CURRICULUM VITAE

July 12, 2016

Name
Roland L Dunbrack, Jr.

Address:
1912 S. 12th St.
Philadelphia, PA 19111

Citizenship:
United States (Born: Waltham, 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, Philadelphia, PA	2016-date
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
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	2008-date

Diseases (SSGCID), Seattle, WA
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

R01 GM111819 (PI: Dunbrack) 8/1/2015 - 7/31/2019
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 with collaborators.

R01 GM084453 (PI: Dunbrack) 12/14/2001 – 04/30/2017
NIH Role: Principal Investigator
Bayesian Statistics and Algorithms for Homology Modeling
The major goals of this project are: 1) Non-parametric regression of bond angles in protein side chains and modeling of structural heterogeneity of side chains; 2) Automatic protein family and superfamily assignments of proteins in the PDB and web-based homology modeling of protein complexes; 3) Identification of kinase autophosphorylation complexes in protein crystals and experimental testing of proposed complexes.

P30 CA006927-50 (PI: Fisher) 05/31/2001 – 06/30/2016
NIH Role: Facility Director
Comprehensive Cancer Center Program at Fox Chase

This is an Institutional grant from the National Cancer Institute which provides salary support to Dr Dunbrack as Facility Director of the Organic Synthesis Facility and as Facility Director of the Molecular Modeling Facility

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.

Previous
R03 CA167264 (PI: Egleston) 3/1/2013 - 02/28/2015
NIH Role: Co-PI (5% effort)
Clinical Trials with Exclusions Based on Race, Ethnicity, and English Fluency
The major goals of this project are: 1) To identify and describe characteristics of clinical trials that have explicit inclusion or exclusion criteria related to race or ethnicity; and 2) To identify and describe characteristics of clinical trials that have explicit inclusion or exclusion criteria related to language.

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

Non-Federal, Non-Industry Funding History (ACS, sub-specialty group, other):

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.
13. Armand P, Kirshenbaum K, Falicov A, **Dunbrack RL Jr.**, Dill, KA, Zuckermann RN, Cohen, FE. Chiral N-substituted glycines can form stable helical conformations. *Fold, Des* **2:**369-375, 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.
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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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28. Shan X, **Dunbrack RL Jr.**, Christopher SA, Kruger WD. Mutations in the regulatory domain of cystathionine β-synthase can functionally suppress patient-derived mutations in *cis. Hum Mol Genet* **10**:635-643, 2001.
29. Fischer D, Elofsson A, Rychlewski L, Pazos F, Valencia A, Rost B, Ortiz AR, **Dunbrack RL Jr.** CAFASP2: the second critical assessment of fully automated structure prediction methods. *Proteins: Structure, Function, Genetics* **5**:171-183, 2001.
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33. Grant JD, **Dunbrack RL Jr.**, Manion FJ, Ochs MF. BeoBLAST: distributed BLAST and PSI-BLAST on a Beowulf cluster. *Bioinformatics* **18**:765-766, 2002.
34. Cheng JD, **Dunbrack RL Jr.**, Valianou M, Rogatko A, Alpaugh RK, Weiner LM. Promotion of tumor growth by murine FAP, a serine protease, in an animal model. *Cancer Res* **62**:4767-4772, 2002.
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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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43. Canutescu AA, **Dunbrack RL Jr.** MollDE: a homology modeling framework you can click with. *Bioinformatics* **21**:2914-2916, 2005.
44. Wang G, **Dunbrack RL Jr.** PISCES: recent improvements to a PDB sequence culling server. *Nucleic Acids Res* **33**:W94-W98, 2005.
45. Kahsay RY, Wang G, Gao G, Liao L, **Dunbrack RL Jr.** Quasi-consensus based

comparison of profile hidden Markov models for protein sequences. *Bioinformatics* **21**:2287-2293, 2005.

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66. Bourne PE, Beran B, Bi C, Bluhm W, **Dunbrack R,** Prlic A, Quinn G, Rose P, Shah R, Tao W, Weitzner B, Yukich B. Will widgets and semantic tagging change computational biology? *PLoS Comput Biol* **6**:e1000673 2010. PMCID: PMC2829027.
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Editorials, Reviews, and Chapters:

