

## Curriculum Vitae

JEFFREY SKOLNICK, Ph.D.

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**EDUCATION:** B.A. in Chemistry, Summa Cum Laude,  
Washington University, St. Louis, MO, 1975  
M. Phil. in Chemistry, Yale University, 1977  
with Professor Marshall Fixman  
Ph.D. in Chemistry, Yale University, 1978  
with Professor Marshall Fixman; Ph.D.  
Thesis: "Investigations on a Rod Like Polyelectrolyte Model"

**RESEARCH INTERESTS:** Computational Systems Biology & Bioinformatics including the development of algorithms and their application to proteomes for the prediction of protein structure and function, the prediction of small molecule ligand-protein interactions with applications to drug discovery and the prediction of off-target uses of existing drugs with applications to aging, cancer and chronic fatigue syndrome, cancer metabolomics, precision medicine, fundamental studies on the nature and completeness of protein structure space and the exploration of the interplay between protein physics and evolution in determining protein structure and function, prediction of protein-protein and protein-DNA interactions, and molecular simulations of subcellular processes.

### PROFESSIONAL EXPERIENCE:

2008-present	Mary and Maisie Gibson Chair in Computational Systems Biology
2006-present	Director, Center for the Study of Systems Biology, Georgia Institute of Technology
2006-present	GRA Eminent Scholar, Computational Systems Biology
2006-present	Professor, School of Biological Sciences, Georgia Institute of Technology
2015-2016	Co-Director, Integrative Biosystems Institute, Georgia Institute of Technology
2010-2015	Director, Integrative Biosystems Institute, Georgia Institute of Technology
2007-2012	Adjunct Professor, School of Chemistry & Biochemistry, Georgia Institute of Technology
2007-2012	Adjunct Professor, College of Computing, Computational Science & Engineering Division, Georgia Institute of Technology
2008-2010	Associate Director, Integrative Biosystems Institute, Georgia Institute of Technology
2002-2005	Director, Buffalo Center of Excellence in Bioinformatics
2002-2005	Professor, Structural Biology, University at Buffalo
1999-2002	Director, Computational/Structural Biology, Danforth Plant Science Center
1999-2002	Adjunct Professor of Biochemistry, Washington University, St. Louis
1998	Member, Advanced Study Institute, The Hebrew University, Jerusalem
1993	Member, Institute of Theoretical Physics, UCSB

1989-1999	Professor, The Scripps Research Institute
1988-1989	Professor of Chemistry, Washington University, St. Louis
1986-1989	Director, Institute of Macromolecular Chemistry
1985-1988	Associate Professor of Chemistry, Washington University, St. Louis
1982-1985	Assistant Professor of Chemistry, Washington University, St. Louis
1979-1982	Assistant Professor of Chemistry, LSU, Baton Rouge, Louisiana
1978-1979	Postdoctoral Research Fellow, Bell Laboratories, Murray Hill, NJ
1976-1978	Research Assistant, Yale University
1975-1976	Teaching Assistant, Yale University

**EDITORIAL BOARDS:**

2017	Co-Guest Editor, <i>Emerging Topics in Life Science</i>
2017-present	Editorial Board, <i>Scientific Reports</i> in the field of Chemical Biology
2016-present	Editorial Board, <i>Journal of Data Mining in Genomics &amp; Proteomics</i>
2015-present	Editorial Board, <i>Computational Drug Discovery</i>
2014	Co-Editor, <i>Israel Journal of Chemistry, Special Volume, 2013 Nobel Prize in Chemistry</i>
2012-2015	Editorial Board, <i>PeerJ</i>
2012-present	Structural Biology Section Editor, <i>Biology Direct</i>
2012-present	Editorial Board, <i>Journal of Metabolomics &amp; Metabolites</i>
2011-present	Editorial Board, <i>Current Bioinformatics</i>
2005-present	Editorial Board, <i>Biology Direct</i>
2005-present	Editorial Board, <i>Protein Science</i>
2003-2007	Editorial Board, <i>Biopolymers</i>
2001-2007	Editorial Board, <i>Applied Genomics and Proteomics</i>
1998-present	Editorial Board, <i>Proteins</i>
1997-2003	Editorial Board, <i>Biophysical Journal</i>
1993-1996	Editorial Board, <i>Journal of Chemical Physics</i>

