

QING ZHANG

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(U.S. Permanent Resident)

Education **Ph.D.**, Computational Biomolecular Chemistry, January 2005 (GPA=3.9/4.0)
New York University, Department of Chemistry, New York, NY
B.S., Physics with minor in Computer Science, July 1999 (GPA=3.5/4.0)
Fudan University, Department of Physics, Shanghai, P. R. China

Research Experience **Senior Scientist**, 2008-present
GlaxoSmithKline R&D China, Informatics and Structural Biology, Zhangjiang Hi-tech Park, Shanghai

- Supporting target validation, lead discovery, and lead optimization through structural modeling and molecular docking.
- Supporting antibody engineering including affinity maturation through structural modeling, computational library design, and coordinating structural biology projects.

Research Associate (Postdoc), 2005-2008

The Scripps Research Institute, Department of Molecular Biology, La Jolla, CA

Advisor: Prof. Arthur J. Olson

- Fragment-based lead discovery, protein-ligand docking, algorithm development
(collaborator: Prof. Charles D. Stout, X-ray crystallographer)
Developed a docking-based program to automate interpretation of X-ray density maps from fragment screening.
Applied the program to fragment cocktail screening of HIV protease. Optimized hits theoretically through growth, linkage and substructure search.
- Signaling pathway, GPCR modeling, protein-peptide docking, molecular dynamics
(collaborator: Prof. Wolfram Ruf, biologist, department of immunology)
Built a homology model of protease-activated receptor PAR-2 and modeled its interactions with extracellular proteins to understand its signaling pathway.
- Protein-protein interaction, protein-protein docking, algorithm development
(collaborator: Prof. Michel Sanner, software developer)
Developed a multi-resolution Gaussian surface and studied the effects of surface

smoothing on shape complementarity of protein-protein complexes.

Mentored one graduate student on developing an electrostatic scoring term for protein-protein docking.

Assistant Research Scientist (Postdoc), 2004-2005; **Graduate Student**, 1999-2004

New York University, Department of Chemistry, New York, NY

Advisor: Prof. Tamar Schlick

- Macroscopic modeling, Brownian dynamics and Monte Carlo simulations, algorithm development
Developed a protein bead model for modeling flexible histone tails of nucleosome to enable computer simulations of chromatin fiber.
Mentored one Ph.D., one graduate student, and one undergraduate student in chromatin-related modeling projects.
- Microscopic modeling, molecular dynamics simulation, free energy calculation
(collaborator: Prof. Suse Broyde, biologist, department of biology)
Interpreted the stereochemistry and position-dependent effects of carcinogen benzo[a]pyrene on transcription initiation-required TATA-TBP binding.
- Mesoscopic modeling, implicit-solvent electrostatics, algorithm development
Generalized the Discrete Surface Charge Optimization (DiSCO) algorithm, which simplifies electrostatic representations of macromolecules, by developing an irregular surface building method and the DiSCO software.
Applied the software to supercoiled DNA-protein complexes and chromatin fibers.

Software Development Experience

- **MapDock**: automated fitting of ligands on X-ray density maps to interpret ligand binding positions and conformations on proteins, 2007-2008.
Language: Python
- **ShapeFit**: building multi-resolution Gaussian surfaces and performing protein-protein docking (contributed partially), 2005-2006.
Language: Python
- A program to simulate chromatin with Brownian dynamics and Monte Carlo (contributed partially), 2004-2005.
Language: FORTRAN
- **PCCMD**: computing AMBER-compatible partial charges of carcinogen-modified B-deoxynucleotides in order to simulate cancer adducts, 2002.
Language: Perl
Download: <http://monod.biomath.nyu.edu/~qzhang/Research.htm>
- **DiSCO**: building discrete surface charge models in order to increase efficiency of

macromolecular electrostatics calculations, 2000-2001.

Languages: C, FORTRAN

Download: <http://monod.biomath.nyu.edu/index/software/DiSCO>

- **ViewModel:** visualizing DiSCO models, 2001.

Languages: Matlab, C

Download: <http://monod.biomath.nyu.edu/~qzhang/Softwares.htm>

Leadership Experience

[President, 2002-2003](#)

Chinese Culture Club, New York University, New York, NY

- Tripled annual events to 21 [[Summary](#), [Details](#)]
- Increased membership from 300 to 740.
- Increased annual funding from the university by 25%.
- Started volunteer services for new Chinese students, including airport pickup, temporary housing, and living guides.
- Co-Founded and managed an online [Bulletin Board System](#) that served 700 users.
- Led a 12-member committee by coordinating daily agendas, conducting regular meetings, and encouraging leadership development.
- Promoted club's publicity and influence by establishing good relationships with Graduate School of Arts and Science, outside student and scholar organizations, professional organizations, Chinese consulate, and media.

Teaching Experience

Teaching Assistant, 1999-2003.

Department of Chemistry, New York University, New York, NY

- Instructed Molecular Modeling (graduate course, 20 students) for two semesters; edited and improved homework assignments with students' feedback; participated in exam design.
- Instructed General Chemistry Lab (undergraduate course, 180 students) for four semesters.

Computer Skills

- **Certificate:** Programmer Rank of Computer Software (national), P. R. China, 1997.
- **Programming Languages:** Python, C, C++, Perl, Matlab, FORTRAN, and HTML.
- **Software:** AutoDock, Modeler, AMBER, InsightII, APBS, DelPhi, CCP4, Gaussian.
- **Operating Systems:** UNIX (5 years), Linux (8 years), and Windows (11 years).

