CURRICULUM VITAE

Yibing Shan, PhD

Current Appointments:

Currently
Sr. Research Scientist: D. E. Shaw Research (10/2002–present)
北京计算科学研究中心讲座教授 （Part time 08/2013–present）
Member of the Board of Reviewing Editors of eLife （3/2015–present）

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Education and Training:

1990	Shanghai University of Sci. and Tech.	B.S.	Mech. Engineering
1998	Drexel University	M.S.	Physics
1999	Drexel University	M.S.	Computer Science
2001	Drexel University	Ph.D.	Biophysics

3/2001-10/2002: Research Scientist: Structural GenomiX, San Diego, CA

Awards

Gordon Bell Prize (Special Achievement) 2009

Best Paper Award, ACM/IEEE Conference on Supercomputing (SC09) 2009

Best Paper Award, ACM/IEEE Conference on Supercomputing (SC06) 2006

中组部第九批创新短期千人计划 （2013）

RESEARCH ACTIVITIES

Publications

Computational biophysics and biology:

Needham, S. R., Roberts, S. K., Arkhipov, A., Mysore, V. P., Tynan, C. J., Zanetti-Domingues, L. C., … Martin-Fernandez, M. L. (2016). EGFR oligomerization organizes kinase-active dimers into competent signalling platforms. ***Nature Communications***, *7*, 13307. http://doi.org/10.1038/ncomms13307 **[Correspondent Author]**

Ingram J.R., Knockenhauer K.E., Markus B.M., Mandelbaum J., Ramek A., Shan Y.B., Shaw D.E., Schwartz T.U., Ploegh H.L., Lourido S. (2015). Allosteric activation of apicomplexan calcium-dependent protein kinases. ***Proceedings of the National Academy of Sciences*** 112, E4975-E4984

Foda Z.H., Shan Y.B., Kim E.T., Shaw D.E., Seeliger M.A., (2015). A dynamically coupled allosteric network underlies binding cooperativity in Src kinase. ***Nature Communication***. **6**, 5939 doi:10.1038/ncomms6939 **[Correspondent Author]**

Shan Y.B., Gnanasambandan K., Ungureanu D., Kim E.T., Hammarén H., Yamashita K., Silvennoinen O., Shaw D.E., Hubbard S.R. (2014). Molecular basis for pseudokinase-dependent autoinhibition of JAK2 tyrosine kinase. ***Nature Structural & Molecular Biology*** 21, 579-584 **[Correspondent Author]**

Littlefield P., Liu L., Mysore V., Shan Y.B., Shaw D.E., Jura N. (2014). Structural analysis of the EGFR/HER3 heterodimer reveals the molecular basis for activating HER3 mutations. ***Science Signaling***, 7, RA114,

Kavran J.M., McCabe J.M., Byrne P.O., Connacher M.K., Wang Z., Ramek A., Sarabipour S., Shan Y.B., Shaw D.E., Hristova K., Cole P.A., Leahy D. (2014). How IGF-1 activates its receptor. ***eLIFE***: e03772

Arkhipov A., Shan Y.B., Kim E.T., Shaw D.E. (2014). Membrane Interaction of Bound Ligands Contributes to the Negative Binding Cooperativity of the EGF Receptor. ***PLoS computational biology***: e1003742 **[Correspondent Author]**

Ferrao R., Zhou H., Shan Y.B., Liu Q., Li Q.,, Shaw D.E., Li X., Wu H. (2014). IRAK4 dimerization and trans-autophosphorylation are induced by myddosome assembly. ***Mol. Cell*** 55, 891-903

Pan A.C., Weinreich T.M., Shan Y.B., Scarpazza D.P., Shaw D.E. (2014). Assessing the accuracy of two enhanced sampling methods using EGFR

kinase transition pathways: the influence of collective variable choice. ***J. Chem. Theory Comput.*****,** *10* (7), 2860–2865

Arkhipov A., Shan Y.B., Eric T. Kim, Ron Dror, Shaw D.E. (2013). Her2 activation mechanism reflects evolutionary preservation of asymmetric ectodomain dimers in the human EGFR family. ***eLIFE*** 2:e00708 **[Correspondent Author]**