1. **Dunbrack RL Jr.**, Gerloff DL, Bower M, Chen X, Lichtarge O, Cohen FE. Meeting review: The second meeting on the critical assessment of techniques for protein structure prediction (CASP2), Asilomar, CA, December 13-16, 1996. *Fold Des* **2**:R27-R42, 1997.
2. **Dunbrack RL Jr.** Bayesian statistics in molecular and structural biology In: Computational Biochemistry and Biophysics (MacKerell A, Watanabe M, Roux B, Becker OM, eds.), pp. 313-349, Marcel Dekker, Inc, New Your, 2000.
3. **Dunbrack RL Jr.**, Dunker K, Godzik A. Protein structure prediction in biology and medicine. *Pac Symp Biocomput* **2000**:93-4, 2000.
4. **Dunbrack RL Jr.** Homology modeling in biology and medicine In: Bioinformatics: From Genomes to Drugs (Lengauer, T, ed), pp. 145-235, Wiley VCH Press, Berlin, 2001.
5. Bove B, Sauder JM, **Dunbrack RL Jr.**, Godwin, AK. BRCA1, BRCA2, and hereditary breast cancer In: Breast Cancer: Prognosis-Treatment-Prevention (Pasqualini, J, ed) pp. 555-624, Marcel Dekker, New York, 2002.
6. **Dunbrack RL Jr.** Rotamer libraries in the 21st century. *Curr Opin Struct Biol* **12**:431-440, 2002.
7. **Dunbrack RL Jr.** Book review: A scoundrel's refuge: Structural Bioinformatics, P E Bourne, H Weissig, eds, *Nature Struct Biol* **10**:590, 2003.
8. **Dunbrack RL Jr.** Homology modeling and structural genomics In: Structural Proteomics (Edwards, Al, Sundstrom, M, Norin, M, eds), pp. 109-136 Marcel Dekker, 2005.
9. **Dunbrack RL Jr.** Sequence comparison and protein structure prediction. *Curr Opin Struct Biol* **16**:374-384, 2006
10. **Dunbrack RL Jr.** Homology modeling in biology and medicine In: Bioinformatics: From Genomes to Therapies, Volume 1 (Lengauer, T, ed.), pp. 297-350, Wiley VCH Press, Berlin, 2007.
11. Mehra R, Serebriiskii IG, **Dunbrack RL Jr.**, Robinson MK, Burtness B, Golemis EA. Protein-intrinsic and signaling network-based sources of resistance to EGFR- and ErbB family-targeted therapies in head and neck cancer. *Drug Resist Updat* **14**:260-279, 2011. PMCID: PMC3195944.
12. Nikonova AS, Astsaturov I, Serebriiskii IG, **Dunbrack RL Jr.**, Golemis EA. Aurora-A (AURKA) kinase in normal and pathological cell growth. *Cell Molec Life Sciences* **70:**661-687, 2013. PMCID: PMC3607959.
13. Shapovalov MV, **Dunbrack RL Jr.** Non-Parametric Statistical Analysis of the Ramachandran Map. In: Biomolecular Forms and Functions: 50 Years of the Ramachandran Map (Bansal, M, Srinivasan, N, eds.). World Scientific. Singapore, 2013.
14. Shagisultanova E, **Dunbrack RL Jr.**, Golemis EA. Issues in interpreting in vivo activity of Aurora A. *Expert Opin Ther Targets* **19**:187-200, 2015. PMCID: PMC4294965.

Invited Talks, Participation in Conferences (2006-2016):