**PROFESSIONAL SERVICE:**

2017	Ad hoc Member, NIH MSFD Study Section
2017	Ad hoc Member and Alternate Chair, NIH MIRA for New and Early Stage Investigators Study Section
2016-present	External Scientific Advisory Committee, Cancer Systems Therapeutics (CaST), Columbia University
2016	Ad hoc Member, NIH K99 Pathway to Independence Study Section
2016	Faculty Member, Theory & Simulation, Structural Biology Faculty, F1000 Faculty
2016	Ad hoc Member, NIH MIRA for New and Early Stage Investigators Study Section
2015-present	Member, International Advisory Board of the Drug Discovery & Therapy World Congress 2016 & 2017
2015	Chair, NIH Special Study Section: MSFC - Macromolecular Structure and Function C Study Section
2015	Ad hoc Member, NIH R21 Glycan Tools Study Section
2014	Program Committee Member, ISMB 2014
2014	Program Committee Co-Chair, Biopolymers <i>in vivo</i> Subgroup, Biophysical Society
2013	Member, NRC Committee for Anton Proposal Review
2013	NIH Special Study Section, ZRG1 IMST-G (11), Small Business Biological Chemistry, Biophysics and Drug Discovery
2011	Chair, NIH Special Study Section
2010-2012	Advisory Board Member, UIUC NIH Research Resource

2010	Member, Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics
2010	External Reviewer, Computational Biology Initiative, George Washington University
2010	Chair, Two NIH Special Study Sections
2010-present	Member, NIH College of Scientific Reviewers
2009-present	Ad hoc Member, NIH MSFD Study Section
2006-2008	Chair, NIH MSFB Study Section
2007	Member, Israel Cancer Research Fund's Scientific Review Panel
2004-2007	Member, Advisory Committee of the National Research Program for Genomic Medicine of Taiwan
2004-2007	Advisory Board Member, NIH Resource for Macromolecular Modeling and Bioinformatics
2004-2007	Member, Biophysical Society Publications Committee
2004-2006	Board Member, Great Lakes Bioinformatics Consortium
2004-2006	Member, Northeast Biodefense Center Governing Council
2004	Chairman, Advisory Board, University of Illinois, Urbana-Champaign, NIH Research Resource for Macromolecular Modeling and Bioinformatics
2002-2005	Nominations Committee, Protein Society
2001-2004	Member, Scientific Advisory Board of the Proteome Society
2000-2004	Member, NIH BCCA Study Section
1989-1990	Member, Two NIH Special Study Sections
1999	Scientific Founder, Geneformatics
1999	Chairman, Advisory Boards of Cornell and University of Illinois, Urbana-Champaign NIH Research Resources
1997	Advisory Board Member of the NIH Parallel Processing Resource for Biomedical Scientists at the Cornell Theory Center at Cornell University
1998	Advisory Board Member of the NIH Resource for Macromolecular Modeling and Bioinformatics at the University of Illinois, Urbana-Champaign, Illinois
1999	Member, 4 NIH Special Study Sections
1998	Member, 3 NIH Special Study Sections
1997	Member, 2 NIH Special Study Sections
1996	Ad hoc Member NIH BCCA Study Section & Member, NIH Special Study Section
1993	Chairman, NIH Special Study Section; Member on 3 NIH Special Study Sections
1991	Member of 2, Chairman of 1, NIH Special Study Sections; Review Panel for Division of Computer Research & Technology
1990	Member, 2 NIH Special Study Sections
1988-1990	NSF Graduate Fellowship Evaluation Panel in Chemistry

#### **HONORS AND AWARDS:**

2014	Southeastern Universities Research Association (SURA), Distinguished Scientist Award
2004	Biophysical Society Fellow
2003	Stockton Kimball Award, University at Buffalo, Medical Alumni Award
2002	Joseph F. Foster Lecturer, Purdue University
2001	Fellow Academy of Science of St. Louis
2001	American Association for the Advancement of Science Fellow
1983	Alfred P. Sloan Foundation Research Fellow
1978	Richard Wolfgang Memorial Prize for the Most Outstanding Graduate Student in Chemistry, Yale University
1975	Summa Cum Laude, Washington University

