Robin M. Betz

SF Bay Area, USA
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EDUCATION

Ph.D. Biophysics
Stanford University
Ron Dror Lab
Thesis: Methods development for computational simulation of protein-ligand binding

B.S. Bioinformatics
University of California San Diego
Minor in Mathematics

SOFTWARE EXPERIENCE

I have over 20 years of experience programming and enjoy both using and developing tools and libraries for scientific computing.

Tools I know well:

- **Languages:** C, C++, CUDA, Python, Perl, Bash, FORTRAN, MPI, OpenMP, Java, mySQL, LaTeX
- **Libraries:** PyTorch, numpy, pandas, rdkit, ray, netCDF, Qt, AWS, Spa
- **Software:** AMBER, Schrodinger Maestro, Gaussian, OpenMM, GAMESS, ADF, many others.

Open source contributions:

- **Dabble** - Constructs molecular dynamics systems with a lipid bilayer.
  dabble.robinbetz.com
- **redun** - Contributed to workflow engine development while at insitro.
  github.com/insitro/redun
- **vmd-python** - Python backend for popular molecular dynamics analysis package. 200k+ downloads.
  vmd.robinbetz.com

WORK EXPERIENCE

Staff Engineer 2019 - 2025
Insitro
South San Francisco, CA

As a member of the Scientific Pipelines team, I collaborated with both lab scientists and machine learning researchers to solve scientific and technical problems and build supporting infrastructure. I worked with many data modalities including microscopy, small molecule, and genomic datasets.

Selected accomplishments:

- Wrote enumeration engine for DNA-encoded libraries that scales to libraries of 10B+ molecules.
- Wrote optimized CUDA kernels for experimental transformer architectures.
- Reduced runtime of image tiling pipeline from weeks to hours.
- Grew software infrastructure from 20 to 200+ employees.
- Conducted over 100 technical interviews.
- Mentored a summer intern who was later hired as a full-time employee.

Consultant 2018 - 2019
Various companies

I consulted for several startups on molecular dynamics simulation setup and analysis, including parametrizing small molecules for simulation. I also built infrastructure and tooling on AWS as needed.

PUBLICATIONS

Kapse, S.; **Betz, R.M.**; Sivanandan, S.; "Fast Vision Mamba: Pooling Spatial Dimensions for Accelerated Processing", *arXiv preprint*, February 2025

Betz, R.M.; Dror, R.O.; "How effectively can adaptive sampling methods capture spontaneous ligand binding?", *Journal of Chemical Theory and Computation*, January 2019

Venkatakrishnan, A.J.; Ma, A.; Fonseca, R.; Latorraca, N.R.; Kelly, B.; **Betz, R.M.**; Asawa, C.; Kobilka, B.K.; Dror, R.O.; "Diverse GPCRs exhibit conserved water networks for stabilization and activation" *Proceedings of the National Academy of Sciences*, February 2019

Schmidt, H.R.; **Betz, R.M.**; Dror, R.O.; Kruse, A.C.; "Structural basis for sigma-1 receptor ligand recognition", *Nature Structural and Molecular Biology*, October 2018

Bjij, I.; Khan, S.; **Betz, R.M.**; Cherqaoui, D.; Soliman, M.E.S.; "Exploring the structural mechanism of covalently bound E3 ubiquitin ligase: Catalytic or allosteric inhibition?", *The Protein Journal*, September 2018

Khan, S.; Bjij, I.; **Betz, R.M.**; Soliman, M.E.S.; "Reversible versus irreversible inhibition modes of ERK2: a comparative analysis for ERK2 protein kinase in cancer therapy", *Future Medicinal Chemistry*, April 2018

McCorvy, J.D.; Butler, K.V.; Kelly, B.; Rechsteiner, K.; Karipak, J.; **Betz, R.M.**; Kormos, B.L.; Shoichet, B.K.; Dror, R.O.; Jin, J.; Roth, B.L.; "Structure-inspired design of β-arrestin-biased ligands for aminergic GPCRs", *Nature Chemical Biology*, December 2017

