University of California
Brian Shoichet, Curriculum Vitae

Name: **Brian Shoichet, Ph.D.**
Position Professor, Step VII, Dept. of Pharmaceutical Chemistry

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Citizenship Canada, Born: 06/27/63 US Permanent Resident

Education

1981-1985 Massachusetts Institute of Technology
B.Sc. in Chemistry; B.Sc. in History

1986-1991 University of California, San Francisco
Ph.D. in Pharmaceutical Chemistry, Advisor Professor Irwin Kuntz

Postdoctoral Research

1992 University of California, San Francisco, Professor Irwin Kuntz
1993-1996 Institute of Molecular Biology, Eugene, Oregon, Professor Brian Matthews

Principal Positions Held:

1996-2002 Assistant Professor of Molecular Pharmacology & Biological Chemistry
2002-2003 Associate Professor (tenured), Mol. Pharmacology & Biological Chemistry
Northwestern University

2003-2005 Associate Professor of Pharmaceutical Chemistry
2005-2013 Professor (Step VII) of Pharmaceutical Chemistry
2011-2012 Vice Chair, Dept. of Pharmaceutical Chemistry, UCSF
2012-2013 Director, California Institute for Quantitative Biology of UCSF (QB3)
2013-2014 Adjunct Professor of Pharmaceutical Chemistry (WOS)
University of California, San Francisco

2013-2014 Professor, Faculty of Pharmacy
2014-Present Adjunct Professor, Faculty of Pharmacy (Courtesy Appt)
University of Toronto

2014-Present Professor of Pharmaceutical Chemistry, Step VII
University of California, San Francisco

Keywords: Molecular recognition, drug discovery, structure-based inhibitor discovery, computational chemical biology, systems pharmacology, molecular docking, promiscuous inhibition, G-Protein Coupled Receptors.

Honors & Awards

1993-1996 Damon Runyon-Walter Winchell Cancer Research Fellow
1997-1999 PhRMA Foundation Career Development Award
1998-2003 National Science Foundation CAREER Award
2001 Dean's Award for Teaching Excellence (Northwestern University)
2004 Astra Lectureship, University of Ottawa
2006-2007 Novartis Chemistry Lecturer (Cambridge, Basel, Vienna, Horsham, Tsukuba, Emeryville)
2008 Swiss Universities 3e Cycle en Chimie (Lausanne, Bern, Friborg, Geneva)
2009 Abbott Lectureship, Yale University
2011 Society for Biomolecular Sciences Accomplishment Award

2011 Topliss Lectureship, University of Michigan
2013 Distinguished Scientist Seminar, University of Pittsburgh
2014 Distinguished Scientist Lectureship, University of Ohio School of Pharmacy
2014 Center for Mol. Innovation in Drug Discovery, Northwestern University, Annual Keynote
2015 Cambridge Healthtech 10*th Annual Drug Discovery Chemistry*, Plenary Keynote.
2015 Arthur Broom Lecture, University of Utah School of Pharmacy.
2015 International Chair of Therapeutic Innovation, CNRS, Paris.
2016 Molecular Graphics & Modeling Society, Erlangen, Germany. Plenary Keynote.
2016 Partnership for Excellence in Structural Biology Annual Symposium, UConn. Keynote

Professional & Scientific Activity

Editorial Service

1993-present Ad hoc reviewer for *J. Mol. Biol.*, *Proc. Natl. Acad. Sci.*, *Chemistry & Biology*, *Protein Sci.*, *Proteins*, *J. Am. Chem. Soc., J. Med. Chem., J. Chem. Inf. Modeling, Protein Eng., J.Biol. Chem., Nature Biotech.*, *Nature Struct. Biol.*, *Nature Chemical Biology, Nature Chemistry, Nature,* and *Science.*
1999-2000 Editorial Board of *Journal Of Computer-Aided Molecular Design*
1999-2003 Editorial advisory board of *PharmSci*, Amer. Assoc. of Pharmaceutical Sciences
2001-2003 Faculty of 1000 (Ligand-Macromolecular Interactions & Inhibitor Design)
2001-2003 Editor-in-Chief of *Journal Of Computer-Aided Molecular Design*
2005-present International Advisory Board *Molecular Biosciences, Royal Soc. Chem.*
2005-2010 Editorial Advisory Board *Journal of Medicinal Chemistry*
2016-2017 Editorial Advisory Board, *Journal of Chemical Information & Modeling*
2016-2017 Editorial Advisory Board, *ACS Chemical Biology*

