experience BioEngineering”. 2001, 2002.

Outreach Committee.

- *Speech at Lions Township High School, IL: Introducing Bioengineering as a major for potential recruits for UIC undergraduate program. Presentation of bioinformatics research at UIC.*

- *High school students summer training.* I have worked with two high school student for summer research experience in my lab. Student Sarah Cheng has continued to study CS at MIT, and Cem Onyuksel has continued to study EE at Carnegie-Mellon U.
- *Flossmore High School, II.* I have been working with science teacher Jean Barker in guiding the SMART team students in developing science project focusing on target three-dimensional models for developing anti-infectious tereapeutics.

Papers in Peer Reviewed Journals

Zheng Ouyang and Jie Liang. Predicting protein folding rates from geometric contact and amino acid sequence. *Protein Science*, Accepted.

Youfang Cao and Jie Liang, Optimal enumeration of state space of finitely buffered stochastic molecular networks and accurate computation of steady state landscape probability. *BMC Systems Biology*, Accepted.

Jerry Osagie Ebalunode, Zheng Ouyang, Jie Liang, and Weifan Zheng. A novel approach to structure-based pharmacophore search using computational geometry and shape matching techniques. *J. Chemical Information and Modeling*. Accepted.

Jian Zhang, Ming Lin, Rong Chen, Wei Wang, and Jie Liang Discrete state model and accurate estimation of loop entropy of RNA secondary structures. *J. Chem. Phys.* Accepted.

Ming Lin, Rong Chen, and Jie Liang. Statistical geometry of lattice chain polymers with voids of defined shapes: Sampling with strong constraints. *J. Chem. Phys.* Accepted.

Joe Dunda, T Andrew Binkowski, Bhaskar DasGupta, and Jie Liang. Topology independent protein structural alignment. *BMC Bioinformatics* 2007, 8:388, doi:10.1186/1471-2105-8-388 (15 October 2007)

Hsiao-Mei Lu and Jie Liang (2007) A model study of protein nascent chain and cotranslational folding using hydrophobic-polar residues. *Proteins*. Accepted.

Yan Yuan Tseng and Jie Liang (2007) Predicting enzyme functional surfaces and locating key residues automatically from structures. *Annals of Biomedical Engineering*. 35(6):1037-42..

Jinfeng Zhang, Ming Li, Rong Chen, Jie Liang, and Jun Liu (2007) Monte Carlo sampling of near-native structures of proteins with applications. *Proteins*. 66(1):61-68.

Larisa Adamian, Zheng Ouyang, Yan Yuan Tseng, Jie Liang (2006) Evolutionary Patterns of Retinal-binding Pockets in Rhodopsins and Their Functions. *Photochem Photobiol*. 82(6):1426-1435

Ronald Jackups, Jr. Sarah Cheng and Jie Liang.(2006) Sequence motifs and anti-motifs in beta-barrel membrane proteins from a genome-wide analysis: the Ala-Tyr dichotomy and chaperone binding motifs *J. Mol. Biol.*, 363(2):611-23.

Larisa Adamian and Jie Liang.(2006) Prediction of transmembrane helix orientation in polytopic membrane proteins. *BMC Structural Biology*. 6:13.1-17, doi:10.1186/1472-6807-6-13

Joe Dundas, Zheng Ouyang, Jeffery Tseng, Andrew Binkowski, Yaron Turpaz and Jie Liang. (2006) CASTp: computer atlas of surface topography of proteins with structural and topographical mapping of functionally annotated residues. *Nucleic Acids Research*, W116-118.

Sema Kachalo, Hsiao-Mei Lu and Jie Liang.(2006) Protein folding dynamics via quantification of kinematic energy landscape. *Physical Review Letters*. 96:058105.1-4.

Jinfeng Zhang, Rong Chen, and Jie Liang.(2006) Empirical potential function for simplified protein models: Combining contact and local sequence-structure descriptors. *Proteins*, In press.

Larisa Adamian and Jie Liang.(2006) Prediction of buried helices in multispans alpha helical membrane proteins. *Proteins*, 63(1):1-5.

Yan Yuan Tseng and Jie Liang.(2005) Estimation of amino acid residue substitution rates at local spatial regions and application in protein function inference: A Bayesian Monte Carlo approach. *Mol. Biol. Evo.* 23:421-436.

Ronald Jackups, Jr. and Jie Liang.(2005) Interstrand pairing patterns in beta-barrel membrane proteins: the positive-outside rule, aromatic rescue, and strand registration prediction. *J. Mol. Biol.*, 354:979-993. (doi:10.1016/j.jmb.2005.09.094, selected as Editor's Choice by the *Science* magazine, Nov. 4, 2005).

T. Andrew Binkowski, Andrzej Joachimiak, and Jie Liang.(2005) Protein surface analysis for function annotation in high-throughput structural genomics pipeline. *Protein Science*, 14:2972-2981.

Larisa Adamian, Vikas Nanda, William F. DeGrado, and Jie Liang. (2005) Empirical lipid propensities of amino acid residues in multispans alpha helical membrane proteins. *Proteins*. 59(3):496-509.

Xiang Li, and Jie Liang.(2005) Geometric cooperativity and anti-cooperativity of three-body interactions in native proteins. *Proteins*. 60:46-65.

