Izhar Wallach

10 King's College Rd., Room 3302
Toronto, Ontario, Canada, M5S-3G4
+1-416-558-7680

izharw@cs.toronto.edu
http://www.cs.toronto.edu/~izharw

Education

Ph.D. Candidate — University of Toronto
Computer Science — *Jan 2009 – Jun 2012 (expected)*

My research focuses on improving posing and ranking of molecular docking. Particularly, developing algorithms for:
- Small-molecule binding-mode prediction
- Reduce bias in structure-based high-throughput screening
- Pharmacophore inference and protein binding-site similarity

Additionally, I have worked on analyzing large quantities of chemical genomics and genetic interaction data. Particularly, developing algorithms for:
- Genome-wide drug combination effect
- Combining structure- and pathway-based network models for the analysis of adverse drug reactions
- Synthetic Genetic Array analysis (yeast/E.coli)

Advisor: Ryan Lilien

M. Sc. — University of Toronto
Computer Science — *Sep 2007 – Jan 2009*

Algorithms for predicting binding site similarities and inference of protein–small-molecule interaction patterns

Advisor: Ryan Lilien

B. Sc. (4-year track) — Israel Institute of Technology (Technion)
Computer Science — *Sep 1999 – Apr 2004*

Developed a framework for computational inference of RNA secondary structure similarity

Advisor: Zohar Yakhini

Work Experience

Researcher — University of Toronto
Michael Brudno's group — *May 2011 – Present*

Develop novel structure-based algorithms to identify the effect of genomic variation in heterogeneous population on the efficacy of drugs. Worked on integrating genomic and proteome information into a framework that identifies drugs that may show altered efficacy profiles due to variation in the binding sites of their primary targets. My research involved:
- Identifying of potential genomic variants in drug targets and building alternative structural models
- Developing novel docking algorithms and decoy-based normalization techniques
- Performing molecular-dynamics simulations and calculating binding-free energies of potentially affected drugs

Algorithm Developer — Ashkelon, Israel
Keddem Bioscience — *May 2004 – Jul 2007*

Algorithm developer at *Keddem Bioscience*, a small-molecule drug discovery company. Experience with cheminformatics technologies for drug design such as pharmacophore analysis, molecular similarity and scaffold hopping, computational QSAR, molecular clustering and docking optimization.
Specifically, I led or was involved in the following projects:
- Design of a chemical universal screening library for protein binding site probing
- Algorithms for protein active site mapping using protein-ligand interaction analysis
- Algorithm for active site reconstruction that utilizes information obtained from high-throughput screening
- Pharmacophore-based small-molecule docking algorithm

Unix System Administrator — Haifa, Israel
Intel Development Center — *Aug 2001 – May 2004*

- UNIX/Linux system administration
- Development of internal data management tools
- Development of monitoring and administration scripts

Skills

Cheminformatics/Bioinformatics Solid theoretical and practical knowledge of 2D and 3D methods of cheminformatics, statistical modeling, pharmacophore inference, ligand- and structure-based virtual screening, small-molecule–protein interaction, docking and scoring, genetic and protein interactions, pathway analysis, molecular network models, and large-scale -OMICS data.

Molecular modeling tools Accelrys, Schrodinger, OpenEye, Tripos

Docking packages Extensive experience with Glide, eHiTS, Dock, AutoDock, Amber

Cheminformatics/Bioinformatics software development OpenBabel Chemical ToolBox, Bioperl, PerlMol, Pymol scripting interface

Programming languages High proficiency in C/C++, R, Perl, UNIX Shells, LaTeX
Others: Matlab, Python/NumPy/SciPy, Java, SQL.

Databases Extensive work with: PDB, MMDB, PubChem, ChEMBL, KEGG, DrugBank

Operating systems High proficiency in development under UNIX and Linux

Publications

- **Izhar Wallach**, Navdeep Jaitly, Kong Nguyen, Matthieu Schapira, Ryan Lilien, *Normalizing Molecular Docking Rankings using Virtually Generated Decoys*, Journal of Chemical Information and Modeling, 51(8):1817-1830, (2011)
- **Izhar Wallach** and Ryan Lilien, *Virtual Decoy Sets for Molecular Docking Benchmarks*, Journal of Chemical Information and Modeling, 51(2):196-202, (2011)
- **Izhar Wallach**, *Pharmacophore Inference and its Application to Computational Drug Discovery*, Drug Development Research, 72(1):17-25, (2010)
- **Izhar Wallach**, Navdeep Jaitly, Ryan Lilien, *A Structure-Based Approach for Mapping Adverse Drug Reactions to the Perturbation of Underlying Biological Pathways*, PLoS ONE 5(8), (2010)
- **Izhar Wallach** and Ryan Lilien, *Predicting Multiple Ligand Binding Modes Using Self-Consistent Pharmacophore Hypotheses*, Journal of Chemical Information and Modeling, 49(9):2116-2128, (2009)
- **Izhar Wallach** and Ryan Lilien, *Prediction of Sub-Cavity Binding Preferences Using an Adaptive Physicochemical Structure Representation*, Bioinformatics, 25:i296-304 (2009)
  Article also appeared as:
  Izhar Wallach and Ryan Lilien, *Prediction of Sub-Cavity Binding Preferences Using an Adaptive Physiochemical Structure Representation*, Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB), Stockholm, Sweden, (2009)
- **Izhar Wallach** and Ryan Lilien, *The protein – small-molecule database, a non-redundant structural resource for the analysis of protein-ligand binding*, Bioinformatics, 25(5):615-20 (2009)

Oral Presentations

- *Virtual Decoy Sets for Molecular Docking Benchmarks and Ranking*, The American Chemical Society (ACS) meeting, Anaheim, California (2011)
- *Predicting Multiple Ligand Binding Modes Using Self-Consistent Pharmacophore Hypotheses*, The American Chemical Society (ACS) meeting, San-Francisco, California (2010)
- *Prediction of Sub-Cavity Binding Preferences Using an Adaptive Physiochemical Structure Representation*, International Conference on Intelligent Systems for Molecular Biology (ISMB), Stockholm, Sweden, (2009).

Awards & Fellowships

- C.C. Gotleib (Kelly) Graduate Fellowship in the Department of Computer Science (2008).
- Helen Sawyer Hogg Graduate Admission Award (2007).

Teaching Experience

Teaching Assistant University of Toronto
Sep 2007 – Present

- CSC209 – Software Tools and Systems Programming
- CSC192 – Computer Programming, Algorithms, Data Structures and Languages
- CSC148 – Introduction to Computer Science
- CSC108 – Introduction to Computer Programming