Wang, S.; Wacker, D.; Levit, A.; Che, T.; **Betz, R.M.**; McCorvy, J.D.; Venkatakrishnan, A.J.; Xi-Ping, H.; Dror, R.O.; Shoichet, B.K.; Roth, B.L.; "D4 dopamine receptor high-resolution structures enable the discovery of selective agonists", *Science*, October 2017

Komolov, K.E.; Du, Y.; Nguyen, N.M.; **Betz, R.M.**; Rodrigues, J.P.G.L.M.; Leib, R.D.; Patra, D.; Skiniotis, G.; Adams, C.M.; Dror, R.O.; Chung, K.Y.; Kobilka, B.K.; Benovic, J.L.; "Structural and Functional Analysis of a β2-Adrenergic Receptor Complex with GRK5", *Cell*, April 2017

Wacker, D.; Wang, S.; McCorvy, J.D.; **Betz, R.M.**; Venkatakrishnan, A.J.; Levit, A.; Lansu, K.; Schools, Z.L.; Che, T.; Nichols, D.E.; Shoichet, B.K.; Dror, R.O.; Roth, B.L.; "Crystal structure of an LSD-bound human serotonin receptor", *Cell*, January 2017

Betz, R.M.; Walker, Ross C; "Paramfit: Automated optimization of force field parameters for molecular dynamics simulations," *Journal of Computational Chemistry*, January 2015

D.A. Case, V. Babin, J.T. Berryman, **R.M. Betz**, Q. Cai, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, H. Gohlke, A.W. Goetz, S. Gusarov, N. Homeyer, P.

Janowski, J. Kaus, I. KolossvÁry, A. Kovalenko, T.S. Lee, S. LeGrand, T. Luchko, R. Luo, B. Madej, K.M. Merz, F. Paesani, D.R. Roe, A. Roitberg, C. Sagui, R. Salomon-Ferrer, G. Seabra, C.L. Simmerling, W. Smith, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu and P.A. Kollman, "AMBER 14", University of California, San Francisco, 2014

Betz, R. M.; Walker, Ross C; "From Punch Cards to Continuous Integration: Streamlining Development of a Multi-million Line Computational Chemistry Code," *Computing in Science and Engineering*, February 2014

Betz, R.M.; DeBardeleben, N.A.; Walker, R.C.; "An investigation of the effects of hard and soft errors on graphics processing unit-accelerated molecular dynamics simulations," *Concurrency and Computation: Practice and Experience*, March 2014

Dickson, C.J.; Madej, B.D.; Skjevik, A.A.; **Betz, R.M.**; Teigen, K.; Gould, I.R.; Walker, R.C.; "Lipid14: The Amber Lipid Force Field", *Journal of Chemical Theory and Computation* January 2014

Dickson, C.J; Rosso,L.; **Betz, R.M.;** Walker,R.C.; Gould, I.R. "GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid," *Soft Matter*, 2012

CONFERENCES

Walker, R.C.; **Betz, R.M.**; "An investigation of the effects of error correcting code on GPU-accelerated molecular dynamics simulations," *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery (XSEDE 13)*, July 22, 2013

Lenhardt, C.; Blanton, B.; Idaszdak, R.; **Betz, R.**; Promoting Scientific Software Best Practices, *Earth Science Information Partners Summer Meeting*, July 2013

Betz, R.M; Walker, R.C.; "Implementing Continuous Integration Software in an Established Computational Chemistry Software Package.", International Workshop on Software Engineering for Computational Science and Engineering, May 18, 2013

Betz, R.M.; Walker, R.C.; "Paramfit: A program for automated forcefield parameter generation using a genetic algorithm," *American Chemical Society National Meeting*, 2012

AWARDS

NVIDIA Fellow	2017
NSF Graduate Research Fellow	2014
DOE Computational Science Graduate Fellow	2014 *(declined)*
Best Paper & Best Presentation, IEEE SE-CSE	2013
Amgen Scholar	2013
Calit2 Undergraduate Fellow	2011

TEACHING

Physical Biology of the Cell Teaching Assistant	2016
Biophysics NSF GRF Application Workshops	2015
Cell Biology Teaching Assistant	2014
Bioinformatics Algorithms Coursera Community Teaching Assistant	2013
Metabolic Biochemistry Teaching Assistant	2013
Molecular Biology Teaching Assistant	2012