Xiang Li, Ozlem Keskin, Buyong Ma, Ruth Nussinov and Jie Liang. (2004) Protein-protein interactions: Hot spots and structurally conserved residues often locate in complemented pockets that are pre-organized in the unbound states. Implications to docking *J. Mol. Biol.* 344:781-795

Nathan Stitzel, Brenton G. Mar, Jie Liang, and Carol Westbrook.(2004) Membrane-associated and secreted genes in breast cancer. *Cancer Research*. 64:8682-8687.

Moon Jung Song, Seungmin Hwang, Wendy Wong, June Round, DeeAnn Martinez-Guzman¹, Yaron Turpaz, Jie Liang, Ben Wong, Reid C. Johnson, Michael Carey, and Ren Sun. (2004) The DNA architectural protein HMGB1 facilitates RTA-mediated viral gene expression in gamma2 herpesviruses. *J. Virology*. In press.

Changyu Hu, Xiang Li, and Jie Liang.(2004) Developing optimal nonlinear scoring function for protein design *Bioinformatics*. 20(17):3080-3098.

Jinfeng Zhang, Yu Chen, Rong Chen and Jie Liang (2004) Importance of chirality and reduced flexibility of protein side chains: A study with square and tetrahedral lattice models. *J. Chem. Phys.* 121:592-603.

T. Andrew Binkowski, Patrick Freeman and Jie Liang (2004) pvSOAR: Detecting similar surface patterns of Pocket and Void Surfaces of Amino Acid Residues on proteins. *Nucleic Acid Research*. 32:W555-W558.

Yan Yuan Tseng and Jie Liang (2004) Are residues in a protein folding nucleus evolutionarily conserved? *J. Mol. Biol.* 335:869-880.

Nathan O. Stitzel, T. Andrew Binkowski, Yan Yuan Tseng, Simon Kasif and Jie Liang (2004) topoSNP: A topographic database of non-synonymous single nucleotide polymorphisms with and without known disease association. *Nucleic Acid Research*. 32:D520-D522.

Xiang Li, Changyu Hu, and Jie Liang. (2003). Simplicial edge representation of protein structures and alpha contact potential with confidence measure. *Proteins*. 53:792-805.

T. Andrew Binkowski, Larisa Adamian and Jie Liang. (2003) Inferring functional relationship of proteins from local sequence and spatial surface patterns. *J. Mol. Biol.* 332:505-526.

T. Andrew Binkowski, Shapor Naghibzadeh, and Jie Liang. (2003). CASTp: computed atlas of surface topography of proteins. *Nucleic Acid Research*. 31(13):3352-3355. Abstract

Nathan O. Stitzel, Yan Yuan Tseng, Dimitri Pervouchine, David Goddeau, Simon Kasif, and Jie Liang. (2003) Structural location of disease-associated single nucleotide polymorphisms. *J. Mol. Biol.* 327:1021-1030.

J. D. Lear, H. Gratkowski, L. Adamian, J. Liang, and W.F. DeGrado. (2003) Position-dependence of stabilizing polar interactions of asparagine in transmembrane helical bundles. *Biochemistry*. 2003 42(21):6400-6407.

Larisa Adamian, and Jie Liang. (2003) Interhelical hydrogen bonds in transmembrane region are important for function and stability of Ca²⁺-transporting ATPase. *Cell Biochemistry and Biophysics*. 39:1-12.

Larisa Adamian, Ronald Jackups, Jr, T. Andrew Binkowski, and Jie Liang. (2003) Higher order interhelical spatial interactions in membrane proteins. *J. Mol. Biol.* 327:251-272.

Jinfeng Zhang, Rong Chen, Chao Tang, and Jie Liang. (2003) Origin of scaling behavior of protein packing density: A sequential Monte Carlo study of compact long chain polymers. *J. Chem. Phys.* 118(13):6102-6109.

Jie Liang, Jinfeng Zhang and Rong Chen. (2002) Statistical geometry of packing defects of lattice chain polymer from enumeration and sequential Monte Carlo method. *J. Chem. Phys.*, 117:3511-3521. Selected by (*Virtual Journal of Biological Physics Research*–August 1, 2002 Volume 4, Issue 3).

Jie Liang and Sema Kachalo. (2002) Computational Analysis of Microarray Gene Expression Profiles Clustering, Classification, and Beyond. *Chemometrics and Intelligent Laboratory Systems*, 62:199-216.

Larisa Adamian, and Jie Liang. (2002) Interhelical hydrogen bonds and spatial motif in membrane proteins: Polar clamps and serine zippers. *Proteins*, 47:209-218

Maria P. McGee, Jie Liang, and J. Luba. (2002) Hydration effects of heparin on antithrombin probed by osmotic stress. *Biophys. J.*, 82:1040-1049

M. P. McGee and J. Liang. (2002) Factor X, Coagulation. *Wiley Encyclopedia of Molecular Medicine*. John Wiley & Sons.

L. Adamian and J. Liang. (2001) Helix-helix packing and interfacial pairwise interactions of residues in membrane proteins. *J. Mol. Biol.*, 311:891-907

J. Liang and K.A. Dill. (2001) Are proteins well-packed? *Biophys. J.*, 81:751-766

M. P. McGee and J. Liang. (2001) Regulation of glycosaminoglycan function by osmotic potentials. Measurement of water transfer during antithrombin activation by heparin. *J. Biol. Chem.*, 276:49275-49282

I. Gomes, T. L. Sharma, J. D. Kapp, S. Edassery, N. Fulton, J. Liang, R. Hoffman, and C.A. Westbrook. (2001) Highly abundant genes in the transcriptome of human and baboon CD34 antigen-positive bone marrow cells. *Blood*, 98:93-99.