Arkhipov A., Shan Y.B., Das R., Endres N.F., Eastwood M.P., Wemmer D.E., Kuriyan J., Shaw D.E. (2013). Architecture and membrane interactions of the EGF receptor. ***Cell*** 152 (3) 557-569 **[Correspondent Author] [*Faculty 1000* Recommendation]**

Endres N.F.**,** Das R.**,** Smith A.W.**,** Arkhipov A.**,** Kovacs E., Huang Y., Pelton J.G.**,** Shan Y.B., E. Shaw D.E.**,** Wemmer D.E., Groves, J.T., Kuriyan J. (2013). Conformational Coupling across the Plasma Membrane in Activation of the EGF Receptor. ***Cell*** 152 (3) 543-556 **[*Faculty 1000* Recommendation]**

Shan Y.B., Arkhipov A., Kim E.T., Pan A.C., Shaw D.E. (2013). Transitions to catalytically inactive conformations in EGFR kinase. ***Proceedings of the National Academy of Sciences*** 110**:**7270-7275 **[Correspondent Author]**

Shan Y.B., Eastwood M.P., Kim E., Zhang X.W., Jumper J., Kuriyan J., Shaw D.E. (2012). Oncogenic Mutations Counteract Intrinsic Disorder in the EGFR Kinase and Promote Receptor Dimerization. ***Cell*** 149 (4) 860-870 **[Correspondent Author] [*Faculty 1000* Recommendation]**

Bandaranayake R.M., Ungureanu D., Shan Y.B., Shaw D.E., Silvennoinen O., Hubbard S.R. (2012). Crystal structures of the JAK2 pseudokinase domain and the pathogenic mutant V617F. ***Nature Structural & Molecular Biology*** 19, 754-759 **[*Faculty 1000* Recommendation]**

Yang M.H., Nickerson S., Kim E.T., Liot C., Laurent G., Spang R., Philips M.P., Shan Y.B., Shaw D.E., Bar-Sagi D., Haigis M.C., Haigis K.M. (2012). Regulation of RAS oncogenicity by acetylation. ***Proceedings of the National Academy of Sciences*** 109 (27) 10843-48

Shan Y.B., Kim E., Eastwood M.P., Seeliger M.A., Shaw D.E. (2011). How does a drug molecule find it target binding site? ***Journal of the American Chemical Society*** 133: 9181-9183 **[*Faculty 1000* Recommendation]**

Dror R.O., Pan A.C., Arlow D.H., Borhani D.W., Maragakis P., Shan Y.B., Xu H., Shaw D.E. (2011). Pathway and mechanism of drug binding to G protein–coupled receptors. ***Proceedings of the National Academy of Sciences*** 108: 13118-13123 **[*Faculty 1000* Recommendation]**

Shaw D.E., Maragakis P., Lindorff-Larsen K., Piana S., Dror R.O., Eastwood M.P., … Shan Y.B., Wriggers W. (2010). Atomic-Level Characterization of the Structural Dynamics of Proteins. ***Science*** 330:341-346 **[*Faculty 1000* Recommendation]**

Jura N., Shan Y.B., Cao X., Shaw D.E., Kuriyan J. (2009). Structural analysis of the catalytically inactive kinase domain of the human EGF receptor 3. ***Proceedings of the National Academy of Sciences*** 106**:**21608-613

Wriggers W., Stafford K.A., Shan Y.B., Piana S., Maragakis P. … Eastwood M.P., Dror R.O., Shaw D. E., Automated Event Detection and Activity Monitoring in Long Molecular Dynamics Simulations. ***Journal of Chemical Theory and Computation*** 5:2595-605 (2009)

Shan Y.B., Seeliger M.A., Eastwood, M.P., Frank F., Xu H.F., Jensen M.Ø, Dror R.O., Kuriyan J., Shaw D.E. (2009). A conserved protonation-dependent switch controls drug binding in the Abl kinase. ***Proceedings of the National Academy of Sciences*** 106**:**139-144 **[*Faculty 1000* Recommendation]**