1. Mar 9, 2006 *Predicting the Structure of Proteins and Protein Complexes* Chemical

Biophysics Mini-Symposium, University of Pennsylvania, Philadelphia PA

2. May 1-2, 2006 *The future of CASP* CASP65 Meeting Dept of Biochemistry and Biophysics, Columbia University, New York NY
3. Jun 26, 2006 *PSI2 Modeling Families* Workshop on Target Selection for the Protein Structure Initiative, NIH Bethesda MD
4. July 4, 2006 *Improving methods of structure prediction of proteins and protein complexes* MODREF 2006, Barcelona, Spain
5. Sep 26 2006 *Structure prediction of proteins and protein complexes of biology and medicine* COMBIO 2006, Brisbane, Queensland, Australia
6. Sep 30, 2006 *Methods for Protein Structure Prediction* Phylogica, Inc, Perth, Western Australia
7. Oct 4, 2006 *Methods for Protein Structure Prediction* University of Sydney, Sydney, New South Wales, Australia
8. Oct 24, 2006 *Protein structure prediction in biology and medicine* Ursinus College, Collegeville, PA
9. Oct 26 2006 *Protein Structure Prediction in Biology and Medicine* Baylor College of Medicine, Houston TX
10. Nov 8, 2006 *Protein Structure Prediction in Biology and Medicine* Greater Philadelphia Bioinformatics Alliance, Drexel University, Philadelphia PA
11. Dec 1, 2006 *Molecular Modeling in Cancer Biology* 7th Meeting on the Critical Assessment of Protein Structure Prediction (CASP7) Asilomar, Pacific Grove, CA
12. Mar 12, 2007 *Protein interactions in crystal structures: how do we identify biologically relevant interfaces?* Dept of Biology, Columbia University, New York, NY
13. July 20, 2007 *Structural bioinformatics identifies probable biologically relevant interfaces in protein crystals* 3DSIG, Conference on Intelligent Systems in Molecular Biology (ISMB), Vienna, Austria
14. July 24, 2007 *Using electron density in structural bioinformatics* Highlights Session, ISMB, Vienna, Austria
15. July 24, 2007 *Structural Bioinformatics Reveals Probably Biological Interfaces in Protein Crystals* Public Library of Science Highlights Session (PLOS), ISMB, Vienna, Austria
16. Aug 23, 2007 *Identifying biologically relevant interfaces in protein crystals* American Chemical Society Meeting, Boston, MA
17. Oct 1, 2007 *Identifying biological interfaces in protein crystal structures* Modeling of Protein Interactions (MPI2007), University of Kansas, Lawrence, KS
18. Nov 19, 2007 *Statistical analysis and algorithms for prediction of protein side-chain conformations* Department of Biomedical Engineering, Boston University, Boston MA
19. Jun 5, 2008 *Statistical Analysis of Protein Structures: Electron Density, Conformational Analysis, and Protein-protein Interfaces* American Crystallographic Association Meeting (ACA08), Knoxville TN
20. Jun 30, 2008 *Methods for Protein Structure Prediction* Baker Center for Bioinformatics and Biological Statistics, Iowa State University

21. July 11, 2008 *Applications of molecular modeling in cancer biology* Workshop on Applications of Protein Models in Biomedical Research, UCSF, San Francisco, CA
22. July 19, 2008 *The Next Generation of the Backbone-dependent Rotamer Library* 3DSIG, Conference on Intelligent Systems in Molecular Biology (ISMB), Toronto, Canada
23. July 24, 2008 *New Ramachandran Maps and the Next Generation of the Backbone-Dependent Rotamer Library* University of Washington Rosetta Conference (RosettaCON), Leavenworth, WA
24. Sep 26, 2008 *Statistical analysis of protein structures: electron density, conformational analysis, and protein-protein interfaces* Conference on Theoretical and Computational Chemistry (TACC), Shanghai, China
25. Oct 14, 2008 *Statistics and Algorithms for Prediction of Protein Side-chain Conformations* INFORMS Conference, Washington, DC
26. Nov 12, 2008 *Structural Bioinformatics and Protein Structure Prediction* BIOMAPS (Biological, Mathematical and Physical Sciences Program), Rutgers Univ
27. Dec 10, 2008 *New methods for high-resolution comparative modeling* Annual Meeting of the Protein Structure Initiative, NIH, Bethesda, MD
28. Feb 26, 2009 *The next-generation of the backbone-dependent rotamer library* Dept of Biochemistry, University of Washington, Seattle, Seattle WA
29. Mar 19, 2009 *Methods for Structure Prediction of Proteins and Protein Complexes* Mount Sinai School of Medicine, New York, NY
30. Jun 15, 2009 *Method development for protein structure prediction and design* Telluride Science Research Center, Telluride, CO
31. Jun 30, 2009 *Comparative analysis of crystal interfaces of homologous proteins* ISMB, Stockholm, Sweden
32. Aug 6, 2009 *Statistical potentials in Rosetta* RosettaCon 2009, Leavenworth, WA
33. Dec 9, 2009 *Refinement in structure determination and comparative modeling* Annual Meeting of the Protein Structure Initiative, NIH, Bethesda, MD
34. Jan 28, 2010 *Statistical analysis of structures of proteins and protein complexes* NCBI, NIH, Bethesda, MD
35. Mar 21 2010 *Non-parametric density estimates for protein backbone and side-chain sampling* American Chemical Society Annual Meeting, Boston, MA
36. Apr 8, 2010 *Statistical analysis of protein structures: electron density, conformational analysis, and protein-protein interfaces* Argonne National Lab, Argonne, IL
37. Apr 25, 2010 *Structure prediction of proteins and protein complexes* ASBMB, Anaheim, CA
38. Jun 15, 2010 *Applications of molecular modeling* Workshop on Theoretical Structural Models Validation, Rutgers University, New Brunswick, NJ
39. July 9, 2010 *Neighbor-dependent Ramachandran probability distributions of amino acids developed from a hierarchical Dirichlet process model* 3DSIG, ISMB, Boston, MA
40. Sep 29, 2010 *Non-parametric statistics and clustering methods in structural biology* Dept of Physics, City College of New York, New York, NY