C. Yuan, O. Kuwata, J. Liang, S. Misra, S.P. Balashov, T.G. Ebrey. (1999) Chloride binding regulates the Schiff base pK in gecko P521 cone-type visual pigment. *Biochemistry*, 38:4649-4654.

M.P. McGee, H. Teuschler and J. Liang. (1999) Electrostatic interactions during activation of coagulation factor IX via the tissue factor pathway: effect of univalent salts. *Biochim. Biophys. Acta*, 1453:239-253

J. Liang, H. Edelsbrunner, and C. Woodward. (1998) Anatomy of protein pockets and cavities: Measurement of binding site geometry and implications for ligand design. *Protein Science*, 7 , 1884-1897.

H. Edelsbrunner, M. Facello and J. Liang. (1998) On the definition and the construction of pockets in macromolecules. *Disc. Appl. Math.* 88:83-102

- J. Liang, H. Edelsbrunner, P. Fu, P.V. Sudhakar and S. Subramaniam. (1998) Analytical shape computing of macromolecules II: identification and computation of inaccessible cavities inside proteins. *Proteins*. 33, 18-29
- J. Liang, H. Edelsbrunner, P. Fu, P.V. Sudhakar and S. Subramaniam. (1998) Analytical shape computing of macromolecules I: molecular area and volume through alpha shape. *Proteins*. 33, 1-17.
- J. Liang and M.P. McGee. (1998) Mechanisms of coagulation factor Xa inhibition by antithrombin. Correlation between hydration structure and water transfer during reactive loop insertion. *Biophys. J.*, 75 , 573-582.
- M.P. McGee, H. Teuschler, and J. Liang. (1998) Effective electrostatic charge of coagulation factor X in solution and on phospholipid membranes: implications for activation mechanisms and structure-function relationships of the Gla domain. *Biochem. J.*, 330 , 533-539.
- J. Liang and S. Subramaniam. (1997) Computation of molecular electrostatics with boundary element methods. *Biophys. J.*, 73 , 1830-1841.
- S. Kim, J. Liang, and B.A. Barry. (1997) Chemical complementation identifies a proton acceptor for redox-active tyrosine D in photosystem II. *Proc. Natl. Acad. Sci. USA*, 94 , 14406-14411.
- J.W. Lewis, J. Liang, T.G. Ebrey, M. Sheves, N. Livnah, O. Kuwata, S. Jager, and D.S. Kliger. (1997) Early photolysis intermediates of gecko and bovine artificial visual pigments. *Biochemistry*, 36 , 14593-14600
- J. Lewis, J. Liang, T.G. Ebrey, M. Sheves and D.S. Kliger. (1995) Chloride effect on the early photolysis intermediates of a gecko cone-type visual pigment. *Biochemistry* 34 , 5817-5823. (899 KB)
- J. Liang, G. Steinberg, N. Livnah, M. Sheves and T.G. Ebrey. (1994) The pKa of the protonated Schiff base of gecko cone and octopus visual pigments. *Biophys. J.* 67 , 848-854.
- J. Liang, R. Govindjee, and T.G. Ebrey. (1993) Metarhodopsin intermediates of the gecko cone pigment P521. *Biochemistry*, 32(51) , 14187-14193. (802 KB)
- W. Lin, C. Ma, Z. Luo, W. Fan, Y. Chen and J. Liang. (1987) Study on the radiosensitization of AT1727 on human lung adenocarcinoma cell line SPC-A- 1. *Chin. J. Radiat. Res. Radiat. Processing*, 5 , 58-62.

Papers in Peer Reviewed Conference Proceedings

- Youfang Cao and Jie Liang. An optimal algorithm for enumerating state space of stochastic molecular networks with small copy numbers of molecules. *Conf Proc IEEE Eng Med Biol Soc*, 2007, 1:4599–602.
- Hsiao-Mei Lu and Jie Liang. Perturbation-based Markovian Transmission Model for Macromolecular Machinery in Cell. *Conf Proc IEEE Eng Med Biol Soc*, 2007, 1:5029–34.

Zheng Ouyang and Jie Liang. Detecting Positively Selected Sites From Amino Acid Sequences: An Implicit Codon Model. *Conf Proc IEEE Eng Med Biol Soc*, 2007, 1:5302–5306.

Joe Dundas, T.A. Binkowski, Bhaskar DasGupta and Jie Liang, Topology Independent Protein Structural Alignment 7th Workshop on Algorithms in Bioinformatics, R. Giancarlo and S. Hannenhalli (Eds.), LNBI 4645, Springer-Verlag Berlin Heidelberg, pp. 171–182, September 2007.

Yan-Yuan Tseng and Jie Liang.(2006) Automated method for predicting enzyme functional surfaces and locating key residues with accuracy and specificity. *Conf Proc IEEE Eng Med Biol Soc*. 1:4552-5.

Jeffrey Tseng and Jie Liang. Estimating evolutionary rate of local protein binding surfaces: a Bayesian Monte Carlo approach. *IEEE EMBS 2005 Conference Proceeding*, 739 - 742..

Sema Kachalo, Hsiao-Mei Lu, and Jie Liang. Protein folding dynamics in lattice model with physical movement. *IEEE EMBS 2005 Conference Proceeding*, 4449 - 4452.

Xiang Li, and Jie Liang. (2005) Computational design of combinatorial peptide library for modulating protein-protein interactions. *Pacific Symposium on Bio-computing*. 2005, 28-39.

