

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and other significant contributors in the order listed on Form Page 2.
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NAME John J. Irwin	POSITION TITLE Adjunct Assistant Professor
eRA COMMONS USER NAME irwinj	

EDUCATION/TRAINING (Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)

INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
University of Toronto, Toronto, Canada	B.Sc.	1981-1985	Chemistry/Biochem.
University of Toronto, Toronto, Canada	M.Sc..	1986-1987	Inorganic Chemistry
Swiss Federal Institute of Technology, Zurich	Ph.D.	1988-1991	Organic Chemistry
MRC Lab. of Molecular Biology, Cambridge, UK	Postdoc	1994-1998	Structural Biology

A. Positions and Honors:

02/91-06/93 Product Line Manager
BioStructure SA
Strasbourg, France

03/94-09/98 Postdoctoral Research Fellow
MRC Laboratory of Molecular Biology
Cambridge, UK

01/98-09/98 Head of IT
Global Phasing Ltd
Cambridge, UK

10/98-06/00 Staff Scientist
European Bioinformatics Institute
Hinxton, Cambridge, UK

07/00-04/03 Senior Research Associate
Northwestern University Medical School
Chicago IL

05/03-09/04 - Senior Research Associate
Dept. of Pharmaceutical Chemistry
University of California, San Francisco CA

10/04-present – Adjunct Assistant Professor
Dept. of Pharmaceutical Chemistry
University of California, San Francisco CA

Honors

None.

Federal Government Public Advisory Committee Service

ad hoc reviewer for NSF (2005, 2007)
ad hoc reviewer for NIH/CSR (2006)

Editorial Service

BMC Chemistry Central, Editorial Advisory Board and Section Editor, Cheminformatics and Molecular Modeling

B. Peer-reviewed publications (in chronological order)

1. Bogdan P.L., **Irwin J.J.**, and Bosnich B, "Asymmetric Synthesis. Molecular Graphics and Enantioselection in Asymmetric Catalytic Hydrogenation," *Organometallics*, 1989, 8, 1450-1453.
2. Burrow T., **Irwin J.J.** and Farrar D.H., "Computer Modelling of Steric Effects in Organometallic Chemistry," *Inorg. Chim Acta*, 1991, 181, 65-72.
3. **Irwin J.J.**, Ha T-K., Dunitz J.D., "Stereolectronic Aspects of the Anomeric Effect in Fluoromethylamine," *Helv. Chim. Acta*, 1990, 73, 1805-1817.
4. Weston S.A., Camble R., Colls J., Rosenbrock G., Taylor I., Egerton M., Tucker A.D., Tunnicliffe A., Mistry A., Mancina F., de La Fortelle E., **Irwin J.J.**, Bricogne G., Pauptit R.A., Crystal structure of the anti-fungal target N-myristoyl transferase. *Nat Struct Biol.* 1998 Mar;5(3):213-21.
5. Roversi P., **Irwin J.J.** and Bricogne G. "Accurate charge density studies as an extension of Bayesian crystal structure determination". *Acta Crystallographica A*54, Part 6, Number 1 , 971-996, (1998).
6. Atreya C.E., Johnson E.F., **Irwin J.J.**, Dow A., Massimine K.M., Coppens I., Stempliuk V., Beverley S., Joiner K.A., Shoichet B.K., Anderson K.S., A molecular docking strategy identifies eosin B as a non-active Site Inhibitor of protozoal bifunctional thymidylate synthase-dihydrofolate reductase, *J Biol Chem.* (2003) 278(16):14092-100
7. **Irwin J.J.** and Shoichet B.K., ZINC – A free database of commercially available compounds for virtual screening, *J. Chem. Inf. Model.*, 2005, 45, 177-82.
8. **Irwin JJ**, Raushel FM and Shoichet BK, Virtual Screening against metalloenzymes for inhibitors and substrates, *Biochemistry*, **44**(37), 12316-28 (2005)
9. Brenk R, **Irwin JJ**[‡] and Shoichet BK, Here be dragons: docking and screening in an uncharted region of chemical space. *J Biomol Screen*, **10**(7), 667-74 (2005). [‡] Denotes co-first author
10. Huang N, Kalyanaraman C, **Irwin JJ** and Jacobson MP, Physics-based scoring of protein-ligand complexes: enrichment of known inhibitors in large-scale virtual screening, *J. Chem. Inf. Model*, **46**(1), 243-53 (2006)
11. Huang N, Shoichet BK*, **Irwin JJ***, Benchmarking sets for Molecular Docking, *J. Med. Chem.*, **49**(23), 6789-6801 (2006).
12. Hermann JC, Gahanem, E, Li Y, Raushel FM, **Irwin JJ*** and Shoichet BK, Predicting Substrates by Docking High-Energy Intermediates to Enzyme Structures, *J.Am.Chem.Soc.* 128(49), 15882-91 (2006).
13. Keiser MJ, Roth BL, Armbruster BN, Ernsberger P, **Irwin JJ*** and Shoichet BK*, Relating protein pharmacology by ligand chemistry, *Nature Biotechnology* (2007) 25(2):197-206

C. Research Support. List selected ongoing or completed (during the last three years) research projects (federal and non-federal support). Begin with the projects that are most relevant to the research proposed in this application. Briefly indicate the overall goals of the projects and responsibilities of principal investigator identified above.

Program Director/Principal Investigator (Last, First, Middle): Irwin, John J. et al.

R01 GM71896 (Shoichet, PI)

8/1/04 – 07/31/08

NIH/NIGMS

A Web-Based Automatic Molecular Docking System

The major goals are to develop community-accessible databases of dockable molecules and an automated computational platform to allow the community to undertake docking calculations. This is the current application.