

# Robert L. Jernigan

Baker Center for Bioinformatics and Computational Biology  
Plant Sciences Institute  
112 Office and Laboratory Building  
Iowa State University  
Ames, Iowa 50011-3020  
515-294-3833

## Education

- 1963* – B.S. in Chemistry, California Institute of Technology
- 1968* – Ph.D. in Chemistry, Stanford University  
Thesis on Statistical Mechanics of Polymers.  
Advisor: P. J. Flory (Nobel Laureate)
- 1968* – Postdoctoral Fellow, Stanford University, with P. J. Flory
- 1968* – *1970* NIH Postdoctoral Fellow, University of California, San Diego, with B. H. Zimm
- 1970* – *1974* Senior Staff Fellow, Physical Sciences Laboratory, Division of Computer Research and Technology, National Institutes of Health
- 1974* – *1975* Senior Staff Fellow, Laboratory of Theoretical Biology, National Cancer Institute, National Institutes of Health

## Professional Positions

- 1975* – *2002* Physical Chemist, Laboratory of Experimental and Computational Biology, National Cancer Institute, National Institutes of Health
- 1989* – *2002* Deputy Chief, Laboratory of Experimental and Computational Biology
- 1992* – *2002* Chief, Section on Molecular Structure
- 2002* – *Pres.* Director, Laurence H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University
- 2002* – *Pres.* Professor, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University

## Committees

- 1984* – *1988* Chairman, NIH Advisory Committee on Computer Usage
- 1989* – *2002* Time Allocation Group for supercomputer time at the Advanced Scientific Computing Laboratory, FCRDC, Frederick
- 1989* – *2002* NCI-Advanced Scientific Computing Laboratory Coordination Group
- 1993* – *1998*, *2000* – *2002* NIH Inter-Institute Structural Biology Steering Group

- 1993 – 2002 Resource Advisory Committee for Parallel Processing Resource, Cornell University Theory Center
- 1994 – Award Committee - Biophysical Society
- 1995 – 1997 NIH Telecommunications Committee
- 1995 – Pres. Editorial Advisory Board of Journal *Biochemistry*
- 2001 – Pres. Publications Committee, Biophysical Society overseeing Biophysical Journal
- 2003 – Pres. Chairman, Publications Committee, Biophysical Society
- 2003 – 2008- Editorial Advisory Board of Journal of Biological Chemistry
- 2002 – Pres. Plant Sciences Institute Council, Iowa State University
- 2002 – Pres. Supervisory Committee, Bioinformatics and Computational Biology Program
- 2003 – Pres. Biochemistry, Biophysics and Molecular Biology Department - Computing Committee
- 2005 – National Advisory, Minnesota Supercomputing Institute, Univ. Minn.
- 2005 – Pres. - External Advisory Committee, Tuskegee University (NSF HBCU-HP)

### Professional Memberships

American Association for the Advancement of Science  
 American Chemical Society  
 Biophysical Society  
 Protein Society  
 American Society for Biochemistry and Molecular Biology  
 International Society for Computational Biology

### Awards

NIH Special Achievement Cash Award 1982

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Calculations of Preferred Ligands of the HIV-1 Protease Surface", 1990-1 and 1991-2

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Enzyme Binding Sites for Peptides", 1992-3; 1993-1994

Grant from United States-Israel Binational Science Foundation "Structure and Sequence Variability Evaluated with a Computer-Vision Method" (#91-00219) 1992-1995 (with R. Nussinov)

EEO Officers Recognition Award, 1993

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Improving Peptide Inhibitors for Receptor Targets", 1994-5, 1995-6

NIH Merit Award, 1995 *"in recognition of research contributions on protein and nucleic acid structures leading to deeper comprehension of conformations and biological functions"*

Grant, United States-Israel Binational Science Foundation “Probing Immunoglobulin Polyreactivity via Highly Efficient Docking, Fold Recognition and Kinetics” 1997-2000 (with R. Nussinov and H. Woolfson)

Grant, NATO Collaborative Research Grants Programme, 1996-1997 (with I. Bahar)

Fellow, The Institute for Advanced Studies, Hebrew University, Jerusalem, 1998-1999

Grant, “Deriving Structures for Lead Drug Discovery from Cell-Line Screens”, DAMD17-98-1-8323, US Army Breast Cancer 1998-2001

Fellow, AAAS, 1999- Pres.

