Donald S. Berkholz

Structural biologist

612-991-1321—berkhold@science.oregonstate.edu

Education

Ph.D. Biochemistry & Biophysics, **Oregon State University** 2009
Dissertation: Modeling protein structure at atomic resolution

B.S. Biochemistry & Molecular Biology, **University of Richmond** 2004
B.A. Chemistry, **University of Richmond** 2004

Research experience

Postdoctoral fellow, Mayo Clinic 2009–
● Advisers: **James R. Thompson** and **Grazia Isaya**. Crystallography and drug design.

Doctoral student, Oregon State University 2005–2009
● Adviser: **P. Andrew Karplus**. Structural bioinformatics, structural enzymology, and homology modeling. Crystallographically dissected reaction mechanism at atomic resolution in the flavoenzyme glutathione reductase. Characterized & leveraged broader backbone-dependent geometry trends in proteins at atomic resolution.

Undergraduate researcher, University of Richmond / Gustavus 2000–2004
● Adviser: **J. Ellis Bell**. Enzymology. Changed understanding of the mechanism of 3-phosphoglycerate dehydrogenase by characterizing native and active-site mutants.
● Adviser: **Jonathan M. Smith**. Molecular modeling. To understand biologically relevant conformations of the neurotransmitter serotonin, used experimental & computational approaches including laser spectroscopy and quantum mechanics.
● Adviser: **Brian O'Brien**. Organic synthesis. To test electronic effects of substituent groups, synthesized cesium 4-*tert*-butylphthaloylphosphanide.

NSF-REU researcher, University of Minnesota 2001
● Adviser: **Len Banaszak**. Optimized procedure for mitochondrial isolation for AFM analysis. Created and characterized a PGDH mutant.

Honors & awards

● Best Student Talk award—West Coast Protein Crystallography Workshop 2009
● Finn Wold award—Protein Society 2008
● College of Science Student Travel Award—OSU 2008
● 1st prize undergraduate poster—ASBMB 2002
● John C. Johnson Award (poster)—Tri-Beta biological honor society national meeting 2002
● Partners in Scholarship ($12,500/year)—Gustavus 2000
● Presidential Scholarship ($10,000/year)—Gustavus 2000
● National Merit Scholar 2000
● Eagle Scout 1999

Peer-reviewed publications

(**5 published, 1 in press**, 4 in preparation)

Berkholz DS, Bell JK, Grant GA, Banaszak LJ, Bell JE. “Probing the active site of 3-phosphoglycerate dehydrogenase: the role of acid-base catalysis and the local charge environment of the transition state in V-type regulation by serine.” *J Biol Chem* (in preparation).

Berkholz DS, Driggers CM, Karplus PA. “On the (non)planarity of the peptide bond.” (in preparation).

Tronrud DE, Berkholz DS, Karplus PA. “Using a conformationally dependent stereochemical library in refinement.” *Acta Cryst D* (in preparation).

Berkholz DS, Bretscher A, Karplus PA. “An expert-created model of the tumor-suppressor merlin suggests novel critical regions.” *J Mol Biol* (in preparation).

Berkholz DS, Krenesky PB, Davidson JR, Karplus PA. “Protein Geometry Database: a flexible engine to explore backbone conformations and their relationships to covalent geometry.” *Nucleic Acids Res* (in press).

Berkholz DS, Shapovalov MV, Dunbrack Jr RL, Karplus PA. “Conformation dependence of backbone geometry in proteins.” *Structure* **17**: 1316 (2009). **One of only 2 papers in the issue highlighted with a news story.**

Hollingsworth SA, Berkholz DS, Karplus PA. “On the occurrence of linear groups in proteins.” *Protein Science* **18**: 1321 (2009). **Highlighted in front of issue; only 3-4 papers each issue are honored in this fashion.**

Berkholz DS, Faber HR, Savvides SN, Karplus PA. “Catalytic cycle of human glutathione reductase near 1 Å resolution.” *J Mol Biol* **382**: 371 (2008).

Karplus PA, Shapovalov MV, Dunbrack Jr RL, Berkholz DS. “A forward-looking suggestion for resolving the stereochemical restraints debate: ideal geometry functions.” *Acta Cryst D***64**: 335 (2008).

Benison G, Berkholz DS, Barbar E. “Protein assignments without peak lists using higher-order spectra.” *J Magn Reson* **190**: 8 (2007).

