CURRICULUM VITAE

April 16, 2021

Name

Roland L Dunbrack, Jr.

Address:

1912 S. 12th St.
Philadelphia, PA 19111

Citizenship:

United States (Born: Newton, Massachusetts, July 25, 1963)

Education:

Harvard College, Cambridge, MA	A.B., Chemistry *(summa cum laude)*	1981-1985
University of Cambridge, Cambridge, UK		1985-1987
Undergraduate study in biochemistry		
Graduate study in theoretical chemistry		
Harvard University, Cambridge, MA	Ph.D., Biophysics	1987-1993

Supervisors: Professor Martin Karplus, Department of Chemistry
Professor Jack Strominger, Department of Biochemistry and Molecular Biology

Postgraduate Training:

Postdoctoral Fellow, Supervisor, University of California, San Francisco, CA 1993-1997

Supervisors: Professor Frederick Cohen, Department of Pharmacology
Professor Kenneth Dill, Department of Pharmaceutical Chemistry

Faculty Appointments:

Assistant professor, Institute for Cancer Research, Fox Chase Cancer Center, Philadelphia, PA	1997-2003
Associate professor, Institute for Cancer Research, Fox Chase Cancer Center, Philadelphia, PA	2003-2011
Professor, Institute for Cancer Research, Fox Chase Cancer Center, Philadelphia, PA	2011-date
Adjunct assistant professor of Biochemistry and Molecular Biophysics, University of Pennsylvania School of Medicine, Philadelphia PA	2000-2006
Adjunct associate professor of Biochemistry and Molecular Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA	2006-2012
Adjunct professor of Biochemistry and Molecular Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA	2012-date
Adjunct associate professor of Biochemistry, Drexel University College of Medicine, Philadelphia, PA	2004-date
Adjunct professor of Biochemistry, Temple University School of Medicine,	2016-date

Philadelphia, PA

Director, Molecular Modeling Facility, Fox Chase Cancer Center	2003-date
Director, Organic Synthesis Facility, Fox Chase Cancer Center	2003-date

Awards and Honors:

John Harvard Scholarship	06/1982, 06/1984
Harvard College Scholarship	06/1983, 06/1985
National Science Foundation Predoctoral Fellowship (1987-1990)	03/1985
Herchel Smith Fellowship, awarded by Harvard College for 1-5 years study at Emmanuel College, University of Cambridge (1985-1987)	03/1985
Phi Beta Kappa, Harvard College, *Alpha* Chapter of Massachusetts	06/1985
National Institute of Health Postdoctoral Fellowship (1993-1996)	08/1993
Senior Research Excellence Award, Temple University School of Medicine	09/2012
Special Contributor Award, Fox Chase Cancer Center	02/2014

Membership in Professional and Scientific Societies:

International Society for Computational Biology (ISCB)

Federal Grant Review Committee Service:

NIH MSF-D Study Section, Regular member 10/2009-10/2011

NIH Study Sections and Site Visit Panels (ad hoc):

BBCB	Biochemistry and Biophysics B	02/2001
SSS-6 (10)	SBIR proposals	03/2002
BBCA	Biochemistry and Biophysics A	06/2002
MDCN-A (05)	Special Emphasis Panel	12/2003
YZW-A (M1)	NIAMS R03 Panel	03/2004
BBCA	Biochemistry and Biophysics A	06/2004
BCMB-Q (02)	Computational Biochemistry and Biophysics	10/2005
BCMB-G (91)	Special Emphasis Panel	11/2005
BST-L (51)	Software maintenance proposals	01/2006
BCMB-C (40)	P01 review	03/2006
BCMB-Q (90)	Computational Biochemistry and Biophysics	06/2006
BRT-9	K99 proposals	08/2006
BCMB-Q (90)	Computational Biochemistry and Biophysics	10/2006
BCMB-A (92)	Special Emphasis Panel	12/2006
BCMB-N	Computational Biochemistry and Biophysics	02/2007
CBB-3 (HM)	PSI 2 Molecular Modeling proposals	05/2007
BCMB-H (40)	Center for Synchrotron Biosciences, Brookhaven NY	03/2008
MSF-D	Macromolecular Structure and Function D	10/2008
BCMB-P (58)	ARRA proposals	06/2009
BCMB-P (40)	Competitive Revisions of P41 Grants	03/2012
BCMB-H	Special Emphasis Panel	04/2013
MSF-D	Macromolecular Structure and Function D	10/2014