1975 John W. Sowden Prize for Outstanding Work in Chemistry, Washington Univ.  
 1971-1975 University Scholar at Washington University

#### MEMBERSHIP IN SCIENTIFIC SOCIETIES:

American Association for the Advancement of Science  
 American Chemical Society  
 Biophysical Society  
 Protein Society

#### REFeree FOR THE FOLLOWING JOURNALS:

Biochemistry	Journal of Molecular Biology
Bioinformatics	Journal of Molecular Evolution
Biophysical Journal	Journal of Physical Chemistry
Biopolymers	Journal of Polymer Science
Chemical Physics Letters	Macromolecules
FASEB	Nature
International Journal of Biological Macromolecules	Protein Science
Journal of the American Chemical Society	Proteins
Journal of Chemical Physics	Science

#### CURRENT GRANT SUPPORT

NIH R35 GM118039 (Skolnick, PI)	5/6/16-4/30/21	Direct Costs	\$310,340/year
Title: Interplay of inherent promiscuity and specificity in protein biochemical function with applications to drug discovery and exome analysis			
UCB Pharma (Skolnick, PI)	6/1/16-5/31/17	Direct Costs	\$62,393/year
Title: Novel approaches to improved virtual screening			
Amgen Inc. (Skolnick, PI)	8/1/16-2/22/17	Direct Costs	\$12,210/year
Title: Virtual Screening of HIGLYRA1 proteins by FINDSITE and PoLi.			

#### GRADUATE STUDENTS AND POSTDOCTORAL SCHOLARS:

Total number of Post-docs: 58

S. Tonddast-Navaei	2014-2017	
B. Srinivasan	2012-2017	Postdoctoral Fellow, Instituto Gulbenkian de Ciencia, Portugal
A. Roy	2012-2015	Research Scientist, Vertex Pharmaceuticals
S. Chaudhury	2014-2015	Senior Consultant, Life Sciences at IBM
S. Mukherjee	2013-2015	Data Scientist, Flipkart
A. Hussain	2012-2014	
J. Grahnen	2012-2013	Data Scientist, Capella Biosciences
N. Kumar	2010-2012	Postdoctoral Computational Biologist, National Institute of Immunology, Delhi, India
A. Freed	2011-2012	Senior Analyst, Laureate International Universities
T. Ando	2008-2012	Junior Associate Professor, Tokyo University of Science, Japan
M. Baxa	2010-2011	Staff Scientist, The University of Chicago
A. Guerler	2010-2011	Senior Software Engineer, John Hopkins University
M. Gao	2006-2011	Research Scientist II, Georgia Institute of Technology
S. Lee	2005-2010	Research Engineer, LG Chemical Ltd.

