Michael K. Gilson, Ph.D., M.D.

Professor
Skaggs School of Pharmacy and Pharmaceutical Sciences
University of California, San Diego
9500 Gilman Drive, MC 0736
La Jolla, CA 92093-0736
Voice: 858.822.0622
mgilson@ucsd.edu

Research Interests

- Computer-aided drug design
- Molecular recognition
- Physical chemistry and statistical mechanics of biomolecules
- Modeling and design of host-guest systems
- Chemical and biological databases and informatics.

Employment

- Professor and Chair in Computer-Aided Drug Design, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA, 1/2010—present.
- Professor, Center for Advanced Research in Biotechnology, University of Maryland Biotechnology Institute, Rockville, MD, 7/2001 – 2009.
- Co-Founder and Member, VeraChem LLC, Germantown, MD, 6/2000 – present.
- Associate Professor, Center for Advanced Research in Biotechnology, University of Maryland Biotechnology Institute, Rockville, MD, 1/2000 – 7/2001.
- NIST Research Chemist, National Institute of Standards and Technology, Gaithersburg, MD, and Adjunct Assistant Professor, Center for Advanced Research in Biotechnology, University of Maryland Biotechnology Institute, 7/1994 – 12/1999.

Education and Training

- Postdoctoral research, Department of Chemistry, University of Houston. Advisor: Dr. J. Andrew McCammon, 8/1991-6/1994.
- Internal Medicine Residency (Clinical Investigator Pathway): Stanford University Hospital 7/89-7/91 and Baylor College of Medicine, 8/1991 – 6/1993 (continuity clinic only).
- Medical School, Columbia University College of Physicians and Surgeons, M.D. 5/1989, 9/1981-6/1983 and 11/1987-5/1989.
- Graduate School, Columbia University, Ph.D. Biochemistry and Molecular Biophysics 1/88. Dissertation title: *Theory of Electrostatic Interactions in Proteins.* Advisor: Dr. Barry Honig. 7/1983-11/1987.
- Undergraduate, Harvard College, A.B. Bioengineering, 6/1981, Magna cum Laude, 9/1977-6/1981.

Medical Certifications

- California Medical License G069466 (current).
- Maryland Medical License D47320, 1995 (allowed to lapse).

- American Board of Internal Medicine certification, 1993 (lapsed).

Research Recognition and Honors

- NetWatch brief regarding BindingDB, Science 311: 1529, 2006
- Article on BindingDB, Drug Discovery News, May, 2006, p. 12.
- Digital Brief on BindingDB, Chemical & Engineering News 84:51, 2006.
- Howard Hughes Medical Institute Physician Research Fellowship, 1991-1994
- The Louis Gibofsky Memorial Prize for research, Columbia University College of Physicians and Surgeons, 1989
- Associated Medical Schools of New York award for biomedical research, 1987.
- Alfred Steiner Award for medical student research, 1987.
- NIH Medical Scientist Training Program, Columbia University, 1981-1989.
- A.B. Magna cum Laude, Harvard College, 1981.
- Tau Beta Pi Engineering Award, Harvard College, 1981.
- Woods Hole Oceanographic Institute Summer Student Fellowship, 1979.
- John Harvard Scholarship, 1979.
- Detur Prize for academic achievement, 1978.
- John Harvard Scholarship, 1978
- National Merit Scholarship, 1977.

Extramural Funding

Current

- National Institutes of Health R01 GM070064, *BindingDB: A Tool for Drug Discovery, Methods Development and Chemical Biology*, 2009-2012, $346K direct costs first year. No-cost extension and carryover allow continuation through 2013. Competitive renewal pending review.
- European Commission Seventh Framework Program, *PSIMEx Proteomics Standards International Molecular Exchange – Systematic Capture of Published Molecular Interaction Data*, 9/10-2/13, $48,000 total costs to our UCSD component of this multi-center data project.
- National Institutes of Health R01 GM061300: *Theory and Modeling of Noncovalent Binding*, 2010-2014 242,000 direct costs first year.
- National Institutes of Health Fast-Track SBIR R44GM088867, *Multilevel parallelization of software for accurate protein-ligand affinities*, (co-Investigator; S. Webb PI, VeraChem LLC) Phase II 12/2010 – 4/2014, $1,338,364 total costs (est).