NIH-NSF Grant - BBSI: Summer Institute in Bioinformatics and Computational Biology (2002-2006) \$645,000

NIH Grant - Discovering Protein Sequence Structure Function Relationships (2003-2007) \$1,022,000

NIH Grant - Coarse-Grained Models of Protein (2004-2008) \$1,168,000

Sun Microsystems - Academic Equipment Grant (2004) \$86,880

NSF Grant - CNS MRI: Acquisition of a 512-node BlueGene/L Supercomputer for Large-Scale Applications in Genomics and Systems Biology (2005-2008) \$645,000

NIH - Modeling Ribosomal Control, Function and Assembly (2007-2011) \$1,060,380

NIH-NSF Grant - BBSI: Summer Institute in Bioinformatics and Computational Biology (2006-2008) \$499,999

10<sup>th</sup> most cited paper in the journal *Macromolecules*  
[http://pubs.acs.org/journals/mamobx/promo/40th/most\\_cited.html](http://pubs.acs.org/journals/mamobx/promo/40th/most_cited.html)

ISU - Center for Integrated Animal Genomics - Comparative Genomics to Improve Livestock Gene Annotations (2007-2009) \$100,000

## Interests

Elucidation of the molecular details of biochemical and biophysical processes through the study of macromolecular conformations

Computer modeling and simulations

Development of coarse-grained structural principles

Application of advanced computing to molecular calculations

Protein and Cell Engineering and drug design

Development of a combined experimental and theoretical methods to elucidate structures of proteins and nucleic acids

Computer simulations of protein and RNA folding. Conformation enumeration of all chain tracings in restricted space of a given shape

Effects of external conditions, including solvent and temperature, on the relative stabilities of macromolecular conformations

Molecular interactions, recognition and specificity

Nucleic acid conformational properties and their relationship to function, recombination and regulation

Utilizing sequence similarities in conformational calculations

Conformational transitions between ordered and disordered states, and between various ordered states

Molecular visualization

Dynamics of complex molecular assemblages, with the goal of constructing models of cellular processes such as mitosis

Understanding protein sequence through structure

Gene annotation through structural modeling

Genome comparisons

Bioinformatics methods

Systems Biology

**Scientific  
Accomplishments**

Methods for averaging over conformations of flexible macromolecules

Dynamic programming to choose optimum combination of protein secondary structures

Matrix methods for calculating electro-optic properties

Equilibrium pathway model for protein folding

Coarse graining of structures

Residue-residue interaction energies for proteins

Demonstration of weaker base pairings within promoter sequences

Large conformational fluctuations for different DNA sequences

Solvation model including structural water bridges

Calculation of sequence dependence of DNA double helix preferences for forms A or B

Generating and counting large numbers of diverse chain tracings for proteins and nucleic acids

Demonstration that intra-molecular interactions and solvation effects favor observed sequence dependences of DNA double helix groove variabilities

Derivation of amino acid substitution matrix from crystal structures

Treating RNA folding in three dimensions by generating chain tracings on lattice points

Treating peptide binding to surfaces of other macromolecules by generating peptide conformations on neighboring lattice sites

Modeling the bending of nucleic acid double helices around proteins

Calculations of favorable conformations of peptides and agreeing with NMR results

Description of TATA sequence box as a "swivel joint"

Identifying specific interacting pairs in a protein to effect conformational

changes

Discovery of unique base triplets, with implications for recombination and replication

Discovery of high regularity of coordination geometry of protein ligands around cations

Established correlations between fluctuations in coarse-grained proteins and X-ray temperature factors and hydrogen exchange protection

Development of regular lattice from observed packing in protein crystals

Elastic networks and normal mode analyses to identify functional motions of coarse-grained proteins

Development of methods to calculate large scale motions in proteins

Establishing a connection between largest scale motions in Reverse Transcriptase and the nucleic acid processing steps

Identifying “wobble” motions in tubulin, related to its behavior

Identifying critical cavity surface changes arising from GroEL/GroES motions

Identifying critical motions of the ribosome and relating them to translocation

Networks as unifying models in biology

Systems biology applications of networks

Comprehending the highly coordinated motions of the ribosome

### Meetings Organized

1990 – Organizer of Workshop in NIH Research Festival on Nucleic Acid-Protein Interactions

1990 – Co-organizer with H. Scheraga of Cold Spring Harbor Conference on Computational Aspects of Protein Folding

1992 – Co-organizer of NSF Molecular Dynamics Conference (Puerto Rico)