Jinfeng Zhang, Rong Chen, and Jie Liang. (2004) Potential function of simplified protein models for discriminating native proteins from decoys: Combining contact interaction and local sequence-dependent geometry. *IEEE EMBS 2004 Conference*.

Thomas Andrew Binkowski, Bhaskar DasGupta, and Jie Liang. (2004) Order independent structural alignment of circularly permuted proteins. *IEEE EMBS 2004 Conference*.

Herbert Edelsbrunner, Michael Facello and Jie Liang. (1996) On the Definition and the Construction of Pockets in Macromolecules. *Pacific Symposium on Bio-computing*. 1996.

Herbert Edelsbrunner, Michael Facello, Ping Fu and Jie Liang. (1995) Measuring proteins and voids in proteins. *Proc. 28th Ann. Hawaii Intl. Conf. System Sci*. Vol. 5. 256-264.

Review Articles

Jie Liang, Larisa Adamian, and Ronald Jackups, Jr.(2005) The membrane-water interface region of membrane proteins: structural bias and the anti-snorkeling effect. *Trends in Biochemical Sciences*. 30(7):355-357.

Jie Liang. (2002) Experimental and computational studies of the determinants of membrane protein folding. *Current Opinion in Chemical Biology*. 6:878-884

Book Chapters

Xiang Li and Jie Liang. (2006) Knowledge-based energy functions for computational studies of proteins. *Computational methods for protein structure prediction and modeling. Volume 1: Basic characterization* (Eds: Ying Xu, Dong Xu, and Jie Liang). p.71–124. Springer, 2006.

Jie Liang. (2006) Computation of protein geometry and its applications: Packing and function prediction. *Computational methods for protein structure prediction and modeling. Volume 1: Basic characterization* (Eds: Ying Xu, Dong Xu, and Jie Liang). p.181–206. Springer, 2006.

Dong Xu, Jie Liang, and Ying Xu. Resources and infrastructure for structural bioinformatics. *Computational methods for protein structure prediction and modeling. Volume 2: Structure prediction* (Eds: Ying Xu, Dong Xu, and Jie Liang). p.207–228. Springer, 2006.

Yang Dai and Jie Liang. Mathematics and statistics for studying protein structure. *Computational methods for protein structure prediction and modeling. Volume 2: Structure prediction* (Eds: Ying Xu, Dong Xu, and Jie Liang). p.299–316. Springer, 2006.

Invited Talks

“Detecting geometric pattern and evolutionary signal from protein structure for understanding biological functions and predicting protein-protein interaction surfaces”, Center of Bioinformatics, University of Kansas, Lawrence, KS, May 6, 2008.

“Computational systems bioengineering: from single molecule, interaction networks, to cellular pattern formation.” Dept. of Bioengineering, University of California at Riverside, April 17, 2008.

“Geometric potential for protein structure and binding prediction”, The 2008 NIH Protein Structure Initiative “Bottlenecks” Workshop, Bethesda, Maryland, April 14, 2008.

Statistics Seminar. “Entropy, folding, and function of biomolecules through Monte Carlo sampling.” Dept. of Mathematics, University of Illinois at Chicago, April 2, 2008

“Dynamics in systems biology: from single molecule, macromolecular machines, regulatory networks, to cellular pattern formation.” Dept. of Biomedical Engineering, Northwestern University, March 13, 2008.

“Characterizing entropic effects, transition state ensemble, and folding dynamics of biomolecules.” Condensed Matter Colloquim, Dept. of Physics, University of Illinois at Chicago, March 12, 2008.

“Discovery of geometric pattern and evolutionary signal from protein structure for understanding biological functions and predicting protein-protein interactions.”

Center for Computational Biology and Bioinformatics, Indiana University, School of Medicine. Feb. 11, 2008. Indianapolis, IN.

1st Midwest Symposium on Computational Biology & Bioinformatics (MSCBB), “Exact computation of probability landscape of small molecular networks with full stochasticity: An alternative to Gillespie simulation and Fokker-Planck approximation”, Oct. 6, 2007. Northwestern University, Evanston, IL.

“Bayesian estimation of functional residues substitution rates and optimal-structure derived global protein fitness landscape”, The Ecology and Evolution Natural History Seminar, U of Chicago, Oct. 2, 2007.

“Exact stochastic behavior of molecular networks and realistic simulation of cellular pattern formation”, Dept of Mathematics, University of California at Irvine, Sept. 26, 2007, Irvine, CA.

“Understanding how proteins work in cell: A computational approach” July 2, 2007. Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan.

Bioinformatics Symposium - Recent advances and breakthroughs in bioinformatics research, Morning keynote speech. “Spatial patterns of structures for understanding protein folding, evolution, and biological functions”, Institute of Bioinformatics and Molecular Bioinformatics Center, National Chiao-Tung University, July 3, 2007. Hsin-Chu, Taiwan.

Bioinformatics Symposium - Recent advances and breakthroughs in bioinformatics research, Afternoon keynote speech. “Improved sampling and discrimination for characterizing protein transition state ensemble, designing phage display library, and for predicting physical protein-protein interactions” Institute of Bioinformatics and Molecular Bioinformatics Center, National Chiao-Tung University, July 3, 2007. Hsin-Chu, Taiwan.

“Transition state ensemble of protein folding and evolutionary selection pressure through Sequential Monte Carlo and MCMC”. 3rd Harvard Monte Carlo Workshop, Harvard University, Boston, May 13, 2007.