Completed

- CDC-NIOSH: *Configurational Entropy in Receptor-Ligand Binding: The MIE-NN Method*. 2008-2009, $55K direct costs.
- National Institutes of Health Fast-Track SBIR (co-Investigator; M. Potter PI, VeraChem) *Software for Accurate Ligand-Protein Affinities*. Phase I: 8/1/2005-7/31/2006. Phase II 8/2006-10/2010.
- National Institutes of Health R01, *BindingDB: A Tool for Structure-Based Drug Discovery*, 2004-2009, $270K direct costs first year.
- National Institutes of Health R01, *Ensemble-Based Design of Novel HIV Protease Inhibitors*, $1,124,833 total cost 7/1/02-6/30-07. This R01 was the CARB part of a program project grant involving 5 other laboratories at U. Mass. Medical School, M.I.T., U. North Carolina, and Stanford.

- National Institutes of Health, Phase II STTR to VeraChem LLC: *Inexpensive, Interactive Molecular Modeling Software*, ~$1,922,129 total costs, 5/2002- 4/2005. This grant included a subcontract from VeraChem LLC to my lab at CARB, $399,403 total costs.
- National Institutes of Health R01: *Theory and Modeling of Noncovalent Binding*, $800K direct costs, 9/1/2005- 8/31-2009.
- National Institutes of Health R01: *Theory and Modeling of Noncovalent Binding*, $700K direct costs, 9/1/2000- 8/31-2004.
- National Institutes of Health, Phase I STTR to VeraChem LLC: *Inexpensive, Interactive Molecular Modeling Software*, $100K 7/1/2000- 6/30/2001.
- National Science Foundation: *A Public Molecular Recognition Database*, $600K total costs, 9/1/1998 - 8/31/2001.
- National Institutes of Health R29: *Theory of Noncovalent Protein-Ligand Binding*, $300K direct costs, 5/1/1996-8/31/2000.
- Howard Hughes Medical Institute Physician Research Fellowship: *A Novel Theoretical Approach to the Conformational Energetics of Biological Molecules*, 200K, 8/1991-6/1994.

Service (selected)

Extramural

- Co-Organizer, Telluride Workshop on Free Energy Simulation: From academic research to industrial application, 2011.
- Co-Organizer SAMPL3 workshop on computational prediction of experimental observables, Stanford University, Palo Alto, CA, 7/2011.
- Associate Editor PLoS Computational Biology, 2011 - present
- Member, National Biomedical Computation Resource Advisory Committee, 2010-
- Guest Editor, Folding and Binding issue of Current Opinion in Structural Biology 2010.
- Organizer, Keystone Symposium on Computer-Aided Drug Design, 4/2010.
- Chair, NIH MSFD study section focusing on theoretical and computational biochemistry and biophysics, 2007 – 2009.
- Member, NIH BCMB-Q, BCMB-N, SSS-H and other study sections, June 2001-2009.
- Editorial Advisory Board Journal of Medicinal Chemistry, 2008 - present
- Editorial Advisory Board Journal of Chemical Information and Modeling, 2006- present
- Editorial Advisory Board, Biopolymers, 2001- present.
- Editorial Advisory Board, Journal of Molecular Recognition, 1998 – present.
- Editorial Advisory Board Chemical Biology & Drug Design, 2006 – present
- Technology Advisory Board, Locus/Ansaris Pharmaceuticals, Bluebell, PA, 2007 – 2011.
- Advisory Board, Community Structure-Activity Resource, U. Michigan, 2008 – present.
- External reviewer for multiple faculty promotion and tenure committees.

Intramural

- Director, UCSD Drug Discovery Institute, 2010 – present.
- UCSD Medical Scientist Training Program, 2011— present
- Co-chair, UCSD Research Cyberinfrastructure (RCI) Oversight Committee
- Member, Executive Committee of UCSD Health Sciences Research Council, 2010 – present.
- Member, UCSD Health Sciences Research Council, 2010 – present
- Member, Skaggs School of Pharmacy and Pharmaceutical Sciences Research Council, 2010 – present.
- Co-chair, Skaggs Stewardship Committee, 2011- present.