1992 – Co-organizer of Workshop for NIH Research Festival on Structure Prediction with S. Bryant

1992 – Co-organizer of Nucleic Acid Conference with V. SasiSekharan, N. Leonard (Fogarty Scholars-in-Residence) and H. T. Miles

1993 – Program Committee, Biophysical Society National Meeting

1993 – Program Chair, NIH Inter-Institute Structural Biology Group

1994 – Co-organizer of Cold Spring Harbor Meeting - Protein Folding and Design

1994 – Co-organizer of Conference, "Frontiers in Biological Physics", La Jolla International School of Physics, The Institute for Advanced Physics Studies

1999 – Organizing Committee, Eleventh Conversation in Biomolecular Stereodynamics

2001 – Organizing Committee, 12<sup>th</sup> Conversation in Biomolecular Stereodynamics

2003 - Iowa Bioinformatics Workshop

2003 - Organizing Committee, 13<sup>th</sup> Conversation in Biomolecular Stereodynamics

2004 - Iowa Bioinformatics Workshop

2005 - Organizing Committee, 14<sup>th</sup> Conversation in Biomolecular Stereodynamics

2005 - Iowa Bioinformatics Workshop

2005 - Integration of Structural and Functional Genomic, ISU  
 2006 - Steenbock Symposium on Dynamics of Proteins and Macromolecular Assemblies, Madison, WI

### Theses

1987 – Regine Bohacek - Chemistry Department, Rutgers University  
 1991 – David Bisant - Genetics Program, George Washington University  
 2000–2001 – Isabelle Soury-Lavergne - Ecole Normal, Paris  
 2002 – Committee of Sangyoon Lee - Johns Hopkins University, School of Engineering  
 2004 – Moon-ki Kim - Johns Hopkins University, School of Engineering  
 2005 - Haitao Cheng -M.S., Computer Science, ISU  
 2006 - Peter Vedell - Ph.D., Mathematics and Bioinformatics and Computational Biology, ISU  
 Currently - Five Ph.D. graduate students at Iowa State University

### Presentations and Invitations - last 10 years

1996 – Invitation to speak, Computational Aspects of the Human Genome Project, Israel

1996 – Invited Speaker, Telluride Workshop on Structure and Dynamics of Biophysical and Condensed Matter Systems

1996 – Invited Speaker, Fall Chemistry Colloquium Series, Boston University

1996 – Invited Speaker, Molecular Graphics and Modeling Society Electronic Symposium

1996 – Invited Speaker, Symposium on Protein Folding Methods, Chapel Hill, NC

1997 – Invited Speaker, American Chemical Society Symposium on Molecular Modeling of Biological Systems Polymers

1997 – Invited Speaker, Theoretical Chemistry in Biology, Satellite Symposium Int. Congress of Quantum Chemistry, Savannah

1997 – Invited Speaker, Structural Biology Symposium, Cornell University

1998 – Invited Speaker, Biophysical Society, Kansas City, Symposium, Bioinformatics: Computer-Based Predictions of Protein Structure and Binding

1998 – Invitation to speak, “Protein Structure, Stability, and Folding. Fundamental and Medical Aspects”, Moscow

1998 – Invited Speaker, Symposium for New Center for Structural Biology, Tel Aviv University

1998 – Invited Speaker, Washington University, St. Louis

1998 – Invited Speaker, Weizmann Institute, Rehovot, Israel

1998 – Invited Speaker, Structural Biology Seminar, University of California, Berkeley

1999 – Plenary Lecturer – Conversation on Biomolecular Structure and Dynamics, Albany, NY