Conferences & Sessions Organized

1998 *Midwest Enzyme Chemistry Conference*, Northwestern University.
2001 *Computational Structural Biology (Session on Docking)*, FSU, Tallahasse FL
2001 *Docking & Testing Session*, ACS National Meeting, Chicago IL
2002 *Structure-based drug design*, Cambridge HealthTech Institute, Boston MA
2003 *Structure-based drug design*, Cambridge HealthTech Institute, Boston MA
2005 *NIH Meeting on Docking & Scoring*, Washington DC (co-chair)
2006 *Structure-Based Drug Design Keystone Conference*, Whistler BC (co-chair)
2007 *Gordon Research Conference in Computer-Aided Drug Discovery*, New Hampshire (vice chair)
2009 *ASBMB National Meeting*, New Orleans LA (co-chair), April 18-22
2009 *Gordon Research Conference in Computer-Aided Drug Discovery*, New Hampshire (chair). July 19-24
2009 *Nature Chem. Biol. Drug Discovery Meeting*, Boston MA (co-chair)
2010 *Gordon Research Conference in Biomolecular Interactions and Methods,* session chair in drug discovery (January, Galveston Tx)
2015-2016 Scientific Advisory Board of the 21st EuroQSAR Symposium

Scientific Advisory Boards, Consulting & Companies Founded

1998-2003 SAB Synergix, Cue Biotech, Ctr for Molecular Design (Univ of Toronto)
2001-2003 Consultant for Pharmacia Corp.; Procter & Gamble Pharmaceuticals
2001-2004 Consultant for Protein Pathways, Cytoclonal Pharma, Syrrx, Epix Medical
2002-2008 Consultant for Structural GenomiX
2004-present SAB, NIH RoadMap Chemical Libraries and Screening Initiative
2005 Consultant for Scios; Consultant for Novartis
2005-2006 Consultant for Boehringer Ingelheim
2006-2007 Consultant for CropSolutions Inc.

2006-2008	SAB for Buck Institute.
2007-2009	Consultant for Eli Lilly & Co.
2008-2009	SAB for Chicago Tri-Institutional Center for Chemical Methods and Library Development
2009-2012	Scientific Advisory Group for Corning Life Sciences
2012	Consultant for Alios Pharma
2009-2011	Consultant for Anacor Pharma
2008-2012	Consultant for Vitae Pharmaceuticals
2009-present	Consultant for ZoBio Pharma
2014	Consultant for Astra Zeneca
2015	External Advisory Board, University of Pittsburgh Drug Discovery Institute
2009	Founder, SeaChange Pharmaceuticals

Research Program

An overarching goal of our lab is bringing chemical reagents to biology, using a combination of computational simulation and experiment. Using a protein-centric approach, we search for new ligands that complement protein structures. This typically involves molecular docking and the development of model experimental systems to experimentally test new algorithms that we develop. A new direction adopts a ligand-centric approach that seeks new targets for known drugs. Whereas this lacks the physical foundation of the structure-based docking, it returns to an older, pharmacological view of biological relationships, bringing to it a quantitative model. A biological focus for both areas is the discovery of reagents to modulate GPCRs.