- Organization of UCSD Drug Discovery Institute formal and informal seminar series, 2011- present.
- One of two members of UCSD-Roche EIN Steering Committee, 2011 – present
- Co-organizer, Skaggs School of Pharmacy and Pharmaceutical Sciences workshop on Orthostery and Allostery, 2011.
- Faculty interviewer on Skaggs School interview day, 2011
- Vice-Chair of UMBI Faculty-Staff Senate, 2008-2009.
- CARB representative to UMBI Senate, 2006 – 2009.
- UMBI faculty lead in development of Joint Biophysics Institute with the NIST Physics Laboratory, 2007-2008.
- Member of team to update the UMBI-NIST memorandum of understanding, 2006-2007.
- Member, Executive Committee of the Graduate Program in Molecular and Cellular Biology, University of Maryland College Park, 2000-2002.
- Organizer and Chair, NIST Workshop for a Molecular Recognition Database, Gaithersburg, MD, August 1997.
- Multiple search, promotion and tenure, and other institutional committees, 1994-present.

Panels and Committees

- Panelist, NIST/UMBI conference *Accelerating Innovation in 21st Century Biosciences*, 10/2008.
- Invited participant, Center for Scientific Review (CSR) *Biomolecular Open House Meeting on NIH Peer Review*, NIH, Bethesda, MD, 12/2007.
- Co-organizer, NIST *Workshop on Structure-Based Drug Discovery*, NIST, Gaithersburg, MD, April 19-21, 2006.
- Panelist, NIGMS *Workshop of Structure-Based Drug Design*, NIH, Bethesda, MD, August 26, 2005. (An invitational workshop to organize a strategic attack on the theoretical and computational challenges in computer-aided drug design.)
- NIH *Major Histocompatibility Complex (MHC)-Peptide Database Planning Meeting*, June 5, 2001.
- *Biomarkers Knowledge System*, National Institutes of Health, Bethesda, MD, Sept. 8, 2000.
- *Metabolic Engineering*, National Science Foundation, Arlington, VA, May 31, 2000.
- Panelist and presenter at NIH Symposium on Bioengineering: Building the Future of Biology and Medicine, for panel *Beyond Informatics: The Future of Computation*, February 28, 1998.

Professional Societies
American Chemical Society, American Society for the Advancement of Science, Biophysical Society, International QSAR and Modeling Society, Molecular Graphics and Modeling Society

Teaching and Training (selected)
Classroom

- Co-chair of seminar class "From Molecular Mechanisms to New Medications: The Science of Drug Discovery", winter quarter 2012.
- UCSD pharmacology small group conference facilitator (Integrated Science Curriculum)
  2010-2011: Drug Absorption and Metabolism; Pharmacokinetics
  2011-2012: Cardiovascular; Drug Excretion
- Research presentation in Concepts in Pharmacy Practice, SSPPS, 2011.
- Cheminformatics lectures in UCSD Bioinformatics I/Pharm201, 2010-2011.

- Lectures, problem set, and exam on *Energetics* in team-taught Proteins course in the Molecular and Cellular Biology graduate program at U. Maryland, College Park, February-March 2002 - 2007.
- Lectures and practical session on *Continuum Electrostatic Modeling*, EMBO Practical Course on Biomolecular Simulation, Heidelberg, Germany, July 11, 2000.

Other Didactic Lectures

- Three-lecture series: Bioinformatics Institute, Agency for Science, Technology and Research (A*Star), Singapore, 12/2004.
    - *Biomolecular Electrostatics*
    - *Computer-Aided Drug-Discovery*
    - *Molecular Recognition in Host-Guest Systems: Energy, Entropy and Implications for Drug-Design*
- *Computer-Aided Drug-Design*, U. Md. Baltimore County Myerhoff Scholarship Program, 6/2000, CARB.
- *Computers in Biotechnology*, for Industrial College of the Armed Forces, CARB, February 2000.

Graduate Faculties

- UCSD Bioinformatics and Systems Biology, 2011 – present
- UCSD Biomedical Sciences, 2011 - present
- Molecular and Cellular Biology, U. Maryland, College Park, MD, 1999-2010
- Chemical Physics, U. Maryland, College Park, MD, 2006-2010.