- 1999 – Invited Speaker, Proteins Gordon Conference, Holderness College, NH
- 1999 – Invited Speaker, University of California, San Francisco
- 1999 – Invited Speaker, Second Congress of Biophysicists of Russia, Moscow
- 1999 – Invited Speaker, Russian Biophysics Congress, Ptitsyn Memorial Symposium, Pushchino, Russia
- 1999 – Invited Speaker, Department of Chemistry, Pennsylvania State University
- 1999 – Invited Speaker, Department of Biological Chemistry, State University of New York, Stony Brook
- 2000 – Invited Speaker, MPSA 2000, Methods of Protein Structure Analysis, Charlottesville, VA
- 2000 – Invited Speaker, Danforth Plant Science Center and Washington University, St. Louis
- 2001 – Chair, Conversation on Biomolecular Structure and Dynamics, Albany, NY
- 2001 – Invited Speaker, “Protein folding, structure and design”, International Center for Theoretical Physics, Trieste, Italy
- 2001 – Invited Speaker, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University
- 2001 – Invited Speaker, Laboratory of Chemical Physics, NIDDK, NIH
- 2001 – Invited Speaker, Department of Biochemistry, Texas A&M University
- 2001 – Invited Speaker, Department of Biology, Georgia Tech
- 2001 – Invited Speaker, Department of Chemistry, University of Maryland
- 2001 – Invited Speaker, SUNY Buffalo School of Medicine
- 2001 – Invited Speaker, University of Colorado Health Sciences Center
- 2001 – Invited Speaker, Workshop, “Proteins as Machines”, College Park, MD
- 2001 – Invited Speaker, NEC America
- 2001 – Invited Speaker, Center for Studies in Physics and Biology, Rockefeller University
- 2001 – Invited Speaker, Center for Computational Biology & Bioinformatics, School of Medicine, University of Pittsburgh
- 2002 – Invited Speaker, Laboratory of Molecular Biology, National Cancer Institute

- 2002 – Invited Speaker, School of Engineering, Johns Hopkins University
- 2002 – Plenary Speaker, Joint Conference on Information Sciences, Durham, NC
- 2002 – Invited Speaker, “Proteomes: Structures, Changes, Interactions and Functions”, Ames, Iowa
- 2002 - Invited Speaker - Polymer Division, American Chemical Society
- 2003 - Invited Speaker - Chemistry Department, Iowa State University
- 2003 - Invited Speaker - Animal Breeding Group -Department of Animal Science, Iowa State University
- 2003 - Seventh Johns Hopkins Folding Meeting
- 2003 - Invited Speaker, Physics Department, Iowa State University
- 2003 - Invited Speaker - “Frontiers of Bioinformatics” Symposium, University of Buffalo, NY
- 2003 - Invited Speaker - “ Modeling of Protein Interactions in Genomes”, SUNY, Stony Brook, NY
- 2004 - Invited Speaker - Polymer Symposium, American Chemical Society, New York
- 2003 - Invited Speaker, Chemical Engineering Department, Iowa State University
- 2003 - Invited Speakers, Physics Department, Iowa State University
- 2004 - Invited Speaker, Center for Computational Biology, Washington University
- 2004 - Invited Speaker, Biomedicine Lecture Series, Des Moines University
- 2004 - Invited Speaker - “Frontiers in Chemistry”, Case Western Reserve University
- 2004 - Invited Speaker - “Interplay between Computer Modeling and Experiments on Complex Biological Systems”, American Chemical Society, Anaheim
- 2004 - Invited Speaker - Department of Biochemistry, Georgetown University Medical School
- 2005 - Invited Speaker - Center for Bioinformatics and Computational Biology, University of Iowa State University
- 2005 - Invited Speaker - Midwest Computational Structural Biology Workshop
- 2005 - Invited Speaker - International Center for Theoretical Physics, Trieste, Italy

2005 -Invited Speaker - Center for Bioinformatics and Computational Biology,  
College of Engineering, University of Iowa

2005 -Invited Speaker - Modeling of Protein Interactions in Genomes,  
Lawrence, KS

2005 - Invited Speaker - International Meeting on Relaxations in Complex  
Systems, Lille, France

2005 - Invited Speaker - Computational Biology Symposium - National Cancer  
Institute, Frederick MD

2005 - Invited Speaker - Large Scale Molecular Dynamics, Nanoscale, and  
Mesoscale Modeling: Bridging the Gap, Symposium, American Chemical  
Society, Washington, DC

2005 - Invited Speaker - Multiscale Workshop, Snowbird, UT

2005 - Invited Speaker - Department of Electrical and Computer Engineering,  
ISU

2005 - Invited Speaker - NIGMS, NIH, Bethesda

2006 - Invited Speaker - Biophysical Society, Workshop on Coarse-Grained  
Methods for Biomolecular Structure and Dynamics, Satl Lake City

2006 - Invited Speaker - Department of Chemistry, University of Oregon,  
Eugene

2006 - Invited Speaker - Workshop on Rigidity, Flexibility, and Motion in  
Biomolecules, Tempe, AZ

2006 - Invited Speaker - Workshop on Nanomechanics of Biomolecules,  
Ascona, ETH Conference, Switzerland