ZGM1 PPBC-0 (GL)	Large-Scale Collaborative Project Awards (R24/U54)	03/2015
CE	Cancer Etiology (mail reviewer)	09/2016
MSF-D	Macromolecular Structure and Function D	06/2017
BSF-T (40)	National Technology Research Resource Award (mail)	08/2018

NSF Site Visit Panel: BioGeometry Project, Duke University, Durham, NC 11/2002
NSF Site Visit Panel: RCSB-Protein Data Bank, New Brunswick, NJ 04/2003
NIH Site Visit Panel: Laboratory of Molecular Biology, NCI, Bethesda, MD 2007, 2009

National and International Committee Service:

Assessor for 6th Meeting on the Critical Assessment of Protein Structure Prediction (CASP6); Assessment of fold-recognition models; Assessment of Disorder predictions 2004

External Advisory Board, Seattle Structural Genomics Center for Infectious Diseases (SSGCID), Seattle, WA 2008-date

Advisory Board, RCSB Protein Data Bank, Rutgers Univ., New Brunswick, NJ 2009-date

Assessor for BRCA1/BRCA2 challenge, 3rd Meeting on Critical Assessment of Genome Interpretation, Max Planck Institute, Berlin, Germany 2013

Assessor for 11th Meeting on the Critical Assessment of Protein Structure Prediction (CASP11): (1) Template-based modeling category; (2) Biological inferences from models; (3) Refinement of template-based models category 2014

Editorial Positions:

Editorial Advisory Board, *Protein Science* 2001-2007
Associate Editor, *PLOS Computational Biology* 2008-date

Academic Committees and Activities, Fox Chase Cancer Center:

Biomolecular Structure and Function Faculty Search Committee (Member) 2002-2003
Bioinformatics Facility Oversight Committee (Chair) 2002-2007
Post-doctoral Fellowship Selection Committee (Member) 2003-2008
High-Performance Computing Facility Oversight Committee (Chair) 2006-date
Research Informatics Advisory Committee (Member) 2007-date
Institutional Information Systems Advisory Committee (Member) 2007-date
Molecular Medicine, Faculty Search Committee (Member) 2009-2010
Facility Parent Oversight Committee (Member) 2009-date
2013 Post-doc Day Committee 2012-date
Tenure and Promotions Committee 2015-date

Federal (NIH, DOD, VA) Funding History:

Current

R35 GM122517 (PI: Dunbrack) 04/01/2017 - 03/31/2022
NIH ($370,000 per year in direct costs) Role: Principal Investigator
Structural bioinformatics of proteins and protein complexes and applications to cancer biology
This MIRA (Maximizing Investigator Research Award) grant funds the entirety of the research in my

lab previously funded by NIGMS. The grant is focused on the utilization of structural bioinformatics – the statistical study of experimental structures of proteins and protein complexes – to further our understanding of cancer biology, the effects of mutations discovered in tumor and germline samples, and the development of cancer therapeutics. In particular, we have developed methods for computational antibody design and we are engaged in extensive studies of the structures of protein-protein interactions and protein kinases and their inhibitors.

P30 CA006927 (PI: Fisher) 08/12/2016 - 07/31/2021
NIH Role: Facility Director
Comprehensive Cancer Center Program at Fox Chase
The major goal of this Cancer Center Support Grant is to provide partial salary support for professional personnel, including senior and program leadership, administration, planning and evaluation, and developmental funds, as well as support for 5 established peer-reviewed Research Programs, 12 Shared Research Resources and 1 Support Element.

Previous

R01 GM111819 (PI: Dunbrack) 08/01/2015 - 07/31/2019
NIH Role: Principal Investigator
Development of Methods for Antibody Computational Design
The major goals of this project are: 1) To further develop the structural bioinformatics needed to perform accurate antibody design; 2) To refine our existing code for antibody design and optimize sampling and scoring functions via a novel metric for protein design; and 3) To test our antibody design methods experimentally. This grant will be replaced with R35 MIRA funding from NIGMS.

R01 GM084453 (PI: Dunbrack) 06/01/2013 - 03/31/2018
NIH Role: Principal Investigator
Bayesian Statistics and Algorithms for Homology Modeling
The major goal of this project is to predict the structures of biologically relevant states of proteins and protein complexes and to utilize these in cancer research. The aims of the project are: 1) Non-parametric statistics of protein structure parameters; 2) Comparative modeling of biological assemblies; and 3) The structure of kinase autophosphorylation complexes. This grant was continued under R35 MIRA funding.