Advice for Young Scientists on the WWW
http://pharmacy.ucsd.edu/labs/gilson/advice1a.html

- Giving a Seminar
- Designing Slides
- Writing a Grant Proposal
- Writing a Paper

Lab Trainees and Research Staff

- Neil Sapra, UCSD undergraduate researcher (Chem/Biochem), 2011-present
- Anne Morgan, Harvard Undergraduate Amgen Scholar, Summer, 2011.
- Camilo Velez Vega, Postdoc, UCSD, 2010 – present
- Jamie Chang, UCSD Regents Scholar undergraduate trainee, Chem/Biochem, 2010-present
- Kunal Shah, Undergraduate Research Trainee, UCSD Bioengineering, 2010
- Hari Muddana, Postdoc, UCSD, 2010 – present
- George Nicola, Postdoc, UCSD, 2010 – 2011, Project Scientist, UCSD in my lab.
- Amanda Li, Graduate Student, UCSD Bioengineering and Interface program, 2010 - present
- Crystal Nguyen, Postdoc, UCSD, 2010- present
- Andrew Fenley, Postdoc, UCSD, 2010- present
- Aditya Ravi, undergraduate intern (Indian Institute of Technology), 2007. Currently Account Manger, Richcore Lifesciences Pvt. Ltd., India.
- Sarvin Moghaddam, Research Associate, 4/2007—2010
- Sandeep Somani, Graduate Student, Chemical Physics, 1/2006—2011
- Anna Hung, high school intern and subsequently undergraduate intern, 1/2006—2007.

- Benjamin Killian, Research Associate, 8/2005 – 2009.
- Prasanna Vasudevan, Stanford undergraduate summer intern, 2005, 2006
- Joslyn Kravitz, Research Associate, 4/2005 – 2007. Currently in Cryptanalysis Development Program, National Security Agency.
- Tiqing Liu, Research Associate, 2005- 2006. Currently Lead Developer of BindingDB at UCSD.
- Xin (Sherry) Wen, Faculty Research Assistant, 2005—2007.
- Miguel Fernandes, Research Associate, 2003-2004. Currently *Professor Auxiliar* and Vice-Rector, University of Madeira, Portugal.
- Himan Mookherjee, Graduate Student, Molecular and Cellular Biology Program, University of Maryland, 2002 – 2005.
- Sripriya Chellappan, Graduate Student , Molecular and Cellular Biology Program, University of Maryland, 2002 – 2006. Currently Staff Pharmacist, WA.
- Wei Chen, Research Associate, 2002 – 2006. Currently Senior Scientist, VeraChem LLC.
- Yuhmei Lin, Research Associate, 2001 – 2005, and Lead Curator of BindingDB, 2005-2010.
- Robert Jorissen, Research Associate, 2002-2006. Cur*rently Clinical Bioinformatics Officer, Ludwig Institute for Cancer Research, Melbourne, Australia.*
- Mihail Mihailescu, Research Associate, 2001– 2003.
- Michael J. Potter, Research Associate, 1998 – 2002. Currently CEO, VeraChem LLC.
- Shashi Ratnayake, Undergraduate, 6/2000 – 8/2000.
- Henry Luo, Wootton High School Intern, Summer 2003.
- Visvaldas Kairys, Research Associate,1999 – 2001 and 2002- 2005. Currently staff scientist, Biotechnology Institute, Vilnius University, Vilnius, Lithuania.
- Chia-En Chang, Graduate Student, Department of Chemistry, Physical Chemistry Division, University of Maryland, College Park, MD, 10/1999 - 2003. Research Associate 2003-2004. Winner of CARB Outstanding Graduate Student award, 2002. Currently Assistant Professor, Department of Chemistry, U. C. Riverside.
- Xi Chen, Graduate Student, Molecular and Cellular Biology Program, University of Maryland, 7/1999 – 2001. Currently Patent Attorney, Jones Day LLP.
- Ming Liu, Ph.D., Database programmer, 1/1999 – 10/2000. Currently Director of Cheminformatics, Caliper Life Sciences, Baltimore, MD.
- Kristy Mardis, Ph.D., National Research Council Research Associate, 8/1998 – 7/2000. Currently Associate Professor of Chemistry, Chicago State University.
- Jian Zhong, Graduate Student, M.S. 7/1998 (co-advised with Prof.Todd Cooke, U. Maryland). Currently Chief SOA Architect, Futrend Technology, Inc.
- Ray Luo, Graduate Student, Ph.D. 1998 (co-advised with Prof. John Moult, U. Maryland). Research Associate, 1998 – 11/1999. Currently Associate Professor of Molecular Biology and Biochemistry, U. C. Irvine.
- Laurent David, Ph.D., Research Associate, 11/1996 – 9/1999. Currently Principal Scientist, Computer-Aided Drug Design, H. Lundbeck A/S, Copenhagen, Denmark.
- Martha S. Head, Ph.D., National Research Council Research Associate, 11/1995 – 11/1997. Currently Director of Computational Chemistry USA, Glaxo SmithKline Pharmaceuticals, Collegeville, PA
- James A. Given, Ph.D., Research Associate 10/1994 – 10/1997. Currently Physicist, Naval Research Laboratory, Washington DC.