41. Oct 28, 2010 *Homologous protein-protein interfaces observed in multiple crystal forms* Conference on Modeling of Protein Interactions (MPI), Lawrence, KS
42. Nov 1, 2010 *Statistical analysis of protein structures for structure prediction and protein design* Molecular Biophysics Seminar Series, University of Texas, Austin, Austin TX
43. Nov. 19, 2010 *Non-parametric statistics and clustering methods in structural biology*. Biomolecular Engineering Research Center, Boston University, Boston MA
44. Apr. 22, 2011 *Non-parametric statistics and protein structure determination*. Dept. of Molecular Biology and Biochemistry, Rutgers University, Piscataway NJ
45. Jul. 15, 2011 *Identifying biologically relevant interactions in protein crystals.* Intelligent Systems and Molecular Biology Conference 3DSIG Meeting, Vienna, Austria
46. Aug. 31, 2011 *Common interfaces in multiple crystal forms of proteins and protein complexes associated with biological function.* 242nd American Chemical Society Annual Meeting, Denver CO
47. Oct. 28, 2011. *Statistical analysis of protein structures: backbone conformations, side-chain rotamers and protein-protein interfaces.* The 2nd Biocomputation Forum, Asia University, Taichung, Taiwan
48. Nov. 30, 2011. *Statistical analysis of protein structures for structure prediction and protein design.* Raymond & Beverly Sackler Institute for Biological, Physical and Engineering Sciences, Yale University, New Haven CT
49. Dec. 5, 2011 *A new clustering of antibody CDR loop conformations for structure prediction and design*. IBC Antibody Engineering Conference, San Diego CA
50. Feb. 28 2012 *Structural bioinformatics of antibodies and protein-protein interactions*. Friday Research Discussion, University of Pennsylvania, Department of Biochemistry and Biophysics, Philadelphia PA
51. May 31, 2012 *Conformational analysis of antibody CDRs using diffusion maps*. Mid-Atlantic Regional Meeting, American Chemical Society, Baltimore MD
52. July 11, 2012 *Clustering of antibody complementarity determining region conformations.* EBI Antibody Workshop, European Bioinformatics Institute, Hinxton, UK
53. Sep. 21, 2012 *Protein structure in biology and medicine.* First Annual Temple Biomedical Research Day, Senior Excellence Award Lecture. Temple University School of Medicine, Philadelphia PA
54. Oct. 4, 2012 *Structural bioinformatics of proteins and protein complexes*. Keynote lecture, Computational Structural Bioinformatics Workshop, IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2012). Philadelphia PA
55. Nov. 8, 2012 *Regulation of protein kinases through protein-protein interactions*. Conference on Modeling of Protein Interactions (MPI), Lawrence, KS
56. Dec. 3, 2012 *Structural bioinformatics and protein structure prediction*. Department of Biochemistry, Temple University School of Medicine, Philadelphia, PA
57. Dec. 7, 2012 *Structural bioinformatics and protein structure* prediction. Dipartimento di Scienze Biomolecolari, Università degli Studi di Urbino "Carlo Bo,", Urbino, Italy
58. Dec. 12, 2012 *Structural bioinformatics for protein structure prediction*. 10th Meeting on