S. B. Pandit	2004-2009	Assistant Professor, Indian Institutes of Science Education and Research (IISER)
L. Wroblewska	2008-2008	Senior Scientist, Pfizer
A. Jagielska	2005-2008	Research Scientist, Massachusetts Institute of Technology
M. Brylinski	2006-2008	Assistant Professor, Louisiana State University
J. Borreguero	2005-2008	Scientific Software Engineer, Oakridge National Laboratory
Y. Huang	2005-2008	Bioinformatics Scientist, Regeneron Pharmaceuticals
D. Ivankov	2007-2008	Postdoctoral Researcher, Center for Genomic Regulation, Barcelona, Spain
R. Kim	2005-2008	Scientist, In Silico Solutions
H. Chen	2005-2007	Principal Scientist - Bioinformatics, Pfizer
D. K.C.	2006-2007	Assistant Professor and Graduate Coordinator, North Carolina A&T State University
M. DeVries	2004-2006	Software Engineer, Plexcan Inc.
P. Rotkiewicz	2003-2005	Principal Scientist, Schrodinger
W. Tian	2004-2005	Professor, Institute of Biostatistics, School of Life Sciences, Fudan University
A. Szilagyi	2002-2005	Senior Research Fellow, Institute of Enzymology, Hungarian Academy of Sciences
O. Zimmerman	2003-2005	Staff Member, Jülich Supercomputing Centre
V. Grimm	2003-2005	Projekträger Jülich, Forschungszentrum Jülich
W. Li	2001-2004	
H. Zhou	2005-present	Research Scientist II, Georgia Institute of Technology
A. K. Arakaki	2005-2009	Deceased
E. Bindewald	2001-2004	Senior Computational Scientist; Section Lead Nanotechnology and Structural Biology, Leidos Biomedical Research, Inc. and Adjunct Faculty, Department of Mathematics at Frederick Community College
P. Xavier	2002-2004	Staff Scientist - Corporate Research & Innovation, Computing & Modeling, SABIC, Saudi Arabia
Y. Zhang	2001-2003	Professor, University of Michigan
T-L. Chiu	1999-2001	Research Associate, University of Minnesota
H. Lu	1999-2002	Associate Professor, University of Illinois at Chicago
D. Kihara	1999-2003	Professor, Purdue University
Y. Bukhman	1998-2001	Associate Scientist, Great Lakes Bioenergy Research Center, University of Wisconsin – Madison
M. Betancourt	1999-2001	Assistant Professor, Borough of Manhattan Community College
M. Wojciechowski	1999-2001	Postdoctoral Fellow, International Institute of Molecular and Cell Biology, Warsaw
D. Mohanty	1997-1998	Staff Scientist - VII, National Institute of Immunology, New Delhi, India
B. Reva	1997-1998	Associate Professor, Icahn School of Medicine at Mount Sinai
L. Zhang	1996-1998	Associate Professor, MD Anderson
W-P. Hu	1995-1997	Professor, National Chung Cheng University, Taiwan

A. Ortiz	1996-1998	Deceased
S. DeBolt	1994-1996	Scientist, Agouron
M. Milik	1992-1997	Head of Computational Chemistry, Selvita
K. Olszewski	1994-1996	Sr. Bioinformatics Scientist, Pathwork Diagnostics
A. Rey	1991-1993	Professor of Chemistry, University of Madrid
A. Godzik	1991-1993	Professor, The Stanford/Burnham Institute
G. Nielsen	1989-1990	
T. Yeates	1988-1989	China Lake Naval Research Laboratory
A. Sikorski	1987-1989	Professor, University of Warsaw
B. Pant	1987	Manager Technical, Magnetic and Pressure Sensor Development Group, Honeywell Aerospace
A. Kolinski	1985-1987	Professor, University of Warsaw
D. Perchak	1984-1987	Senior Research Scientist, Eastman Kodak Company

Total number of Ph.D. students: 4

L. Wroblewska	2003-2007	Senior Scientist, Pfizer
W. Tian	1999-2004	Professor, Institute of Biostatistics, School of Life Sciences, Fudan University
L. Lu	1999-2003	Associate Professor, Division of Biomedical Informatics, Cincinnati Children's Hospital Medical Center
M. Vieth	1995	Senior Research Advisor, Eli Lilly and Company

Total number of M.A. students: None

#### INVITED TALKS:

2017	Seminar, Amgen Inc., November 3, Boston, MA
2017	Georgia Bio Innovation Summit, October 24, Atlanta, GA
2017	NIH NCATS Automated Chemical Synthesis Workshop, October 19-20, Bethesda, MD
2017	Seminar, Morehouse School of Medicine, September 5, Atlanta, GA
2017	Seminar, Data-X Seminar Series, Lehigh University, April 19, Bethlehem, PA
2017	“Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling” 253rd ACS National Meeting, April 5, San Francisco, CA
2016	Modeling of Protein Interactions (MPI 2016), October 26-28, Lawrence, KS
2016	Seminar, School of Materials Science & Engineering Seminar Series, Georgia Tech, October 24, Atlanta, GA
2016	Seminar, Laufer Center for Physical and Quantitative Biology, Stony Brook University, October 21, Stony Brook, NY
2016	Innovations in the Management of Locally Advanced Pancreatic Cancer Symposium, Cancer Treatment Centers of America, September 23, Newnan, Georgia
2016	Plenary Lecture, Drug Discovery and Therapy World Congress 2016 / Global Biotechnology Congress 2016, August 25, Boston, MA
2016	Keynote Forum, 6 <sup>th</sup> International Conference On Structural Biology, August 22, New Orleans, LA
2016	17th Tetrahedron Symposium, June 29 – July 1, Sitges, Spain
2016	Seminar, Department of Biochemistry Seminar Series, Emory University, May 5, Atlanta, GA
2016	Seminar, St. Jude Children’s Research Hospital, May 3, Memphis, TN
2016	Seminar, Institute for Applied life Sciences (IALS), University of Massachusetts,