<u>Visiting Scientists and Students</u>

- Dov Barak, Israel Institute for Biological Research, 2008-2009.
- Ky-Youb Nam, Computational Chemist, Drug Design Division, Bioinformatics and Molecular Design Research Center, South Korea, 10/2005 – 2007.
- Steven Brose, Graduate Student, Food Science, U. Minnesota, 1/2007.
- Sune Pedersen, Graduate Student, Dept. of Medicinal Chemistry, U. of Copenhagen, 2006
- Konesh Siva, Graduate Student (Adviser: Dr. Jay Rasaiah, U. Maine), Summers 1998-9.
- Jian Shen, Ph.D. Visiting Scientist from Hoechst, Marion Roussel, 1998.

Graduate Committees

- Member of doctoral committees of Brian Fuglestad, Levi Pierce, Kevin Rynearson, Nick Kosa, Jessica Fullagar, Chun-Chieh Lin, Ryan Hayes, William Sinko, Chung-mao Pan, UCSD, 2010-2011.
- Extramural committee member of dissertation committee of Jaydeep Bardhan, Electrical Engineering and Computer Science, MIT, Cambridge, MA., 2006.
- Graduate committees of multiple students in the Molecular and Cellular Biology program, U. Maryland College Park, 1994-2009.

Public Databases and Software

- *BindingDB*, a major protein-ligand affinity database to support drug discovery, on the WWW since 2001, currently provides 790,000 binding measurements for 350,000 drug-like molecules and 5,600 protein targets, and receives ~35,000 nontrivial hits/month. *http://www.bindingdb.org*.

- Open Source Software (*http://pharmacy.ucsd.edu/labs/gilson/software1a.html*)
    - HYBRID code for solving the multiple titration problem.
    - ACCENT code for extracting configurational entropy from molecular simulation data.
    - M2 software for computing host-guest binding affinities.

Intellectual Property and Commercialization

Entrepreneurship

Founded *VeraChem LLC* (6/2000-present), Germantown, MD, a company developing software and services for molecular analysis in academia and the biotechnology and pharmaceutical industries.

Patents (granted and pending)

- *HIV-1 Protease Inhibitors* (USPTO Patent Application 11/960,120; also submitted through PCT and in Australia, China, Europe and Japan.)
- *Tailored User-Interfaces for Molecular Modeling* (USPTO Patent 6,970,791).
- *Computational Method for Drug Discovery and Receptor Design* (USPTO Patent Application 60/787,522 by VeraChem LLC; patent was allowed November 2011, patent number is pending.)

Commercial Software (co-developed)

- *Vcharge* for calculating partial atomic charges of drug-like compounds
- *Vconf* for conformational analysis of drug-like compounds
- *Vfilter* for accurately removing duplicate conformations of drug-like compounds
- *Vrms* for computing the structural similarities among various conformations of a drug-like compound, while accounting for chemical symmetry

- *Vm2* for computing protein-ligand affinities with the mining minima method.
- *DelPhi*, software for computing electrostatic interactions in macromolecules with the Poisson-Boltzmann theory, licensed to and distributed by Biosym Technologies, San Diego, CA..
- *UHBD*, software for Poisson-Boltzmann molecular electrostatics, distributed by Accelrys, San Diego, CA.