Seeliger M.A., Ranjitkar P., Kasap C., Shan Y.B., Shaw D.E., Shah N.P., Kuriyan J., Maly D.J. (2009). Equally potent inhibition of c-Src and Abl by compounds that recognize inactive kinase conformations. ***Cancer Research*** 69**:**135-148 **[Cover Story; *Faculty 1000* Recommendation]**

Arkin I.T., Xu H.F., Jensen M.Ø., Arbely E., Bennett E.R., Bowers K.J., Chow E., Dror R.O., Eastwood M.P., Flitman-Tene R., Gregersen B.A., Klepeis J.L., Kolossvary I., Shan Y.B., Shaw D.E. (2007). Mechanism of Na^+/H^+ Antiporting. ***Science*** 317:799-803 **[*Faculty 1000* Recommendation]**

Shan Y.B., Klepeis J.L., Eastwood M.P., Dror R.O., Shaw D.E. (2005). Gaussian split Ewald: A fast Ewald mesh method for molecular simulation. ***Journal of Chemical Physics*** 122:054101 **[Correspondent Author]**

Zhou H.X., Shan Y.B. (2001). Prediction of protein interaction sites from sequence profile and residue neighbor list. ***Proteins: Structure, Function, and Genetics*** 44**:**336-343

Shan Y.B., Wang G.L. Zhou H.X. (2001). Fold recognition and accurate query-template alignment by a combination of PSI-BLAST and threading. ***Proteins: Structure, Function, and Genetics*** 42**:**23-37 (2001)

Shan Y.B., Zhou H.X. (2000). Correspondence of potentials of mean force in proteins and in liquids. ***Journal of Chemical Physics*** 112:4794-4798

Design and development of algorithms, software, and specialized supercomputer:

Shaw D.E., Dror R.O., Salmon J.K., Grossman J.P., Mackenzie K.M., Bank J.A., Young C., Deneroff M.M., Batson B., Bowers K.J., Chow E., Eastwood M.P., Ierardi D.J., Klepeis J.K.,, Kuskin J.S., Larson R.H., Lindorff-Larsen K., Maragakis P., Moraes M.A., Piana S., Shan Y.B., Towles B. (2009). Millisecond-scale molecular dynamics simulations on Anton *Proceedings of the ACM/IEEE Conference on Supercomputing (SC09)*, Portland, Oregon

Shaw D.E., Deneroff M.M., Dror R.O., Kuskin J.S., Larson R.H., Salmon J.K., Young C., Batson B., Bowers K.J., Chao J.C., Eastwood M.P., Gagliardo J., Grossman J. P., Ho C.R., Ierardi D.J., Kolossvary I., Klepeis J.L., Layman T., McLeavey C., Moraes M.A., Mueller R., Priest E.C., Shan Y.B., Spengler J., Theobald M., Towles B., Wang S.C. (2008). Anton, A Special-Purpose Machine for Molecular Dynamics Simulation. *Communications of the ACM* 51:91-97

Larson R.H., Salmon J.K., Dror R.O., Deneroff M.M., Young R.C., Grossman J.P., Shan Y.B., Klepeis J.L., Shaw D.E. (2008). High-throughput pairwise point interactions in Anton, a specialized machine for molecular dynamics simulation. *Proceedings of the 14th International Symposium on High-Performance Computer Architecture*, Salt Lake City, Utah

Shaw D.E., Deneroff M.M., R.O. Dror, Kuskin J.S., Larson R.H., Salmon J.K., Young C., Batson B., Bowers K.J., Chao J.C., Eastwood M.P., Gagliardo J., Grossman J.P., Ho C.R., Ierardi D.J., Kolossvary I., Klepeis J.L., Layman T., McLeavey C., Moraes M.A., Mueller R., Priest E.C., Shan Y.B., Spengler J., Theobald M., Towles B., Wang S.C. (2007). Anton: A special-purpose machine for molecular dynamics simulation. *Proceedings of the 34th Annual International Symposium on Computer Architecture*, San Diego, California

Bowers K.J., Chow E., Xu H.F., Dror R.O., Eastwood M.P., Gregersen B.A., Klepeis J.L., Kolossvary I., Moraes M.A., Sacerdoti F.D., Salmon J.K., Shan Y.B., Shaw D.E. (2006). Scalable algorithms for molecular dynamics simulations on commodity clusters. *Proceedings of the 2006 ACM/IEEE Conference on Supercomputing (SC06)*, Tampa, Florida

Patents

Shan Y.B., Kim E.T., Methods for in silico screening. Application Number: US 14/463,435, August 2014

Shan Y.B., Klepeis J.L., Eastwood M.P., Dror R.O. Shaw D.E. Multiple body simulation. Application Number: US20060142980. June 2005.