Awards

- New York University Dean's Dissertation Fellowship, 2003-2004.
- New York University MacCracken Fellowship, 1999-2003.
- Fudan University Triple-Excellent Student Award, 1996-1997, 1998-1999.
- Fudan University JianGuo Fellowship, 1997-1998.
- Fudan University RenMing Fellowship, 1995-1998.

Publications

1. **Zhang, Q.**, Stout, C.D., & Olson, A.J., "MapDock, a program for automated interpretation of X-ray density maps from fragment screening", *in preparation*, 2009.
2. **Zhang, Q.**, Petersen, H.H., Ruf, W., & Olson, A.J., "Molecular Dynamics Simulations and Functional Characterization of the Interactions of the PAR2 Ectodomain with Factor VIIa", *Proteins: Structure, Function, and Bioinformatics*, *in press*, 2009.
3. **Zhang, Q.**, Sanner, M., & Olson, A.J., "Shape complementarity of protein-protein complexes at multiple resolutions", *Proteins: Structure, Function, and Bioinformatics*, 75: 453-467, 2009.
4. Arya, G. *, **Zhang, Q.** *, & Schlick, T., "Flexible histone tails in a new mesoscopic oligonucleosome model", *Biophysical Journal*, 91: 133-150, 2006 (*contributed equally).
5. **Zhang, Q.** & Schlick, T., "Stereochemistry and position-dependent effects of carcinogens on TATA/TBP binding", *Biophysical Journal*, 90: 1865-1877, 2006.
6. Sun, J., **Zhang, Q.**, & Schlick, T., "Electrostatic mechanism of nucleosomal array folding revealed by computer simulation", *Proceedings of the National Academy of Sciences USA*, 102: 8180-8185, 2005.
7. **Zhang, Q.**, "Mesoscopic, microscopic, and macroscopic modeling of protein/DNA complexes", *Ph.D. Thesis*, New York University, January 2005.
8. **Zhang, Q.**, Broyde, S., & Schlick, T., "Deformations of promoter DNA bound to carcinogens help interpret effects on TATA-element structure and activity", *Philosophical Transactions of The Royal Society of London Series A: Mathematical, Physical & Engineering Sciences (special volume on The Mechanics of DNA)*, 362: 1479-1496, 2004.
9. **Zhang, Q.**, Beard, D. A., & Schlick, T., "Constructing irregular surfaces to enclose macromolecular complexes for mesoscale modeling using the discrete surface charge optimization (DiSCO) algorithm", *Journal of Computational Chemistry*, 24: 2063-2074, 2003.
10. Huang, J., **Zhang, Q.**, & Schlick, T., "Effect of DNA superhelicity and bound proteins on mechanistic aspects of the *Hin*-mediated and *Fis*-enhanced

inversion", *Biophysical Journal*, 85: 804-817, 2003.

11. **Zhang, Q.**, Chen, Y., Wang, Y., & Zhang, G., "Discussion of a small signal in the experiment of NMR by optical pumping", *Physics Experimentation (Chinese)*, 122: 48-49, 2000.

Presentations

1. **Zhang, Q.**, Heaslet, H., Rosenfeld, R., Stout, C. D., & Olson, A. J., "MapDock: a program for automated fitting of fragments on X-ray density maps from fragment screening" (Poster), *Fragment-based Lead Discovery Conference 2008*, San Diego, CA, February 2008.
2. **Zhang, Q.**, Broyde, S., & Schlick, T., "Interpreting carcinogen benzo[a]pyrene's effects on transcription initiation-required TATA/TBP binding using molecular dynamics simulations" (Talk), *The 229th National Meeting, American Chemical Society*, San Diego, CA, March 2005.
3. **Zhang, Q.**, Beard, D. A., & Schlick, T., "Constructing irregular surfaces to enclose macromolecular complexes for mesoscale modeling using the discrete surface charge optimization (DiSCO) algorithm" (Poster), *The 229th National Meeting, American Chemical Society*, San Diego, CA, March 2005.
4. **Zhang, Q.**, "Developing new inhibitors for extracellular signal-regulated kinase ERK2" (Talk), *Original Research Proposal, New York University*, New York, NY, December 2004.
5. **Zhang, Q.** & Schlick, T., "Macroscopic modeling of nucleosomes and chromatin fiber" (Poster), *Undergraduate Research Fair, New York University*, New York, NY, December 2004.
6. **Zhang, Q.**, Beard, D. A., & Schlick, T., "Constructing irregular surfaces to enclose macromolecular complexes for mesoscale modeling using the discrete surface charge optimization (DiSCO) algorithm" (Poster), *Third Metropolitan Area Poster Program for Graduate Students in Chemical Sciences, American Chemical Society*, New York, NY, February 2003.
7. **Zhang, Q.**, "Structural basis of transcription: RNA polymerase II" (Talk), *Biomolecular Chemistry Seminar, New York University*, New York, NY, November 2001.
8. **Zhang, Q.**, "Optimizing ligand charges for maximum binding affinity" (Talk), *Biophysical Chemistry Seminar, New York University*, New York, NY, February 2001.
9. **Zhang, Q.**, Beard, D. A., & Schlick, T., "Computation in discrete surface charge optimization (DiSCO)" (Poster), *Third International Workshop on Methods for Macromolecular Modeling (M³)*, New York, NY, October 2000.
10. **Zhang, Q.**, "NMR by optical pumping" (Talk), *Public Special-Topic Meeting of The 94th Anniversary of Fudan University*, Shanghai, P. R. China, 1999.

11. **Zhang, Q.**, “Optical fiber communication system” (Talk), *Public Special-Topic Meeting of The 93rd Anniversary of Fudan University*, Shanghai, P. R. China, 1998.