Invited Talks (recent and selected)

- *Entropy tales*, Barry Honig 70th birthday symposium, Columbia U., New York, NY, 12/2011.
- *BindingDB, a publicly accessible database for drug design*, 5th US Government Chemical Database and Open Chemistry Meeting, Frederick, MD, 8/2011.
- *Overview of host-guest binding free energy predictions*, SAMPL3 workshop, Stanford University, Palo Alto, CA, 7/2011.
- *Free energy and entropy in molecular recognition*, Purdue University, Lafayette, IN, 4/2011.
- *Computational modeling of host-guest and protein-ligand binding*, CUP XII meeting, Santa Fe, NM, 3/2011.
- *Computer-aided drug design*, UCSD-Taiwan Symposium on Frontiers in Biosciences, U.C. San Diego, La Jolla, CA, 9/2010.
- *Computation of free energy, entropy and mechanical stress in molecular recognition.* Center for Theoretical Biological Physics, U.C. San Diego, La Jolla, CA, 4/2010.
- *Free energy, entropy and stress in molecular recognition*, U. Miami, Coral Gables, FL, 10/2010
- *Free energy, entropy and stress in molecular recognition*, Carnegie Mellon U., Pittsburgh, PA, 10/2010
- *Free energy, entropy and stress in molecular recognition*, Computational Chemistry Gordon Research Conference, Les Diablerets, Switzerland, 9/2010
- *Validation, entropy and stress in molecular recognition*, ACS National Meeting, Boston, MA, 8/2010
- *Free energy, entropy and stress in molecular recognition*, Ecole Polytechnique, Palaiseau, France, 7/2010.
- *Configurational Entropy and Molecular Stress*, Keystone meeting on Computer-Aided Drug Design, Whistler, Canada, 4/2010.
- *Computer-Aided Drug Design: Molecular Recognition and the Role of Entropy*, University of Texas, Austin, TX, 5/2009.
- *Computer-Aided Drug Design: Molecular Recognition and the Role of Entropy*, Northwestern University, Evanston, IL, 4/2009.
- *Computer-Aided Drug Design: Molecular Recognition and the Role of Entropy*, U.C. San Diego, La Jolla, CA, 3/2009.
- *BindingDB*, European Bioinformatics Institute, Hinxton, United Kingdom, 11/2008.
- *Entropy and Affinity in Molecular Recognition*, Maryland Biophysics Program, University of Maryland College Park, 10/2008.
- *Entropy and Affinity in Molecular Recognition*, Division of Molecular Biophysics and Physiology, Rush University Medical Center, 10/2008.
- *Modeling Host-Guest Interactions. Accuracy, Insight and Design*, Procter & Gamble, Cincinnati, OH, 7/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, Center for Computational Biology and Bioinformatics, Indiana U. School of Medicine, 5/2008.

- *Computer-Aided Drug Design. Affinity, Entropy and High-Dimensionality Distributions*. Dept. of Mathematics, Yale University, New Haven, CT, 5/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, Center for Bioinformatics, U. Kansas, Lawrence, KA, 4/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, Pfizer, La Jolla, CA, 2/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, U. California San Diego, La Jolla, CA, 2/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, U. California, Riverside, 2/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, U. California, Irvine, 2/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, California Institute for Quantitative Biosciences, U. California, San Francisco, 2/2008. (Graduate student invitational seminar.)
- *BindingDB*, Druggable Genome Workshop of the European Bioinformatics Institute, Hinxton, United Kingdom, 2/2008.
- *Entropy, Affinity and the Design of Targeted Molecules*, Mini-Symposium of the Webster Center for Molecular Research in Infectious Diseases, University of Otago, Dunedin, New Zealand, 12/2007.
- *Entropy, Affinity and the Design of Targeted Molecules*, MM2007 meeting, Melbourne, Australia, 11/2007.
- *Entropy and Affinity in Molecular Recognition*, Laboratory of Chemical Physics, NIH, Bethesda, MD, 11/2007.
- *Molecular Flexibility and Configurational Entropy*, Gordon Research Conference on Computer Aided Drug Design, Tilton, NH, 8/2007.
- *Targeting Ensembles of Drug Resistant HIV-1 Protease: Computational Design*, 21st Annual Meeting of Groups Studying the Structures of AIDS-Related Systems and their Application to Targeted Drug Design, NIH, Bethesda, MD, 6/2007.
- *Molecular Recognition: Informatics, Entropy, and Design*, Department of Computational Biology, University of Pittsburgh, 5/2007
- *Computational Tools for Computer-Aided Drug-Discovery*, ACS National Meeting, Chicago, IL, 3/2007.
- *Changes in Configurational Entropy on Binding*, ACS National Meeting, Chicago, IL, 3/2007.
- *Changes in Configurational Entropy on Binding*, 47th Sanibel Symposium, St. Simons Island, Georgia, 2/2007.
- *Molecular Recognition: Informatics, Entropy, and Design*, L. H. Baker Center for Bioinformatics & Biological Statistics, Iowa State U., Ames, IA, 1/2007.
- *Molecular Recognition: Informatics, Entropy, and Design*, Biotechnology Division, National Institute of Standards and Technology, Gaithersburg, MD, 1/2007.
- *Entropy and Free Energy in Molecular Recognition*, Locus Pharmaceuticals, Blue Bell, PA, 7/2006.
- *Molecular Recognition: Modeling, Informatics and Design*, Department of Medicinal Chemistry, U. Michigan, Ann Arbor, MI, 4/2006.
- *Challenges in the Calculation of Binding Affinities*, Workshop on Validating Modeling and Experimental Methods to Enable Drug Discovery, NIST, Gaithersburg, MD, 4/2006.
- *Theory and Modeling of Molecular Recognition*, Keystone Symposium on Structure Based Drug Discovery, Whistler, British Columbia, 4/2006.
- *In Silico Design of Mutation-Resistant HIV-1 Protease Inhibitors*, AIDS Structural Biology Meeting, National Institutes of Health, Bethesda, MD, 6/2005.