As part of our research, we have introduced free computational & experimental community resources:

1. The **ZINC** database of commercially available, dockable molecules: http://zinc.docking.org.
2. The **DUD** benchmark of 40 targets, 3000 ligands & 97000 decoys: http://dud.docking.org.
3. **DOCK Blaster**, a web-based community tool for docking: http://blaster.docking.org.
4. **SEA**, a chemoinformatics method for predicting targets for ligands: http://sea.docking.org.
5. Procedures and reagents for counterscreening for **promiscuous aggregation**.
6. Libraries of ligands and decoys for **model binding sites** for testing docking: http://shoichetlab.compbio.ucsf.edu/take-away.php.

Six recent papers representative of the interests of my laboratory:

MJ Keiser, V Setola, JJ Irwin et al., BK Shoichet* & BL Roth*. Predicting new molecular targets for known drugs. ***Nature*, 462**, 175-81 (2009).

J Carlsson et al. BL Roth* & BK Shoichet*. Comparing structure-based ligand discovery from a homology model and the crystal structure of the dopamine D_3 receptor**.** ***Nature Chem. Biol.* 7,** 769-78 (2011).

C Laggner, et al., BL Roth,* RT Peterson* & BK Shoichet*. Chemical Informatics and Target Identification in a Zebrafish Phenotypic Screen. ***Nature Chem. Biol.,* 8,** 144-146 (2012).

E Lounkine†, et al., BK Shoichet* & L Urban* Large Scale Prediction and Testing of Drug Activity on Side-Effect Targets. ***Nature* 486,** 361-7. (2012).

H Lin, MF Sassano, BL Roth* and BK Shoichet*. A Pharmacological Organization of G Protein-coupled Receptors. ***Nature Methods* 10**, 140-6 (2013).

London N, et al., Shoichet BK* & Taunton J*. Covalent docking of large libraries for the discovery of chemical probes. ***Nature Chem Biol*. 10**, 1066-72 (2014).

Peer Reviewed Publications (166 total, Total Cites 22,316, Google Scholar H-index 79)

1. Sowdhamini, R.; Srinivasan, N.; Shoichet, BK.; Santi, DV.; Ramakrishnan, C & Balaram, P*;

Stereochemical Modeling of Disulfide Bridges. ***Protein Engineer***., **3**(2): 95-103 (1989).