R01 GM117437 (PI: Graña, Temple University) 01/01/2016 – 03/31/2017
NIH Role: Co-investigator (10% effort)
Unraveling the complexity of substrate specificity of PP2A/B55A, a major eukaryotic serine/threonine phosphatase
This project is focused on the molecular determinants of substrate specificity of protein phosphatases. Our role in this project is to perform docking calculations of disordered regions of PP2A substrates to the catalytic subunit and the B55 regulatory subunit. This subcontract was relinquished on 3/31/2017 and replaced with R35 MIRA funding. The collaboration will continue after this date.

R01 GM078221 (PI: Gray, JHU) 09/01/2012 - 08/31/2016
NIH Role: Co-PI (5% effort)

Prediction of the Structure of Therapeutic Antibodies with their Antigens
The major goals of this project are to develop new methods for predicting the structures of antibodies and for improved methods of docking antibodies to antigens. My role in this project is to supervise the efforts of graduate student Brian Weitzner in structural bioinformatics analysis of antibody CDRs and the role of beta turns in loop structure prediction.

R01 GM073784 (PI: Dunbrack) 03/01/2006 – 02/28/2010
NIH Role: Principal Investigator
Modeling of Protein Complexes and Missense Mutations
The major goals of this project are: 1) A model for missense mutations in protein complexes; 2) Development of database to aid the structure prediction of protein complexes; and 3) Examination of missense mutations associated with cancer

P20 GM076222 (PI: Dunbrack) 04/01/2006 – 03/31/2010
NIH Role: Principal Investigator
New Methods for High-Resolution Comparative Modeling
The major goal of this proposal is to establish a center for high-resolution modeling of protein structures to improve the quality of comparative models both in the >30% sequence identity regime and in the 10-30% sequence identity regime The focus of the center is on the development of powerful new methodology through the integrated efforts of experts in protein structure modeling with computational and mathematical scientists new to protein structure modeling This project includes five subcontracts

R01 HL057299 (PI: Kruger) 01/16/2001 – 11/30/2006
NIH Role: Co-Investigator
Genetic Modulation of CBS to Lower Plasma Homocysteine
The major goals of this project are: 1) Characterization and additional isolation of missense mutations within the regulatory domain of CBS; 2) Determine if mutant CBS enzymes can lower plasma homocysteine levels in vivo using a mouse model; 3) Identify peptamers which can inhibit activity of the regulatory domain of CBS; and 4) Analysis of Adomet binding to both normal and mutant CBS molecules

R01 GM56250 (PI: Roder) 05/01/2002 – 04/30/2006
NIH Role: Co-Investigator
Kinetics of Early Events in Protein Folding
The major goals of this project are: 1) Barriers and intermediates in the folding of protein G; 2) Fluorescence probes to monitor tertiary structure formation during early stages of SNase folding; and 3) Structural characterization of early folding events in SNase by H-D exchange labeling and NMR

U01 AI058269 (PI: Taylor) 09/01/2003 – 02/28/2008
NIH Role: Co-Investigator
Towards a Novel Strategy Against HBV Infection
The major goals of this project are: 1) Establish conditions for the controlled assembly of HDV and evaluate in two different hepatocyte systems the ability to achieve attachment, entry, and the initiation of replication; 2) Use unmodified and/or modified forms of HBV envelope proteins for virion assembly, and identify determinants necessary for attachment, entry, and initiation of HDV replication; and 3) Test small molecules for interference with attachment and entry, usng high throughput screening assays

R21AI063324 (PI: Jaffe) 04/01/2005 – 03/31/2007
NIH Role: Co-Investigator
Hexameric PBGS as a Bioterrorism Defense
The major goals of this project are: 1) Prepare protein structure models of hexameric PBGS proteins for the target species of PBGS that are proposed to freely equilibrate between the hexameric and octameric forms; 2) Use computational methodfs to screen small molecule structural databases for molecules that will selectively bind to the inactive hexameric forms of PBGS from the target organism; and 3) Test the identified candidate molecules, *in vitro* and in an *in vivo* model system, for the ability to inhibit PBGS activity through stabilization of the hexameric form of the protein

<u>Non-Federal, Non-Industry Funding History (ACS, sub-specialty group, other):</u>

No Number (PI: Dunbrack) 4/1/2020- 03/31/2022
GSK ($150,000 per year in direct costs) Role: Principal Investigator
Structural bioinformatics of antibodies to enhance developability of biologics
The goal of this project is to perform structural bioinformatics and deep learning studies on the variable and constant domains of antibodies to develop methods for enhancing thermostability and reducing aggregation of antibodies.