“Geometry and protein function”. Dept of Computer Science, Ohio State U. May, 2007 .

“Inferring functions and dynamics of biological structures”. Shanghai Center for Bioinformatics, Shanghai, China, November 30, 2006.

“Dynamics of biological systems: From protein folding to large virus particles”, Institute of Biophysics, Dept of Physics, Nanjing University, Nanjing, China, November 23, 2006.

“Inferring biological functions: From molecules to systems” School of Electronic, Information and Electrical Engineering, Shanghai Jiaotong University, Shanghai, China, November 15, 2006.

“Evolutionary matching of surface patterns for predicting protein functions and

binding specificities”. Plenary speaker, WICB 2006, Institute of Intelligent Automation, Chinese Academy of Sciences, Hefei, Nov 13, 2006.

“Protein folding dynamics via quantification of kinematic energy landscape and model simplification.” Zhou Pei-Yuan Center of Applied Math, Tsinghua University, Beijing, October 27, 2006.

“Evolutionary matching of surface patterns for predicting protein functions and binding specificities.” Academy of Mathematics and Systems Sciences, Chinese Academy of Sciences, Beijing, October 27, 2006.

“Combinatorial model for sequence and spatial motif discovery in short sequence fragments: Examples from beta-barrel membrane proteins”. IEEE-EMBS 2006 Conference. August 30 - Sept 3, 2006. New York, NY.

“Automated method for predicting enzyme functional surfaces and locating key residues with accuracy and specificity”. IEEE-EMBS 2006 Conference. New York, NY. August 30 - Sept 3, 2006.

“Evolutionary matching of surface patterns for predicting protein functions and binding specificities”. The 4th International Conference of Structural Genomics, Beijing, October 23, 2006.

“Evolution of protein local surfaces: predicting binding surfaces, key residues, and functions”. The Biomedical Engineering Society (BMES) 2007 Annual Meeting, Chicago, October 12, 2006.

“Protein folding dynamics via quantification of kinematic energy landscape and model simplification.” Dept. of Mathematics, Fudan University, Shanghai, August 17, 2006.

“Evolutionary matching of surface patterns for predicting protein functions and binding specificities.” Shanghai University, August 9, 2006.

“Spatial patterns, folding dynamics, and biological functions of protein molecules.” Institute of Applied Physics, Chinese Academy of Sciences, Jiading, Shanghai, China, July, 11, 2006.

“Understanding how proteins work in cell: A bioinformatics approach.” Life Science Center, University of Missouri at Columbia, May 11, 2006.

“Voids and pockets in proteins: packing, folding, evolution, and biological functions.”. Dept of Computer Science, University of Missouri at Columbia, May 10, 2006.

“Predicting protein functions through evolutionary models of geometrically computed structural binding surfaces”. Bioinformatics Seminar Series, Toyota Institute of Technology, The University of Chicago. April 17, 2006.

“The nature of membrane protein assembly and applications in structure prediction” *Cells and Materials: At the Interface between Mathematics, Biology and*

Engineering Workshop I: Membrane Protein Science and Engineering. Institute of Pure and Applied Mathematics (IPAM). UCLA, March 29, 2006.

“Tessellations of protein structures”. *Workshop: The World a Jigsaw – Tessellations in the Sciences*, Lorentz Centre, Leiden University, The Netherlands, March 6–12, 2006.

“Predicting protein functions through evolutionary models of structural binding surfaces” Center for Bioinformatics and Computational Biology. Institute for Genome Sciences & Policy (IGSP), Duke University. Nov. 30, 2005.

“Geometric patterns and evolution of protein local structures: Predicting protein function and designing peptide modulators for protein-protein interactions” Dept of Biochemistry, University of Wisconsin at Madison, Oct. 3, 2005

“Surface pattern, conformational search, and scoring function for proteins: structure, function, design and evolution.” Dept. of Macromolecular Sciences, Fudan University, Shanghai, China, August 29, 2005.

“Inferring protein functions by local surface matching and similarity assessment”. School of Life Sciences, Beijing University, August 25, 2005.

“Surface pattern, conformational search, and scoring function for proteins: structure, function, design and evolution.” Dept. of Chemistry, Chinese University of Hong Kong, August 22, 2005.

“1. Cavity and voids in proteins and protein functions from geometric computation; 2. Cavity and folding studies of proteins by sequential Monte Carlo sampling; 3. Predicting protein function by evolutionary matching of binding surfaces; and 4. Global protein engineering with optimal empirical potential function and computational design of peptide library.” 5th International Summer School on Biocomplexity: from System to Gene. Dartmouth College, Hanover, NH, July 1, 2005

“Inferring protein functions by local surface matching and similarity assessment”. *3rd Conference of Modeling of Protein Interactions in Genomes*, June 27, 2005, Lawrence, Kansas.

“Protein surface patterns and their functional roles: estimating residue replacement rates and characterizing global design fitness landscape” February 4, 2005. Department of Biostatistics. University of Michigan, Ann Arbor.

“Motifs and Interactions in Alpha-Helical and Beta-Barrel Membrane Proteins”. September 20, 2004. Department of Biochemistry and Molecular Biology. University of Texas, Health Science Center at Houston, Medical School.

“Surface pattern, search method, and scoring function for studying proteins.” Dill Lab, September 1, 2004. U California at San Francisco.

“Simulating protein structures by sequential Monte Carlo.” August 27–28, 2004. The Second Workshop on Monte Carlo Methods. Harvard University, Boston, MA.