Past funding

Research Project Grant (R01), National Institutes of Health (2008). “Empirical conformation-dependent covalent geometry variation in proteins.” I did the preliminary work critical to this grant's successful resubmission. Key personnel. Principal investigator: P. Andrew Karplus. $650,000.

Presidential Student-Faculty Collaboration Grant, Gustavus (2002). “Investigation of stilbene derivatives exhibiting intramolecular charge-transfer: computational and resonance Raman spectroscopic approaches.” Faculty collaborator: Jonathan M. Smith. $7,500.

Teaching experience

Teaching assistant

- Biochemistry 490/590 (biochemistry majors): office hours, grading — 2007
- Biochemistry 450/550 (science majors): recitation, office hours, grading — 2004–2007
- Cellular & molecular biology: recitation, office hours, grading — 2004
- Biochemistry laboratory: in-lab questions, lab prep, grading — 2004

Tutor

- Science-writing specialist, Writing Center — 2001–2002
- General chemistry — 2001

Additional relevant experience

Software engineering
Open-source development; Gentoo Linux development; Python; Bash shell scripting.

Journalism
Writing; story-telling; graphic design; page layout; copy editing.

System administration
Lab manager of the computers (4 Linux and 1 Mac) for the Karplus lab.

High-performance clustering
Cluster architect & administrator for a small prototype cluster.

Leadership
I led ~250 developers as an elected member of Gentoo's 7-member council. I've learned how to work with people from diverse backgrounds. I've also learned how to lead people without having any explicit power, only that provided by my reputation.

Mentoring
I've mentored 1 junior graduate student (Camden Driggers) and 1 undergraduate student (Scott Hollingsworth). I've also mentored 4 new Gentoo developers and continue to mentor 2 of them. I also mentored a Google Summer of Code student who worked full-time on a programming project for a summer.

Invited talks

“Beyond Linus Pauling: Conformation dependence of ideal geometry in proteins.” Seminar speaker for biochemistry & molecular biology program. University of Richmond, April 2009.

“Beyond Linus Pauling: Conformation dependence of ideal geometry in proteins.” Abstract selected for oral presentation. West Coast Protein Crystallography Workshop, April 2009. **Won the Best Student Talk award.**

“How to be a distribution-friendly project.” Invited expert on best practices in software engineering for scientific development. Developer workshop for the ABINIT density-functional theory program. Autrans, France, March 2009.

“Probing the active site of 3-phosphoglycerate dehydrogenase: The value of undergraduate research.” Keynote speaker. Annual meeting of Partners in Scholarship winners, who all perform undergraduate research as part of their scholarships. Gustavus, May 2002.

Presented posters

Berkholz DS, Shapovalov MV, Dunbrack Jr RL, Karplus PA. “Beyond Linus Pauling: Conformation dependence of ideal geometry in proteins.” Protein Society, July 2008.

Berkholz DS, Faber HR, Savvides SN, Karplus PA. “Glutathione reductase catalysis at atomic resolution.” West Coast Protein Crystallography Workshop, April 2007.

Berkholz DS, Smith JM. “Conformations of 5-hydroxytryptamine (serotonin) in solution.” MERCURY Conference in Computational Chemistry, July 2002.

Berkholz DS, Bell JE. “Probing the active site of 3-phosphoglycerate dehydrogenase: the role of acid-base catalysis and the local charge environment of the transition state in V-type regulation by serine.” Tri-Beta (biological honor society) national meeting, June 2002. **John C. Johnson award (2nd place) for best molecular-biology poster.**

Berkholz DS, Bell JE. “Probing the active site of 3-phosphoglycerate dehydrogenase: the role of acid-base catalysis and the local charge environment of the transition state in V-type regulation by serine.” ASBMB national meeting, April 2002. **1st prize undergraduate poster.**

Berkholz DS, Bell JE. “Probing the active site of 3-phosphoglycerate dehydrogenase: the role of acid-base catalysis and the local charge environment of the transition state in V-type regulation by serine.” Tri-Beta (biological honor society) district meeting, May 2002. **John C. Johnson award (1st place) for best poster.**

Advanced coursework

Macromolecular crystallography
Oxidative & nitrative stress
Medicinal chemistry
Quantum chemistry
Genomics & cellular evolution
Protein evolution
Enzyme kinetics
Single-molecule biochemistry
Mathematical basis of statistics
Linear algebra
Computer programming in C