2. BK Shoichet & ID Kuntz.* Protein docking and complementarity. ***J. Mol. Biol***. **221**, 327-346 (1991)
3. Shoichet, BK, Bodian, DL & Kuntz, ID*; Molecular Docking Using Shape Descriptors. ***J. Comput Chem***. **13**, 380-397 (1992).
4. Meng, E.C.; Shoichet, B.K. & Kuntz, I.D.*; Automated Docking with Grid-Based Energy Evaluation. ***Journal of Computational Chemistry*** **13**, 504-524. (1992).
5. Shoichet, B.K**.;** Stroud, R.M.; Santi, D.V.; Kuntz, I.D* & Perry, K.M.; Structure Based Inhibitor Discovery in Thymidylate Synthase. *Science* **259**, 1445-1449 (1993).
6. BK Shoichet & ID Kuntz.* Matching chemistry and shape in molecular docking, *Protein. Engineer*, **6**, 723-32 (1993).
7. U. Schellenberger, VS Francis, P. Balaram, BK Shoichet**,** & DV Santi.* Designed deletion of an entire domain of *Lactobacillus* thymidylate synthase gives a catalytically active enzyme. *Biochemistry*, **33**, 5623-5629 (1994).
8. Shoichet, B.**K;** Baase, W.A.; Kuroki, R. & Matthews, B.W.*; A Relationship Between Protein Stability and Protein Function. ***Proc. Nat. Acad. Sci***. **92**, 452-456 (1995).
9. Zhang, X.J.; Baase, W.A.; Shoichet, B.K**.;** Wilson, K. & Matthews, B.W.*; Incremental Enhancement of Protein Stability by the Combination of Point Mutations in T4 Lysozyme. ***Protein Engineer*** **8**, 1017-1022 (1995).
10. Strynadka, NCJ, Eisenstein, M, Katchalski-Katzir, E, Shoichet, BK**,** et al. & James, MNG*; Molecular Docking Programs Successfully Predict the Binding of a Beta-Lactamase Inhibitory Protein to the TEM-1 Beta-Lactamase. ***Nat. Struct. Biol***. **3**, 233-239 (1996).
11. Gassner, N.C., Baase, W.A., Linstrom, J.D., Shoichet, B.K. & Matthews, B.W*. Isolation and Characterization of Multiple Methionine Mutants of T4 Lysozyme with a Simplified Core. *Techniques in Protein Chemistry*, **VII** 851-863 (1997).
12. Lorber, D.A. & **Shoichet, B.K.*,** Flexible Ligand Docking Using Conformational Ensembles. *Protein Science*, **7**, 938-950 (1998).
13. Morosini, M.-I.; Negri, M.-C.; Shoichet, B.; M.-R. Baquero; Baquero, F. and Blazquez, J.*; An extended-spectrum AmpC-type β-lactamase obtained by in vitro antibiotic selection. *FEMS Microbiology Letters,* **165**, 85-90 (1998).
14. Weston, GS.; Blasquez, J; Baquero, F, and **Shoichet, BK*;** Structure-based Enhancement of Boronic Acid Based Inhibitors of AmpC β-lactamase. *J. Med. Chem*., **41**: 4577-4586 (1998).
15. KC Usher, LC Blaszczak, GS Weston, **BK Shoichet*** & SJ Remington*; The three dimensional structure of AmpC β-lactamase from *Escherichia coli* bound to a transition state analog: possible implications for the oxyanion hypothesis and for inhibitor design. *Biochemistry* **37**,16082-16092 (1998).
16. **Shoichet, B.K.*;** Leach, A. & Kuntz, I.D*; Ligand Solvation Effects in Molecular Docking. *Proteins 34*, 4-16, (1999).
17. BM Beadle, WA Baase, D. Wilson, NR Gilkes & **BK Shoichet*** Comparing the Thermodynamic Stabilities of a Thermophilic and a Mesophilic Enzyme. *Biochemistry* **38**, 2570-2576 (1999).
18. Stout, T.J.; Tondi, D., Rinaldi, M., Barlocco, D., Pecorari, P., Santi, D.V., Kuntz, I.D., Stroud*, R.M., **Shoichet, B.K.*** & Costi, M.P.* Structure-Based Design of Inhibitors Specific for Bacterial Thymidylate Synthase. *Biochemistry* **38**, 1607-1617 (1999).
19. Tondi, D., Slomczynska, U., Watterson, D.M., Costi, M.P., Ghelli, S & **Shoichet, B.K.*,** Structure-Based Discovery and In-Parallel Elaboration of Novel inhibitors of Thymidylate Synthase. *Chemistry & Biology* **6**, 319-331 (1999).