“Geometric representation, conformational search, and scoring function for computational studies of proteins: structure, function, design and evolution”. April 12, 2004, O.M. Stewart Colloquium, Dept of Physics, University of Missouri, Columbia, Missouri.

“Computational molecular topographics: structure, function, folding, design and evolution of proteins.” Fudan Bioinformatics Workshop. December 17, 2003, Fudan University, Shanghai, China.

“Geometric representation, conformational search, and scoring function for computational studies of proteins: structure, function, design and evolution.” University Seminar, December 11, Chongqing Medical University, Chongqing, China.

“Geometric representation, conformational search, and scoring function for computational studies of proteins: structure, function, design and evolution.” December 10, School of Life Science, Chongqing University, Chongqing, China.

“Geometric representation, conformational search, and scoring function for computational studies of proteins: structure, function, design and evolution.” December 4, 2003, Dept. of Biomedical Engineering, Boston University. Boston, MA.

“Structural bioinformatics of protein binding surfaces.” August 19, 2003. Eli Lilly and Company. Indianapolis, IN.

“Inferring functional relationship by discovery of local sequence and spatial patterns of protein surfaces.” Second Conference on Modeling of protein interactions in genomes. June 29, 2003. SUNY at Stony Brook, NY.

“Spatial and Surface Pattern of Proteins and Optimal Potential for Protein Folding and Protein Design.” March 31, 2003. Illinois Institute of Technology, Chicago, IL.

“Statistical potential and kernel model derived from alpha shapes for protein folding ”. 2002 Triangle Biophysics Seminar, Nov. 15, 2002. Duke University/University of North Carolina, Chapel Hill, NC.

“Interhelical interactions in membrane proteins”. Nov. 1, 2002. Dept. of Biochemistry, Wright State University, OH.

“Exploring backbone and side chain packing in lattice models using Sequential Monte Carlo” Sept. 11–12, 2002. 1st Cape Cod Harvard Monte Carlo workshop. Cape Cod, MA.

“Spatial Surface Patterns and Protein Functions.” May 2, 2002. Biosciences Division, Argonne National Laboratory, IL.

“Protein surface topography”. April 22, 2002. Depart. of Anesthesiology, School of Medicine, University of Pennsylvania, Philadelphia, PA.

“Voids in lattice polymers and proteins” April 8, 2002. Department of Physics, North Carolina State University, NC.

“Study protein geometry via sequential Monte Carlo”. Jie Liang, Jinfeng Zhang, and Rong Chen. International Biometric Society ENAR 2002 meeting, March 20, 2002, Arlington VA.

“Contact interactions and spatial voids in proteins”. NEC Research Institute, Princeton, NJ. Jan 8, 2002.

“Helix-Helix Interactions in Membrane Proteins” Depart. of Biochemistry and Biophysics University of Pennsylvania, Dec 14, 2001

“Learning from Protein Structures: Implications for Molecular Recognition and Membrane Protein Assembly” Dept. of Chemistry and Biochemistry, Ohio University, June 1, 2001.

“Specific Pairwise Interactions in Helical Membrane Proteins”, Finch University of Health Sciences/The Chicago Medical School. May 10, 2001.

Bioinformatics Symposium Speaker. “Bioinformatics of Protein Surfaces in the Post-Genomic Era”, Biomedical Engineering Society 2001, Orlando, FL, April 3, 2001.

Computational analysis of gene expression profiles. Genomics Symposium “Microarray technology: Applications and approaches”, Research Resources Center, University of Illinois at Chicago. March 16, 2001.

Analyzing Packing in Membrane Proteins and Mapping Protein Functional Surfaces. Dept. of Medicinal Chemistry, University of North Carolina, December 1, 2000.

Analyzing Packing in Membrane Proteins and Mapping Protein Functional Surfaces Dept. of Computer Science, Duke University, November 30, 2000.

Surface Analysis of Proteins. Dept. of Bioengineering, University of California at San Diego, August, 2000.

The 16th International Conference on Advanced Sciences and Technology (ICAST2000). Fermi Lab, Batavia, June, 2000

Cambridge Research Lab/Compaq, Cambridge, MA, March 14, 2000.

Dept. of Biomedical Engineering, Boston University, March 13, 2000.

Geometric Analysis of Protein Surfaces and Protein Cores: Implications for Molecular Recognition and Protein Stability. Dept. of Biochemistry, University of Illinois at Chicago. Feb. 24, 2000

The geometric structures of protein surfaces. Dept. of Ophthalmology and Visual Sciences, University of Illinois at Chicago. Nov. 10, 1999.

DARPA Workshop on Novel Approaches to Stabilization of Biomaterials, Breckenridge, Colorado, June 9–13, 1999.

CAMP/Nonlinear PDE Seminar. Dept. of Mathematics, University of Chicago, Chicago, Illinois, May, 1999.

Seminar. Biotechnology Center, Virginia Tech, Blacksburg, Virginia, February, 1999.

Seminar. Dept. of Biology, Rensselaer Polytechnic Institute, Troy, New York, January 1999.

Biochemistry Seminar. Dept. of Chemistry & Biochemistry, Worcester Polytechnic Institute, Worcester, Massachusetts, January 1999.

Analyzing Molecular Shapes: Novel Computational Approaches to Receptor Based Ligand Design and Combinatorial Drug Discovery. Dept. of Pharmacology, Case Western Reserve University, Cleveland, Ohio, August 1998.

Biophysics Seminar. *Protein Surface Packing.* Dept. of Physics, Drexel University, Philadelphia, Pennsylvania, August 1998.