(Applied in Anton, the supercomputer specialized for molecule dynamics simulations)

Shaw D.E., Shan Y.B., Klepeis J.L., Eastwood M.P., Dror R.O. Ewald summation method for molecular simulation. Application Number: EP20070000578. May 2005.

Selected Oral Presentations

The Snowmass series of biophysics workshop. Free energy calculations: Three decades of adventure in chemistry and physics. Applying molecular dynamics simualitons for qualitative reasoning in structural biology. Snowmass, CO, July 2015.

Riken. Symposium of Large-scale biological simulations using supercomputers. Structural biology of protein kinases by large-scale Molecular Dynamics Simulations. Kobe, Japan. April 2015

Peking University (北京大学), Introduction to the structural biology of protein kinases. Graduate Lecture, Beijing, China. March 2015

Rutherford Appleton Labatory, Sceince & Technology Facilities Council, Applying molecular dynamics as a tool for structural biology in the study of protein kinases. Feburary 2015, Didcot, UK.

Genentech, Applying large-scale molecular dynamics simulation to structure-based drug discovery, San Francisco, January 2015

Washington University at St. Louis, Dept. of Biochemistry and Molecular Biophysics, Structural Biology of Protein Kinases by Way of Large-scale Molecular Dynamics Simulation, St Louis, MO, September 2014

Peking University (北京大学), Center of quantitative biology. Applying molecular dynamics as a tool for structural biology in the study of protein kinases . Beijing, China. Septemrber 2014

Symposium of Protein Kinases and Phosphorylation, American Chem. Society. Conference. Architectures of the EGF receptor and the molecular effects of oncogenic mutations. San Francisco, CA. August 2014

Telluride Science Research Center, Workshop Proton Transfer in Biology. A proton's role in regulatting conformaitonal change in a protein kianse. Telluride, CO. July 2014

Washington University, Department of Biochemistry and Molecular Biophysics. Structural Biology of Protein Kinases by Way of Large-scale Molecular Dynamics Simulation. St. Louis, MO. September 2014

Karolinska Institute, Department of Biosciences and Nutrition Seminar Series. An investigation using supercomputing: Putative architectures of the EGF receptor and the molecular effects of oncogenic mutations. Stockholm, Sweden, November, 2013

Epidermal Growth Factor Receptor - Future Directions. International Research Conference of the Israel Institute for Advanced Studies. The Hebrew University of Jerusalem, EGFR Architecutre and Oligomorization. Jerusalem, Israel, November, 2013

University of Texas at Austin. Biophysics Seminar Serise. An investigation using supercomputing: Putative architectures of the EGF receptor and the molecular effects of oncogenic mutations. Austin, TX, November, 2013

FASEB Science Research Conference: Protein Kinases and Protein Phosphorylation. Dynamic behavior of EGFR kinase and the effect of cancer mutations. Niagara Falls, NY, July, 2013

Snowmass Biophysics Workshop–Free Energy Calculations: Three decades of Adventure in Chemistry and biophysics. Applying Molecular Dynamics to Computational Structural Biology. Snowmass, CO, July,2013

CHI's 13th Annual Structure-Based Drug Design Conference. How Does a Small-Molecule Inhibitor Bind at the Protein-Protein Interface of Interleukin? Boston, MA, June, 2013

Massachusetts Institute of Technology, Whitehead Institute. Architectures of the EGF receptor and the molecular effects of oncogenic mutations. Boston, MA, May, 2013

EMBO Conference on Allosteric interactions in cell signaling and regulation. Architectures of the EGF receptor and the molecular effects of oncogenic mutations. Paris, France, May, 2013