20. Beadle, B.M., McGovern, S.L., Patera, A. & **Shoichet, B.K.*** Functional Analyses of AmpC β-Lactamase Through Differential Stability. *Protein Science* **8**, 1816-1824 (1999).
21. Powers, R.A., Blazquez, J., Weston G.S., Morosini, M.I., Baquero F. & **Shoichet, B.K.*** The Complexed Structure and Anti-Microbial Activity of a Non- β-Lactam Inhibitor of AmpC β-lactamase. *Protein Science*, **8**, 2330-2337 (1999).
22. A Patera, LC Blaszczak & **BK Shoichet.*** Crystal structures of substrate and inhibitor complexes with AmpC β-lactamase: possible implications for substrate-assisted catalysis. *J. Am. Chem. Soc.* **122**, 10504-10512 (2000).
23. E Caselli, RA Powers, LC Blaszczak, CY Wu, F Prati & **BK Shoichet.*** Energetic, structural & anti-microbial analyses of β-lactam side chain recognition by β-lactamases. *Chem.& Biol* **8**, 10-17 (2001).
24. Su, A.I, Lorber, D.M., Weston, G.S., Baase, W.A, Matthews, B.W. & **Shoichet, B.K.*** Docking Molecules by Families to Increase the Diversity of Hits in Database Screens: Computational Strategy and Experimental Evaluation. *Proteins* **42**:279–293 (2001).
25. Beadle, BM, Nicholas, RA & **Shoichet, BK*** Interaction energies between β-lactam antibiotics and a penicillin binding protein by reversible thermal denaturation. *Protein Science* **10**, 1254-9 (2001)
26. D Tondi, RA Powers, MC Negri, E Caselli, J Blazquez, MP Costi* & **BK Shoichet*** Structure-based design & in-parallel synthesis of inhibitors of AmpC β-lactamase. *Chem. & Biol.* **8**, 593-611 (2001).
27. Trehan, I, Beadle, B.M., & **Shoichet, B.K.*** Inhibition of AmpC β-Lactamase Through a Destabilizing Interaction in the Active Site. *Biochemistry* **40**, 7992-7999 (2001).
28. Powers, R.A., Caselli, E., Focia, P., Prati, F. & **Shoichet, B.K.*** The Structures of Ceftazidime and its Transition-State Analog Bound to AmpC β-lactamase: Implications for Inhibition, Mechanism and Resistance. *Biochemistry* **40**, 9207-14 (2001).
29. Wang, X., Minasov, G. & **Shoichet, B.K**.* Interaction Energies in Covalent Complexes: TEM-1 β-lactamase and β-lactams. *Proteins* **47**, 86-96 (2002).
30. Lorber, D.M., Udo, M.K., & **Shoichet, B.K.*** Protein-Protein Docking with Multiple Ligand Residue Conformations and Multiple Residue Identities. *Protein Science,* **11**, 1393-1408 (2002).
31. BM Beadle, I Trehan, P Focia & **BK Shoichet**.* Structural milestones in the pathway of an amide hydrolase: substrate, acyl, and product complexes of cephalothin with AmpC β-lactamase. *Structure* **10**, 413-424 (2002).
32. SL McGovern, E Caselli, N Grigorieff & **BK Shoichet*** A common mechanism underlying promiscuous inhibitors from virtual and high-throughput screening. *J. Med. Chem*. **45**, 1712-1722 (2002).
33. G. Minasov, X. Wang. & **B.K. Shoichet*** An ultra-high resolution structure of TEM-1 β-lactamase suggests a role for Glu166 as the general base in acylation. *J. Am. Chem. Soc.* **124**, 5333-40 (2002)
34. Doman, T.N*, McGovern, S.L., Witherbee, B.J., Kasten, T.P., Kurumbail, R., Stallings, W.C., Connolly, D.T., & **Shoichet, B.K.*** Molecular Docking and High-Throughput Screening for Novel Inhibitors of Protein Tyrosine Phosphatase-1B. *J. Med. Chem.* **45**, 2213-2221 (2002).
35. Wang, X., Minasov, G., & **Shoichet, B.K.*** Evolution of an Antibiotic Resistance Enzyme Constrained by Stability and Activity Trade-Offs. *J. Mol. Biol.* **320,** 85-95 (2002).
36. Powers, R.A. & **Shoichet, B.K.*** Mapping the Active Site of AmpC β-Lactamase for Hot-Spots. *J. Med. Chem*. **35**, 3222-3234 (2002).
37. Powers, R.A., Morandi, F. & **Shoichet, B.K.*** Structure-based discovery of a novel, non-covalent inhibitor of AmpC β-lactamase. *Structure* **10**, 1013-1023 (2002)
38. B.M. Beadle and **B.K. Shoichet**.* Structural bases of stability-function trade-offs in enzymes. *J. Mol. Biol*. **321,** 285-296 (2002)

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