Biographical Sketch

Name	Position Title
Bruce R. Donald, Ph.D.	**Professor of Computer Science and Biochemistry**

Education/Training

INSTITUTION	DEGREE	YEAR	FIELD OF STUDY
Yale University	B.A.	1980	
Massachusetts Institute of Technology	S.M.	1984	Electrical Engineering & Computer Science
Massachusetts Institute of Technology	Ph.D.	1987	Computer Science

A. Research and Professional Experience

Professional Experience

• 1978-84: Research Analyst, Laboratory for Computer Graphics and Spatial Analysis, GSD, Harvard University. • 1984: Research Staff, Artificial Intelligence Laboratory, MIT. • 1982-1987: Graduate student, Artificial Intelligence Laboratory and Department of EECS, MIT. • 1987-1993: Assistant Professor; 1993-1998: Associate Professor (with tenure), Computer Science Department, Cornell University. • 1995-1996: Consultant and Contractor, Interval Research Corporation, Palo Alto, CA. • 1994-1996: Visiting Professor, Computer Science Department, Stanford. • 1997-1999: Associate Professor (with tenure); 1999-2006: Professor of Computer Science, Dartmouth College. • 1999-2006: M.D.-Ph.D. Committee, Dartmouth College and Dartmouth Medical School. • 2000: Conference chair, Int'l. Workshop on Algorithmic Foundations of Robotics. • 11 NSF Advisory Panels (1990-2003). • 2000-2001: Visiting Scientist, Artificial Intelligence Laboratory and Department of EECS, MIT. • 2000-2002: Scientific Advisory Board, Carta Proteomics, Inc. (now ExSAR). • 2000-2006: Member, Dartmouth Center for Structural Biology and Computational Chemistry. • 2000-2006: Adjunct Professor of Chemistry, Dartmouth. • 2002-2006: Adjunct Professor of Biological Sciences, Dartmouth. • 2002, 2004, 2005: *Ad hoc* Member, NIH Study Sections (BBCA, ALY, ZRG1 CFS). • 2003–2006: Joan and Edward Foley Professor, Dartmouth. • 2006–now: William and Sue Gross Professor of Computer Science, Duke University. • 2006–now: Professor of Biochemistry, School of Medicine, Duke University Medical Center.

Honors and Awards

• 1979: Phi Beta Kappa; 1980: Distinction in the Major, Yale University. • 1980: Graduated *Summa Cum Laude,* Yale. • 1985-1987: NASA/JPL Graduate Student Researcher Fellowship. • 1989-1994: NSF Presidential Young Investigator. • 1997-2000: NSF Challenges in Computer and Information Science and Engineering Grant. • 2001: Guggenheim Fellow, *"Algorithms in Structural Proteomics."* • 2002: Distinguished Lectures, Robert Mueller-Thuns (Univ. Illinois, Urbana-Champaign); Triangle (UNC Chapel Hill, Duke & N.C. State).

B. Selected Peer-reviewed Publications (from a list of 176 total, with 19 in 2005–6)

1. B. R. Donald, D. Kapur, and J. Mundy. *Symbolic and Numerical Computation for Artificial Intelligence*. Academic Press, Harcourt Jovanovich, London, 1992.
2. B. R. Donald, P. Xavier, J. Canny, and J. Reif. Kinodynamic motion planning. *Journal of the ACM*, 40(5):1048–1066, 1993.
3. C. Bailey-Kellogg, A. Widge, J. J. Kelley III, M. J. Berardi, J. H. Bushweller, and B. R. Donald. The NOESY Jigsaw: Automated protein secondary structure and main-chain assignment from sparse, unassigned NMR data. *Jour. Comp. Biol.*, 3-4(7):537–558, 2000.
4. C. Bailey-Kellogg, J. J. Kelley III, C. Stein, and B. R. Donald. Reducing mass degeneracy in SAR by MS by stable isotopic labeling. *Jour. Comp. Biol.*, 8(1):19–36, 2001.