John Hopkins University. School of Medicine, Department of Biophysics and Biophysical Chemistry. Architectures of the EGF receptor and the molecular effects of oncogenic mutations. Baltimore, MD, December, 2012

7th Kinase in Drug Discovery. Oncogenic Mutations Counteract Intrinsic Disorder in the EGFR Kinase and Promote Receptor Dimerization. Boston, MA, May, 2012

OpenEye's 13th Annual CUP Conference. How Does a Drug Molecule Find its Target Binding Site in Kinase. Santa Fe, NM, March, 2012

Sanibel Symposium. Simulation Study of Protein Dynamics and Function. St. Simons Island, GA, February 2012

CHI's 11th Annual Structure-Based Drug Design Conference. How Molecular Dynamics Simulation May be Applied in Structural Based Design of Kinase Drugs. Boston, MA, June 2011

6th Annual Protein Kinases in Drug Discovery. How Molecular Dynamics Simulations may be Applied to the Structure-Based Design of Kinase Drugs. Boston, MA, May 2011

Peking University (北京大学), Center of Theoretical Biology. Investigating functional conformational change and ligand-binding process of kinases using millisecond molecular dynamics simulations. Beijing, China, May 2011

National Institute of Biological Science. Investigating functional conformational change and ligand-binding process of kinase using millisecond molecular dynamics simulations. Beijing, China, May 2011

Dalian University of Technology, School of Life Science and Biotechnology. Functional conformational change and ligand-binding process of kinase. Dalian, China, May 2011

Stony Brook University, Department of Pharmacological Science. Identify intrinsic disorder at EGFR kinase and a molecular-level oncological mechanism of cancer mutants. Stony Brook, April 2011

Osaka University. IPR Seminar: New Era of Biosimulations with Supercomputers Cosponsored by BioSuperComputing Research Community, Apply molecular dynamics to kinase structure-based drug discovery. Osaka, Japan, March 2011

The 5th Annual Protein Kinases in Drug Discovery Conference. Molecular dynamics simulations suggest a molecular-level oncogenesis mechanism shared by several cancer mutants of the EGF receptor kinase. Boston, MA, May 2010

PepCON Conference. The Unique Dynamics of EGFR Kinase and EGFR Activation. Beijing, China, March 2010

NYC Structural Biology Center. Investigating conformational changes of Abl and Src kinases through molecular dynamics simulations. New York, New York, December, 2009

World Cancer Congress. Investigating Protein Kinases Dynamics Using Molecular Dynamics Simulations. Beijing, China, June 2009.

Protein Kinase Targets (CHI Annual Conference). The DFG Motif -- a Protonation-Dependent Conformational Switch in Protein Kinases. Boston, MA, June 2009.

University of Georgia, Department of Biochemistry & Molecular Biology. Studying conformation dynamics of protein kinases using molecular dynamics simulations. Athens, GA. April 2009.

Kinase Symposium 2008, Institute for Complex Adaptive Matter (*ICAM*). A conserved protonation-dependent switch controlling drug binding in Abl kinase. San Diego, CA. December, 2008.

University of Texas Southwestern Medical Center, Biochemistry seminar series, Department of Biochemistry. Frontiers in molecular dynamics and application of biomedical research, Dallas, TX. October 2008

ACS National Meeting. The DFG motif as a central conformational switch controlling drug binding. Philadelphia, PA. August 2008.

University of California at Berkeley, Department of Chemistry. A 40Å-span conserved allosteric network underlying binding cooperativity of Src kinase. Berkeley, CA. May 2008

Florida State University, Department of Biological Science, Computational Science/Molecular Biophysics Seminars. A conserved protonation-dependent switch controlling drug binding in Abl kinase. Tallahassee, FL. April 2008

University of Washington, Department of Biochemistry. *Supermap*--Inferring ligand-binding properties from comparison of protein active sites by empirical descriptors. Seattle, WA. February 2002

Fourth Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (***CASP4***). Fold recognition and accurate query-template alignment by a combination of PSI-BLAST and threading. Asilomer, CA. December 2000