No Number (PI: Dunbrack) 1/1/2017- 12/31/2019
Janssen Pharmaceuticals Role: Principal Investigator
Development of clustering method for molecular dynamics simulations of antibodies
The goal of this project is to provide an implementation of our antibody CDR clustering method for the purpose of clustering CDR conformations from molecular dynamics simulations of antibodies.

No Number (PI: Dunbrack) 1/1/2014 - 12/31/2014
Rosetta Commons Role: Principal Investigator
Development and implementation of statistical scoring functions in Rosetta
The major goals of this project are to develop and test improved statistical scoring functions within Rosetta, including backbone-dependent dihedral and bon angle scoring terms for the backbone and side chains.

69133-01 (PI: Dunbrack) 01/01/2011 – 12/31/2013
Pennsylvania Tobacco Settlement Funds Role: Principal Investigator
Classification and Prediction of Protein-Protein Interactions in Biology and Medicine
The aims of this project are: 1) to improve the assignment of PFAM domains to all proteins of known structure using modern sequence and structure-based methods; 2) to compare and cluster interfaces between domains in all PDB entries; 3) to study the role of specific homodimeric interfaces in activation and inhibition of protein kinases

Keystone Program in Head and Neck Cancer 07/01/2009 –06/30/2011
Fox Chase Cancer Center Role: Co-Principal Investigator
Pilot project on antibody design for head and neck tumor targets

This internal pilot project is a collaboration between Dr Dunbrack's molecular modeling group and investigators in antibody engineering and clinical investigators to design antibodies that target EGFR family proteins

Pilot Project (PI: Roder) 07/01/2008-06/30/2010
Fox Chase Cancer Center Role: Co-Investigator
The role of disordered protein regions in protein function and regulation
This internal pilot project is a collaboration between Dr Dunbrack and Dr Heinrich Roder at Fox Chase to explore the structure, dynamics, and role of the long disordered region in NHERF1 using NMR, electron paramagnetic resonance, fluorescence experiments, and computational modeling

69133-01 (PI: Dunbrack) 01/01/2005 – 6/30/2006
Pennsylvania Tobacco Settlement Funds Role: Principal Investigator
Predicting the effects of disease-associated missense mutations on protein stability and interactions
The goals of this project are to design a statistical model of the effects of missense mutations on protein function, based on changes in protein stability and disruption of protein interactions Structure prediction of complexes and sequence analysis will be used as primary tools

W W Smith Charitable Trust (PI: Dunbrack) 11/01/2000 – 09/30/2002
Role: Principal Investigator
Analysis of Missense Mutations and Polymorphisms in Cancer
The major goal of this project is to examine all identified mutations in several genes associated with cancer and to identify which mutations are most likely to be associated with increased risk of disease using computational methods developed to investigate the evolutionary relationships among related genes, as well as algorithms for predicting the structures of proteins based on their similarity to proteins of known three-dimensional structure The proteins that will be investigated include BRCA1, ATM, APC, the RET proto-oncogene, and TSC2

Bibliography:

Research Publications (peer reviewed):

1. **Dunbrack RL Jr.** Calculation of Franck-Condon factors for undergraduate quantum chemistry. *J Chem Edu* **63**:953-955, 1986.
2. Doyle C, Shin J, **Dunbrack RL Jr.**, Strominger JL. Mutational analysis of the structure and function of the CD4 protein. *Immunol Rev* **109**:17-37, 1989.
3. Shin J, **Dunbrack RL Jr.**, Lee S, Strominger JL. Signals for retention of transmembrane proteins in the ER studied with CD4 truncation mutants. *Proc Natl Acad Sci USA* **88**:1918-1922, 1991.
4. Shin J, **Dunbrack RL Jr.**, Lee S, Strominger JL. Phosphorylation-dependent down modulation of CD4 requires a specific structure within the cytoplasmic domain of CD4. *J Biol Chem* **266**:10658-10665, 1991.
5. **Dunbrack RL Jr.**, Karplus M. A backbone dependent rotamer library for proteins: application to side-chain prediction. *J Mol Biol* **230**:543-571, 1993.
6. Schmidt JM, Brüschweiler R, Ernst RR, **Dunbrack RL Jr.**, Joseph D, Karplus M. Molecular dynamics simulation of the proline conformational equilibrium and dynamics in antamanide using the CHARMM force field. *J Amer Chem Soc* **115**:8747-8756, 1993.