Invited Symposium Speaker. Annual Biophysical Society Meeting. Symposium on Bioinformatics: Computer-Based Predictions of Protein Structure and Binding. *Anatomy of protein binding pockets – implication for drug search and design.* Kansas City, Missouri. Feb. 24, 1998.

Numerical Analysis Seminar. *Molecular Electrostatics through Boundary Integral Equations.* Dept. of Mathematics, University of Minnesota, Minneapolis, Minnesota, March 1997.

Combinatorics Seminar. *Computing Geometric Structures for Molecular Modeling.* Dept. of Mathematics, University of Minnesota, Minneapolis, Minnesota, March 1997.

Novel Computational Methods for Drug Design: Docking and Diversity Management. SmithKline Beecham Pharmaceuticals, King of Prussia, Pennsylvania, February 1997.

Workshop on Voronoi Diagram, Triangulations, Splines. *Applying Novel Computational Methods for Protein Packing, Protein Hydration and Drug Search/Design.* Arizona State University, Tempe, Arizona, Feb. 1997

Protein-Ligand Recognition and Drug Lead Search: Novel Computational Approach. Eli Lilly and Company, Indianapolis, Indiana, Feb. 1997.

The Shape of Molecules and Computational Biology. Pomona College, Claremont, California, Feb. 1997

Shape and Chemistry Based Novel Computational Methods for Compound Diversity Management, Ligand Docking, and Structural Bioinformatics. Pangea Systems, Oakland, California, Jan. 1997

Methods towards Analytic Shapes of Macromolecule and their Applications. Protein Club, Dept. of Biochemistry, University of Minnesota, Oct. 1996

Analytical computing of the molecules: area, volume, void, pocket and more. National Cancer Institute/National Institute of Health, Oct. 1995

Contributed Talks

Biophysic Soc. Meeting *Interhelical side chain and backbone interactions in membrane proteins.* Boston, Feb. 2001.

Pacific Symposium on Biocomputing. Euler: Novel shape descriptors for high-throughput screening and combinatorial drug discovery. Honolulu, Hawaii, Jan. 2000.

Annual Biophysical Society Meeting. *Analytical method for molecular shapes: area, volume, cavities, interface and pockets.* Baltimore, Maryland. Feb. 20, 1996.

Pacific Symposium on Biocomputing. *On the definition and the construction of pockets in macromolecules.* Kohala Coast, Hawaii. Jan. 3, 1996.

Conference Abstracts

Liang, J. A novel class of molecular shape descriptors and a method for validation of chemical diversity. ABSTR PAP AM CHEM S 217: 127-COMP Part 1 MAR 21 1999

Computational analysis of cDNA microarray expression profiles of histiocytic lymphoma cells under the stress of phorbol myristic acid. Y. Turpaz, T. Le, I. Gomes, C. Westbrook, and **J. Liang**. World Congress of Medical Physics and Biomedical Engineering, 2000.

Atlas of topographic surfaces of all known protein structures. S. Naghibzadeh, and J. Liang. World Congress of Medical Physics and Biomedical Engineering, 2000.

Comparability of gene expression between human and baboon CD34+ marrow cells. T. Le, I. Gomes, **J. Liang**, Y. Turpaz, R. Hoffman, and C.A. Westbrook. International Society of Experimental Hematology Meeting, 2000. EXP HEMATOL 28 (7): 88 Suppl. 1 JUL 2000

Identification of Downstream Targets of the Putative Tumor Suppressor Gene on 8p by Differential Gene Expression Analysis. K. Banerjee, Z. Arbieva, L. Usha, T. T. Le, **J. Liang**, I. Gomes, and C. A. Westbrook. 92nd Annual Meeting of American Association for Cancer Research.

Mapping nonsynonymous Single Nucleotide Polymorphism (SNPs) to protein surfaces. N. Stitzel, J. Tseng, and **J. Liang** Student Medical Research Forum, University of Illinois. 2001.

Interhelical side chain and backbone interactions in membrane proteins. J. Liang and L. Kosynkina. *Biophys J.* 2001, 80 Part2: 1482Plat.

Hydrogen bond networks in membrane proteins. **J. Liang** and L. Kosynkina, Biophysical Society Meeting, 2001. *Biophys J.* 2001, 80 Part2: 50a.

CastP: Computed Atlas of Surface Topography of proteins. S. Naghibzadeh, T. A. Binkowski, and **J. Liang**. Biophysical Society Meeting, 2001. *Biophys J.* 2001, 80 Part2: 320a.

Analysis of backbone fold and surface features of viral proteins. Y. Turpaz, and **J. Liang**. Biophysical Society Meeting, 2001. *Biophys J.* 2001, 80 Part2: 323a.

Structure and function of antithrombin analyzed by computational geometry and osmotic stress. M. P. McGee, and **J. Liang** Biophysical Society Meeting, 2001. *Biophys J.* 2001, 80 Part2: 400a.

Compound classification by VARSA shape descriptors: An approach combining. Liang J, Hu CY 2001 August. American Chemical Society Meeting. ABSTR PAP AM CHEM S 222: 91-COMP Part 1 AUG 2001

Aligning genomic sequences to functionally important surface pockets on protein structures for drug discovery. Turpaz Y, Liang J 2001 August. American Chemical Society Meeting. ABSTR PAP AM CHEM S 222: 191-COMP Part 1 AUG 2001

TIGR Computational Genomics Conference. 2001 Oct Plenary Session 5. Protein functions from matching spatial surface patterns. Andrew Binkowski, Larisa Adamian, and Jie Liang. Conference Program and Abstract Book, P.10.