- *Understanding Protein-Ligand Binding*, Incyte Pharmaceuticals, Wilmington, DE, 6/2005.
- *Understanding Protein-Ligand Binding*, Glaxo SmithKline, King of Prussia, PA, 4/2005.
- *Modeling Molecular Recognition*, Department of Pharmaceutical Chemistry, University of Maryland, Baltimore, MD, 4/2005.
- *Calculation of Binding Affinities*, Pfizer, La Jolla, CA, 3/2005.

Publications (out of more than 200)

Velez-Vega, Camilo; Gilson, Michael K. Overcoming dissipation in the calculation of standard binding free energies by ligand extraction. Journal of Computational Chemistry (2013), 34, 2360.

Muddana, Hari S.; Sapra, Neil V.; Fenley, Andrew T.; Gilson, Michael K. The electrostatic response of water to neutral polar solutes: Implications for continuum solvent modeling. Journal of Chemical Physics (2013), 138, 224504/1.

Muddana, Hari S.; Fenley, Andrew T.; Gilson, Michael K. Atomic Stress Propagation Reveals Allosteric Pathways in Proteins. Biophysical Journal (2013), 104, 212.

Gilson, Michael K.; Irikura, Karl K. Entropy-enthalpy transduction caused by conformational shifts can obscure the forces driving protein-ligand binding. Proceedings of the National Academy of Sciences of the United States of America (2012), 109, 20006.

Orchard, Sandra; Binz, Pierre-Alain; Borchers, Christoph; Gilson, Michael K.; Jones, Andrew R.; Nicola, George; Vizcaino, Juan Antonio; Deutsch, Eric W.; Hermjakob, Henning. Ten Years of Standardizing Proteomic Data: A Report on the HUPO-PSI Spring WorkshopApril 12-14th, 2012, San Diego, USA. Proteomics (2012), 12, 2767.

Nguyen, Crystal N.; Kurtzman Young, Tom; Gilson, Michael K. Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit[7]uril.Journal of Chemical Physics (2012), 137, 044101/1.

Nicola, George; Liu, Tiqing; Gilson, Michael K. Public Domain Databases for Medicinal Chemistry. Journal of Medicinal Chemistry (2012), 55, 6987.

Muddana, Hari S.; Daniel Varnado, C.; Bielawski, Christopher W.; Urbach, Adam R.; Isaacs, Lyle; Geballe, Matthew T.; Gilson, Michael K. Blind prediction of host-guest binding affinities: a new SAMPL3 challenge. Journal of Computer-Aided Molecular Design (2012), 26(5), 475.

Muddana, Hari S.; Gilson, Michael K. Prediction of SAMPL3 host-guest binding affinities: evaluating the accuracy of generalized force-fields. Journal of Computer-Aided Molecular Design (2012), 26, 517.

Forrey, Christopher; Douglas, Jack F.; Gilson, Michael K. The fundamental role of flexibility on the strength of molecular binding. Soft Matter (2012), 8, 6385.

Muddana, Hari S.; Gilson, Michael K. Calculation of Host-Guest Binding Affinities Using a Quantum-Mechanical Energy Model. Journal of Chemical Theory and Computation (2012), 8, 2023.