- Amherst, April 26, Amherst, MA
- 2016 Panelist, UCB Supernetworks Conference 2016, April 14-15, Reading, United Kingdom
- 2016 Seminar, UCB Slough Research Site, April 13, Berkshire, United Kingdom
- 2016 “From Dynamics to Function and Back Again: Adventures in Simulating Biomolecules”, Charlie Brooks, 60th Birthday Celebration, 251st ACS National Meeting and Exposition, March 13, San Diego, CA
- 2015 Seminar, Center for Diagnostics and Therapeutics Seminar Series, Georgia State University, December 8, Atlanta, GA
- 2015 Seminar, Grace Wilsey Foundation Principal Investigators Meeting, December 5, San Francisco, CA
- 2015 Seminar, Integrated Cancer Research Center Series, Georgia Tech, October 20, Atlanta, GA
- 2015 Panelist, Health Connect South Symposium, September 16, Atlanta, GA
- 2015 Keynote Speech, Workshop on Genomics and Metagenomics Data Mining, September 9, Atlanta, GA
- 2015 2015 Shanghai International Symposium on Frontiers in Computational Chemistry, NYU Shanghai, August 23 – 26, Shanghai, China
- 2015 Drug Discovery and Therapy World Congress 2015 / Global Biotechnology Congress 2015, July 22 – 25, Boston, MA
- 2015 Albany Conversation, June 9 – 13, Albany, NY
- 2015 Seminar, Revolution Medicines, April 22, Redwood City, CA
- 2015 Grace Wilsey Foundation Inaugural Scientific Conference, March 20, Palo Alto, CA
- 2014 Panelist, Renaissance Weekend, December 28 – January 1, Charleston, SC
- 2014 BioPharm America, September 24, Boston, MA
- 2014 14<sup>th</sup> KIAS Conference on Protein Structure and Function, September 17 – 20, Seoul South Korea
- 2014 J. Clarence Karcher Lecture, September 5, Norman, OK
- 2014 ISMB 3DSig, July 10 – 13, Boston, MA
- 2014 Epilepsy Pipeline Conference, June 4 – 7, San Francisco, CA
- 2014 Seminar, National Academy of Science, May 9, Washington, DC
- 2014 American Academy of Neurology 66<sup>th</sup> Annual Meeting, April 29 – 30, Philadelphia, PA
- 2014 Biophysics Day, University of Texas at Austin, April 7, Austin, TX
- 2014 Seminar, Vertex Pharmaceuticals, February 21, Boston, MA
- 2014 Seminar, Indiana University School of Medicine, February 19, Indianapolis, IN
- 2014 Seminar, Dart NeuroScience, LLC, February 7, San Diego, CA
- 2013 Seminars, School of Mathematics and School of Chemistry, The University of Edinburgh, November 12 – 16, Edinburgh, United Kingdom
- 2013 27<sup>th</sup> Annual Symposium of the Protein Society, July 20 – 22, Boston, MA
- 2013 Seminar, California Institute for Quantitative Biosciences (QB3) and Integrative Program in Quantitative Biology (iPQB) Invitational Speaker Series, University of California, San Francisco, May 16, San Francisco, CA
- 2013 Seminar, Edmond J. Safra Center for Bioinformatics, Tel Aviv University, May 8, Tel Aviv, Israel
- 2013 Computational Biology: Then and Today, Weizmann Institute of Science, May 6 – 9, Rehovot, Israel
- 2013 Frontiers in Systems and Synthetic Biology, March 20 – 24, Atlanta, GA
- 2013 Seminar, University of Georgia Center for Drug Discovery, March 18, Athens, GA
- 2012 Panelist, Renaissance Weekend, December 28 – January 1, Charleston, SC
- 2012 Seminar, University of Southern California, November 15, Los Angeles, CA
- 2012 Modeling of Protein Interactions (MPI 2012), November 8 – 10, Lawrence, KS
- 2012 ACS National Meeting: Materials for Health and Medicine – Simulations of crowding Confinement and Cellular Environments, August 20 – 22, Philadelphia, PA