7. **Dunbrack RL Jr.**, Karplus M. Conformational analysis of the backbone-dependent rotamer preferences of protein side chains. *Nat Struct Biol* **1**:334-340, 1994.
8. Fischer S, **Dunbrack RL Jr.**, Karplus M. Cis-trans imide isomerization of the proline dipeptide. *J Amer Chem Soc* **116**:11931-11937, 1994.
9. Byington CL, **Dunbrack RL Jr.**, Cohen FE, Agabian N. Molecular modeling of phosphofructokinase from *Entamoeba histolytica* for the prediction of new antiparasitic agents. *Arch Med Res* **28**:S86-S88, 1997.
10. Bower MJ, Cohen FE, **Dunbrack RL Jr.** Prediction of protein side-chain rotamers from a backbone-dependent rotamer library: a new homology modeling tool. *J Mol Biol* **267**:1268-1282, 1997.
11. **Dunbrack RL Jr.**, Cohen FE. Bayesian statistical analysis of protein side-chain rotamer preferences. *Protein Sci* **6**:1661-1681, 1997.
12. Byington CL, **Dunbrack RL Jr.**, Whitby FG, Cohen FE, Agabian N. *Entamoeba histolytica:* computer-assisted modeling of phosphofructokinase for the prediction of broad-spectrum antiparasitic agents. *Exp Parasitol* **87**:194-202, 1997.
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15. Williams M, Lyu MS, Yang YL, Lin EP, **Dunbrack RL Jr.**, Birren B, Cunningham J, Hunter K. Ier5, a novel member of the slow-kinetics immediate-early genes. *Genomics* **55**:327-334, 1999.
16. Moraleda G, Seeholzer S, Bichko V, **Dunbrack RL Jr.**, Otto J, Taylor J. Unique properties of the large antigen of hepatitis delta virus. *J Virol* **73**:7147-7152, 1999.
17. **Dunbrack RL Jr.** Comparative modeling of CASP3 targets using PSI-BLAST and SCWRL. *Proteins: Structure, Function, Genetics* **3**:81-87, 1999.
18. Zhang Y-Z, Gould KL, **Dunbrack RL Jr.**, Cheng H, Roder H, Golemis EA. The evolutionarily conserved Dim1 protein defines a novel branch of the thioredoxin fold superfamily adapted to cell cycle regulation. *Physiol Genomics* **1**:109-118, 1999.
19. Jaffe EK, Volin M, Bronson-Mullins CR, **Dunbrack RL Jr.**, Kervinen J, Martins J, Quinlan JF, Jr, Sazinsky MH, Steinhouse EM, Yeung AT. An artificial gene for human porphobilinogen synthase allows comparison of an allelic variation implicated in susceptibility to lead poisoning. *J Biol Chem* **275**:2619-2626, 2000.
20. Sauder JM, Arthur JW, **Dunbrack RL Jr.** Large-scale comparison of protein sequence alignment algorithms with structure alignments. *Proteins: Structure, Function, Genetics* **40**:6-22, 2000.
21. Sauder JM, **Dunbrack RL Jr.** Genomic fold assignment and rational modeling of proteins of biological interest. *Intelligent Systems Mol Biol (ISMB)* **8:**296-306, 2000.
22. Sauder JM, Arthur JW, **Dunbrack RL Jr.** Modeling of substrate specificity of the Alzheimer's disease amyloid precursor protein β-secretase. *J Mol Biol* **300**:241-248, 2000.
23. Kervinen J, **Dunbrack RL Jr.**, Litwin S, Martins J, Scarrow RC, Volin M, Yeung AT, Yoon E, Jaffe EK. Porphobilinogen synthase from pea: expression from an artificial gene, kinetic characterization, and novel implications for subunit interactions. *Biochemistry* **39**:9018-9029, 2000.
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RNA-binding motif proteins that interact with OVCA1, a candidate tumor suppressor. *Genomics* **69**:54-62, 2000.
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40. Canutescu AA, **Dunbrack RL Jr.** Cyclic coordinate descent: A robotics algorithm for protein loop closure. *Protein Sci* **12**:963-972, 2003.
41. Wang G, **Dunbrack RL Jr.** Scoring profile-to-profile sequence alignments. *Protein Sci* **13**:1612-1626, 2004.
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foci and senescence driven by ASFIa and HIRA. *Dev Cell* **8**:19-30, 2005.

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