the Critical Assessment of Protein Structure Prediction (CASP10), Gaeta, Italy

59. Jan. 8, 2013 *Non-parametric statistical estimates on the Ramachandran map: density estimates, classification functions, and regressions*. International Conference on Biomolecular Forms and Functions: A Celebration of 50 Years of the Ramachandran Map. The Indian Institute of Science, Bangalore, India
60. Jan. 18, 2013 *Structural bioinformatics for protein structure prediction*. Department of Biological Sciences and Bioengineering, Indian Institute of Science, Kanpur, India
61. Mar. 13, 2013 *Structural bioinformatics for protein structure prediction*. Mid-Atlantic Computational Chemistry meeting, Bryn Mawr, PA
62. Apr. 17, 2013 *Structural bioinformatics and protein structure prediction*. Department of Biochemistry and Molecular Biology, University of Tennessee, Knoxville, TN
63. Apr. 19. 2013 *Modeling biological assemblies*. Department of Biochemistry and Molecular Biophysics, University of Pennsylvania, Philadelphia, PA
64. Jul. 17, 2013 *Prediction of phenotypes of MRN complex mutations*. Meeting on Critical Assessment of Genome Interpretation (CAGI), Berlin, Germany
65. Jul 17, 2013 *Assessment of predictions of mutations in BRCA1 and BRCA2*. Meeting on Critical Assessment of Genome Interpretation (CAGI), Berlin, Germany
66. Jul. 19, 2013 *Autophosphorylation complexes in crystals of protein kinases*. 3DSIG: Structural Bioinformatics and Computational Biophysics Meeting, Berlin, Germany
67. Nov. 7, 2013 *Computational design of antibodies*. University of Pennsylvania Department of Biochemistry and Molecular Biophysics Annual Retreat, Skytop, PA
68. Dec. 5, 2013 *Statistical Analysis of Protein Structures: Backbone Conformations, Side-Chain Rotamers, Antibodies, and Protein-Protein Interfaces*. ZING Conference on Protein and RNA Structure Prediction, 2013. Xcaret, Mexico
69. Dec. 11, 2013 *New methods for computational antibody design*. IBC Annual Meeting of the Antibody Society/Antibody Engineering and Therapeutics, Huntington Beach, CA
70. Jan. 14, 2014 *Structural bioinformatics and computational antibody design*. Symposium on antibody structure prediction and design. Institute for Protein Research, Osaka University, Osaka, Japan
71. Mar. 13, 2014 *Structural bioinformatics and protein structure prediction*. Department of Chemistry, Temple University, Philadelphia, PA
72. May 19, 2014 *Structural bioinformatics and protein structure prediction*. Ort Braude College, Karmi'el, Israel
73. May 20, 2014 *Structural bioinformatics and computational antibody design*. Department of Microbiology and Molecular Genetics, The Hebrew University of Jerusalem, Jerusalem, Israel
74. May 21, 2014 *Structural bioinformatics for protein structure prediction and design*. Edmund J. Safra Center for Bioinformatics Distinguished Speaker Series, Tel Aviv University, Tel Aviv, Israel
75. May 27, 2014 *Structural bioinformatics for protein structure prediction and design*.

Department of Structural Biology, Weizmann Institute, Rehovot, Israel

76. Jun. 1, 2014 *Structural bioinformatics of protein-protein interactions*. Faculty of Agriculture, the Hebrew University of Jersusalem, Rehovot, Israel
77. Jul. 11, 2014 *Structural bioinformatics and computational antibody design*. Keynote lecture, 3DSIG: Structural Bioinformatics and Computational Biophysics Meeting, Boston, MA
78. Jul. 13, 2014 *Nobel Prize Celebration: A personal perspective on Martin Karplus' lasting influence on my career in science*. Special Talk, Meeting on Intelligent Systems in Molecular Biology (ISMB), Boston, MA
79. Aug. 5, 2014 *The structures of biological assemblies and predicting the effects of missense mutations*. Gordon Research Conference on Single Nucleotide Polymorphisms and Disease, Stonehill College, Easton, MA
80. Oct. 23, 2014 *The structures of biological assemblies and predicting the effects of missense mutations*. Meeting on Modeling of Protein Interactions, University of Kansas, Lawrence, KS
81. Nov. 10, 2014 *Structural bioinformatics and protein structure prediction*. University of Texas Southwestern Medical Center, Dallas, TX
82. Dec. 9, 2014 *Assessment of template-based modeling*. 11th Meeting on the Critical Assessment of Protein Structure Prediction, Riviera Maya, Mexico
83. Dec. 9, 2014 *Assessment of biological implications of structure predictions in CASP11.* 11th Meeting on the Critical Assessment of Protein Structure Prediction, Riviera Maya, Mexico
84. Dec. 10, 2014 *Assessment of protein structure prediction refinement methods*. 11th Meeting on the Critical Assessment of Protein Structure Prediction, Riviera Maya, Mexico
85. Mar. 12, 2015 *Structural bioinformatics for protein structure prediction and design.* Biogen IDEC, Cambridge, MA
86. Jan. 26, 2016. *Autophosphorylation complexes of protein kinases.* Computational and experimental interfaces of Big Data and Biotechnology. King Abdullah University of Science and Technology (KAUST), Jeddah, Saudi Arabia
87. May 17, 2016 *Three-dimensional structures of autophosphorylation complexes in crystals of protein kinases*. University City Science Center, Philadelphia, PA
88. May 19, 2016 *Optimizing and assessing computational antibody design with a unique risk-ratio metric for recovering native CDR sequences and structures*. America's Antibody Congress, Terrapin Inc., San Diego, CA