5. C. Langmead and B. R. Donald. Extracting structural information using time-frequency analysis of protein NMR data. In *Proc. 5th Int'l. Conf. on Research in Computational Molecular Biology (RECOMB)*, pp. 164–175. ACM Press, April 2001.
6. C. Langmead, A. Yan, C. R. McClung, and B. R. Donald. Phase-independent rhythmic analysis of genome-wide expression patterns. *Journal of Computational Biology*, 10(3-4):521–536, 2003.
7. R. Lilien, H. Farid, and B. R. Donald. Probabilistic disease classification of expression-dependent proteomic data from mass spectrometry of human serum. *Journal of Computational Biology*, 10(6):925–946, 2003.
8. C. Langmead, A. Yan, R. Lilien, L. Wang, and B. R. Donald. A polynomial-time nuclear vector replacement algorithm for automated NMR resonance assignments. In *Proc. 7th Int'l. Conf. on Research in Computational Molecuar Biology (RECOMB)*, pp. 176–187, Berlin, Germany, April 2003. ACM Press.
9. C. Langmead and B. R. Donald. 3D structural homology detection via unassigned residual dipolar couplings. In *Proc. IEEE Computer Society Bioinformatics Conference (CSB)*, pp. 209–217, Stanford, Aug. 2003.
10. R. O'Neil, R. Lilien, B. R. Donald, R. Stroud, and A. Anderson. Phylogenetic classification of protozoa based on the structure of the linker domain in the bifunctional enzyme, dihydrofolate reductase-thymidylate synthase. *Jour. Biol. Chem.*, 278(52):52980–52987, 2003.
11. R. O'Neil, R. Lilien, B. R. Donald, R. Stroud, and A. Anderson. The crystal structure of dihydrofolate reductase-thymidylate synthase from *Cryptosporidium hominis* reveals a novel architecture for the bifunctional enzyme. *Jour. Eukaryotic Microbiology*, 50(6):555–556, 2003.
12. C. Langmead and B. R. Donald. An expectation/maximization nuclear vector replacement algorithm for automated NMR resonance assignments. *Jour. Biomolecular NMR*, 29(2):111–138, 2004.
13. L. Wang and B. R. Donald. Exact solutions for internuclear vectors and backbone dihedral angles from NH residual dipolar couplings in two media, and their application in a systematic search algorithm for determining protein backbone structure. *Jour. Biomolecular NMR*, 29(3):223–242, 2004.
14. C. Langmead, A. Yan, R. Lilien, L. Wang, and B. R. Donald. A polynomial-time nuclear vector replacement algorithm for automated NMR resonance assignments. *Jour. Comp. Biol.*, 11(2-3):277–298, 2004.
15. R. Lilien, B. Stevens, A. Anderson, and B. R. Donald. A novel ensemble-based scoring and search algorithm for protein redesign, and its application to modify the substrate specificity of the gramicidin synthetase A phenylalanine adenylation enzyme. In *Proc. Eighth Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, pp. 46–57, San Diego, March 2004.
16. R. Lilien, C. Bailey-Kellogg, A. Anderson, and B. R. Donald. A subgroup algorithm to identify cross-rotation peaks consistent with non-crystallographic symmetry. *Acta Crystallographica Section D: Biological Crystallography*, 60(6):1057–1067, Jun 2004.
17. C. Langmead and B. R. Donald. High-throughput 3D structural homology detection via NMR resonance assignment. In *Proc. IEEE Computational Systems Bioinformatics Conference (CSB)*, pp. 278–289, Stanford, CA, August 2004.
18. L. Wang and B. R. Donald. Analysis of a systematic search-based algorithm for determining protein backbone structure from a minimal number of residual dipolar couplings. In *Proc. IEEE Computational Systems Bioinformatics Conference (CSB)*, pp. 319–330, Stanford, CA, August 2004.
19. R. Mettu, R. Lilien, and B. R. Donald. High-throughput inference of protein-protein interfaces from unassigned NMR data. *Bioinformatics*, 2005; **21**(Suppl. 1):i292–i301.
20. R. Lilien, B. Stevens, A. Anderson, and B. R. Donald. A novel ensemble-based scoring and search algorithm for protein redesign, and its application to modify the substrate specificity of the gramicidin synthetase A phenylalanine adenylation enzyme. *Journal of Computational Biology* 2005; **12**(6-7):740–761.
21. L. Wang and B. R. Donald. An efficient and accurate algorithm for assigning nuclear Overhauser effect restraints using a rotamer library ensemble and residual dipolar couplings. In *Proceedings of the IEEE Computational Systems Bioinformatics Conference (CSB)*, pp. 189–202, Stanford, CA, August 2005.
22. L. Wang, R. Mettu, and B. R. Donald. An algebraic geometry approach to protein backbone structure determination from NMR data. In *Proceedings of the IEEE Computational Systems Bioinformatics Conference*

(CSB), pp. 235–246, Stanford, CA, August 2005.
23. I. Georgiev, R. Lilien, and B. R. Donald. Improved pruning algorithms and divide-and-conquer strategies for dead-end elimination, with application to protein design. *Bioinformatics* 2006; **22**(14):e174–183. Special issue on papers from the Int'l Conf. on Intelligent Sys. for Mol. Biol. (ISMB 2006), Fortaleza, Brazil.
24. L. Wang and B. R. Donald. A data-driven, systematic search algorithm for structure determination of denatured or disordered proteins. In *Proceedings of the LSS Computational Systems Bioinformatics Conference (CSB)*, Stanford, CA, August 2006. Pages 67-78. ISBN 1-86094-700-X.
25. L. Wang, R. Mettu, and B. R. Donald. A polynomial-time algorithm for *de novo* protein backbone structure determination from NMR data. *Journal of Computational Biology*, 2006. In press.
26. S. Potluri, A. Yan, B. R. Donald, and C. Bailey-Kellogg. Structure determination of symmetric homo-oligomers by a complete search of symmetry configuration space using NMR restraints and van der Waals packing. *Proteins: Structure, Function and Bioinformatics*, 2006; 65(1):203–219.