Protein functions from matching sequence patterns derived from spatial surface pockets Biophysical Society Meeting, 2002. Liang J, Binkowski TA, Adamian LA. *BIOPHYS J* 82 (1): 818 Part 2 JAN 2002

High propensity, statistically significant interhelical triple clusters of amino acid residues in membrane proteins Liang J, Jackups R, Adamian LA. Biophysical Society Meeting, 2002. *BIOPHYS J* 82 (1): 2513 Part 2 JAN 2002

Ca²⁺ transporting activity of Ca²⁺-ATPase is correlated with packing interactions of TM helices. Adamian LA, Liang J Biophysical Society Meeting, 2002. *BIOPHYS J* 82 (1): 2564 Part 2 JAN 2002

Geometry and statistics of voids in lattice polymers. Liang J, Chen R, Zhang JF Biophysical Society Meeting, 2002. *BIOPHYS J* 82 (1): 2298 Part 2 JAN 2002

Kernel Model Derived from Simplicial Contact Edges for Protein Folding. Hu C, X Li, Liang J. The 10th International Conference on Intelligent Systems for Molecular Biology, August 2002.

Protein Substructure Comparison: An Efficient Combinatorial Approach. Binkowski A, DasGupta B, Liang J. The 10th International Conference on Intelligent Systems for Molecular Biology, August 2002.

Side chain effect to the geometry of packing defects in lattice chain polymer from enumeration and sequential Monte Carlo method. Jinfeng Zhang, Jie Liang, Yu Chen and Rong Chen. The First Cape Cod Workshop of Monte Carlo Methods, September 2002.

Three body residues and atomic contact interactions in proteins: Additivity, cooperativity, and anticooperativity. Xiang Li and Jie Liang. 2003 Biophysical Society Meeting. San Antonio, TX.

Interstrand spatial interactions in beta-barrel membrane proteins. Ronald R. Jackups, Jr. and Jie Liang. 2003 Biophysical Society Meeting. San Antonio, TX.

Proteins are not optimized to eliminate packing voids. Jinfeng Zhang, Yu Chen, Rong Chen, Chao Tang, and Jie Liang. 2003 Biophysical Society Meeting. San Antonio, TX.

Empirical lipid potentials of amino acid residues in membrane protein Larisa Adamian, Vikas Nanda, William DeGrado, and Jie Liang 2003 Biophysical Society Meeting. San Antonio, TX.

Assessing evolutionary conservation of folding nucleus by continuous time Markov model. Jeffrey Tseng and Jie Liang. 2003 Biophysical Society Meeting. San Antonio, TX.

Nonlinear Kernel Potential Function from Threading for Protein Folding and Protein Design. Changyu Hu, Xiang Li and Jie Liang. 2003 Biophysical Society Meeting. San Antonio, TX.

Interstrand interactions in beta barrel membrane proteins. Ronald Jackups, Jr, and Jie Liang. 2004 Biophysical Society Meeting, Baltimore, MD.

Properties and prediction of lipid-exposed surfaces of membrane proteins. Larisa Adamian and Jie Liang. 2004 Biophysical Society Meeting, Baltimore, MD.

Potential function combining contact interaction and local sequence-structure relationship for simplified protein models. Jinfeng Zhang, Rong Chen and Jie Liang. 2004 Biophysical Society Meeting, Baltimore, MD.

pvSOAR: Pattern of pocket and void surfaces of amino acid residues on proteins. T. Andrew Binkowski, Patrick Freeman, and Jie Liang. 2004 Biophysical Society Meeting, Baltimore, MD.

Geometric mapping and prediction of energetic hot spots and structurally conserved residues in protein-protein interactions. Xiang Li, Ozlem Keskin, Buyong Ma, Ruth Nussinov, and Jie Liang 2004 Biophysical Society Meeting, Baltimore, MD.

Interstrand interactions in beta barrel membrane proteins. Ronald Jackups, Jr, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

pvSOAR: Pattern of pocket and void surfaces of amino acid residues on proteins. T. Andrew Binkowski, Patrick Freeman, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Simplified global nonlinear function for fitness landscape of protein design. Changyu Hu, Yang Dai, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Properties and prediction of lipid-exposed surfaces of membrane proteins. Larisa Adamian and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Potential function combining contact interaction and local sequence-structure relationship for simplified protein models. Jinfeng Zhang and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Predicting residues of the ID2 helix-loop-helix protein that may be important for protein-protein interaction and for its role in BMP-induced bone formation. Yan-Yuan Tseng, Xiang Li, Ying Peng, Quan Kang, Rex C. Haydon, Tong-chuan He, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Geometric mapping and prediction of energetic hot spots and structurally conserved residues in protein-protein interactions. Xiang Li, Ozlem Keskin, Buyong Ma, Ruth Nussinov, and Jie Liang 2004 Chicago Proteomics Symposium. Chicago, IL.

Computational design of combinatorial peptide library predicted to be enriched in protein-protein interactions. Xiang Li, Brian Kay, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

Folding rates of lattice model proteins by solving the master equation. Seman Kachalo and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.

pvSOAR: Pattern of pocket and void surfaces of amino acid residues on proteins. T. Andrew Binkowski, Patrick Freeman, and Jie Liang. 2004 Chicago Proteomics Symposium. Chicago, IL.