2007 - Nebraska Research and Innovation Conference

2007 - 10<sup>th</sup> International Congress on Amino Acids and Proteins, Kallithea,  
Chalkidiki, Greece

2007 - Symposium on Structural Determination, Refinement and Modeling of  
Large Biomolecular Complexes (ACS Meeting)

## Reviews

### Recent Review Panels:

NIH F04B March 2003, November 2003, March 2004 (Biophysics,  
Biochemistry Fellowships Panel)

NIH Special "Roadmap" Study Section for National Centers, ZRG1 BST-C  
May 2004

NSF Science and Technology Center Site Visit Review Committee, June 2004

NIH Computational Biophysics Study Section, October 2004

Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, December  
2004

NIH Special Study Section, 2005

DOE Early Career Principal Investigator Program, 2006

NSF Bioinformatics Postdoctoral Panel, 2006  
 NIH Special Study Section ZRG1 BCMB-B, 2006  
 Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, 2006

**Journals:** Journal of the American Chemical Society, Journal of Biological Chemistry, Biochimica et Biophysica Acta, Journal of Chemical Physics, Science, Nature, Proceedings of the National Academy of Science USA, Biophysical Chemistry, Journal of Molecular Biology, Macromolecules, Biochemistry, Journal of Polymer Science, Biopolymers, Journal of Biomolecular Structure and Dynamics, FASEB Journal, Chemical Physics, Protein Science, Journal of Mathematical Chemistry, Proteins, Journal of Computer-Aided Molecular Design, Europhysics Letters, Journal of Physical Chemistry, Nucleic Acids Research, Computational Polymer Science, Protein Engineering, Folding & Design, Physical Review, IBM Systems Journal and others

**Student Selection, Faculty Tenure and Search Committees:** Pioneer Fellowship Committee - Iowa State University, many NIH committees, Cornell Univ., Boston University, physics search - Iowa State University, Chief Information and Technology Officer search - Iowa State University, and many other academic promotion and tenure reviews (6 during November 2006)

**Grant Reviews:** NIH Special Study Sections including BST-C-R NIH Study Section - National Centers for Biomedical Computing (2004), BST-C Study Section Special Emphasis Panel on Cryo-electron microscopy (2004), NSF Site Visit Science and Technology Center (2004), F04 NIH Ruth L. Kirschstein National Research Service Application Study Section (2003, 2004), World Bank Panel on Biodiversity (2004), Nebraska Research Initiative (2004), Texas A&M Research Initiative, NSF Frontiers in Physics Review Panel, Genome Research Review Committee (NHGRI), The Wellcome Trust (Joint Infrastructure Fund, UK), NIH Biophysical and Chemical Sciences Review Group, NIH Special Study Sections, Plant Sciences Institute ISU, NSF, NIDA, NIH Program Project Special Study Section, NIH Special Emphasis Panel, NIH Fogarty Scholar-in-Residence Program, DOE, NSF Supercomputer Centers, Advanced Scientific Computing Laboratory - FCRDC, NSF Multidisciplinary Research Review Panel, Packard Foundation, Guggenheim Foundation, Petroleum Research Fund and International Science Foundation, NIH CIT Computational Science and Engineering Program Review and others

#### Research Management

Computational Molecular Biology Research Group Initiated  
 Microarray Research Group Initiated  
 Systems Biology Research Group Initiated  
 Organized Seminar Series  
 Organized Advisory Committee  
 Organized Large Grant Applications

#### Present Funding

NIH R33 GM066387 (PI: Honavar) Discovery of Protein Sequence-Structure-Function Relationships (2003-2007) \$1,022,000  
 NIH R01GM72014 (PI: Jernigan) Coarse Grained Proteins (2004-2008) \$1,168,000  
 NIH-NSF Joint EEC-0608769 (PI: Jernigan) BBSI Bioinformatics and Computational Systems Biology Summer Institute at Iowa State (2006-2009) \$499,999  
 NSF-CNS-0521568 Aluru (PI: Aluru) MRI: Acquisition of a 512-node BlueGene/L Supercomputer for Large-Scale Applications in Genomics

and Systems Biology (2005-2008) \$600,000  
NIH R01GM073095 (PI: Jernigan) Modeling Ribosomal Control, Function and  
Assembly, (2006-2010) \$1,060,380  
ISU - Center for Integrated Animal Genomics (PI: Jernigan) Comparative  
Genomics to Improve Livestock Gene Annotations (2007-2009)  
\$100,000