C. Research Projects and Funding

CURRENT SUPPORT

DONALD, BRUCE R. ONGOING
(PI: Donald) 2002-2007
NIH/NIGMS R01 GM-65982
Automated NMR Assignment and Protein Structure

The long-term objective of this project is the development of new computational methods for biomolecular NMR, to be applied in structural genomics. Two main foci are novel algorithms for automated assignments, and algorithms for automated structure determination from solution-state protein NMR.

DONALD, BRUCE R. ONGOING
(PI: A. Anderson, Co-investigator: B. Donald) 2003-2008
NIH (NIGMS & NIAID) R01 GM-067542
Design of C. parvum and T. gondii DHFR-TS Inhibitors

The major goal of this project is to design selective and potent inhibitors against the dihydrofolate reductase (DHFR) domain of dihydrofolate reductase-thymidylate synthase (DHFR-TS) from *Cryptosporidium hominis* and *Toxoplasma gondii.*

Completed Research Support

DONALD, BRUCE R. COMPLETED
(PI: Donald) 2003-2005
NSF EIA-0305444
Algorithmic Challenges in Computational Biology

This grant supported computational research in functional genomics and computational methods in NMR structural biology.

DONALD, BRUCE R. COMPLETED
(co-PI: B. Donald) 1998-2003
NSF NSF 98-02068
Systems Science for Physical Geometric Algorithms

NSF research infrastructure grant. The major goals of this project were to provide research infrastructure for computational science and computational biology in the Computer Science Department. This includes workstations, supercomputing facilities, networking, etc.

DONALD, BRUCE R. COMPLETED
(PI: Donald) 2001-2003
NSF EIA-0102710
Physical Geometric Algorithms and Systems for High-Throughput NMR Structural Biology
The major goals of this project were to develop novel computational methods for biomolecular NMR.

DONALD, BRUCE R. COMPLETED
(PI: Donald) 2001-2003
NSF EIA-0102712
Physical Geometric Algorithms and Systems for Structural Biology using Mass Spectrometry
The major goals of this project were to develop novel computational methods for structural mass spectrometry and proteomics.

DONALD, BRUCE R. COMPLETED
(PI: Donald) 2000-2006
DHS/ODP 2000-DT-CX-K001
Microelectromechanical Systems for Infosecurity
The major goal of this project was the development of novel microelectromechanical systems (”MEMS”) to be useful in micro- and nano-technology applications for homeland security, in particular, information security and micro robotics.

PENDING SUPPORT

DONALD, BRUCE R. PENDING
(PI: D. Madden, Co-investigator: B. Donald) 2007-2012
Submitted to NIH (NIDDK) R01 Application
Keeping CFTR in its Place: An Integrated Small-Molecule Approach
The major goal of this project is to develop an integrated experimental and theoretical approach to identifying small-molecule inhibitors selective for the CAL PDZ domain (a molecular scaffolding protein), which interacts with the cytoplasmic C-terminus of the cystic fibrosis transmembrane conductance regulator protein (CFTR).

DONALD, BRUCE R. PENDING
(PI: J. Hoch, Co-PIs: B. Donald, G. Wagner, A. Alexandrescu, P. Bolton) 2006-2008
Submitted to NSF MRI application
Acquisition of a High Perfomance Computational Resource for NMR Structural Biology.
The major goal of this project is the acquisition of a supercomputer that will be attached to a high field NMR spectrometer in order to facilitate the development of data-directed high-throughput computational protocols for NMR data processing, automated assignment, and structure determination.

DONALD, BRUCE R. PENDING
(PI: B. Donald) 2007-2012
Submitted to NIH (NIGMS) R01 Application
Computational Active-Site Redesign and Binding Prediction via Molecular Ensembles
The major goal of this project is to develop novel algorithms to plan structure-based site-directed mutations to a protein’s active site in order to modify its function. The new algorithms will make progress towards the long-term objective of reprogramming the specificity of non-ribosomal peptide synthetase domains, whose products include natural antibiotics, antifungals, antivirals, immunosuppressants, and antineoplastics.