- 2012 Centre Européen de Calcul Atomique et Moléculaire (CECAM) Workshop: "Towards in silico biological cell: Bridging experiments and simulations", July 8 – 11, Lausanne, Switzerland
- 2012 Molecular Crowding: Chemistry and Physics Meet Biology, June 10 – 14, Ascona, Switzerland
- 2012 Physics, Chemistry, and Biology of Membrane Proteins, May 14 – 16, Tempe, AZ
- 2011 Seminar, Center for Bioinformatics, The University of Kansas, November 21, Lawrence, KS
- 2011 Keynote Address, IEEE International Conference on Bioinformatics and Biomedicine (BIBM), November 14, Atlanta, GA
- 2011 Seminar, Molecular Biophysics Graduate Portfolio Seminar Series, The University of Texas at Austin, November 7, Austin, TX
- 2011 Seminar, Center for Computational Medicine & Bioinformatics, The University of Michigan, November 1, Ann Arbor, MI
- 2011 5th Drug Design and Medicinal Chemistry Conference, October 20 – 22, San Diego, CA
- 2011 Biomedical Engineering Seminar Series, Boston University, September 28, Boston, MA
- 2011 Scheraga 90<sup>th</sup> Birthday Symposium, Cornell University, September 24, Ithaca, NY
- 2011 ACS National Meeting: "Predicting and Disrupting Protein Interactions", August 30 – September 2, Denver, CO
- 2011 From Computational Biophysics to Systems Biology (CBSB11), Celebrating Harold Scheraga's forthcoming 90<sup>th</sup> Birthday, July 20 – 22, Juelich, Germany
- 2011 Macromolecular Crowding, Telluride Science Research Center, June 20 – 24, Telluride, CO
- 2011 Modeling Biomolecular Structures, Interactions and Functions, Telluride Science Research Center, June 13 – 17, Telluride, CO
- 2011 Third Annual Kinase Inhibitor Chemistry: Charting the Chemical Space, April 13 – 14, San Diego, CA
- 2011 American Physical Society Meeting, March 21 – 25, Dallas, TX
- 2011 Colloquium Presentation, Department of Chemistry, University of Cincinnati, February 18, Cincinnati, OH
- 2010 Seminar, Weizmann Institute of Science, November 24, Rehovot, Israel
- 2010 Protein Folding and Dynamics: from Experiment to Theory, Telluride Science Research Center, June 21 – 25, Telluride, CO
- 2010 From Computational Biophysics to Systems Biology (CBSB10), June 5 – 7, Traverse City, MI
- 2010 IEEE International Conference on Bioinformatics and Bioengineering (BIBE), Thomas Jefferson University, June 1 – 3, Philadelphia, PA
- 2010 Principles of Advanced and Distributed Simulations (PADS), May 17 – 19, Atlanta, GA
- 2010 Institute for Biophysical Dynamics Seminar, University of Chicago, April 6, Chicago, IL
- 2010 Seminar, Constellation Pharmaceuticals, January 15, Boston, MA
- 2009 Advances in Macromolecular Modeling, AM<sup>3</sup>, November 11 – 14, Austin, TX
- 2009 Beckman Institute 20<sup>th</sup> Anniversary Symposium, September 21 – 23, Urbana-Champaign, IL
- 2009 CECAM "Coarse-Graining Biological Systems: Towards Large-Scale Interaction and Assembly", September 7 – 10, Lausanne, Switzerland
- 2009 Murray Goodman Symposium, ACS 238<sup>th</sup> National Meeting, August 16 -19, Washington DC
- 2009 20th IEEE International Conference on Application-specific Systems, Architectures and Processors (ASAP 2009), July 6 – 7, Boston, MA
- 2009 Method Development for Protein Structure Predication, Telluride Science Research



- Center, June 14 – 19, Telluride, CO
- 2009 C2B2 Distinguished Speaker Series, Columbia University, April 1, New York, NY
- 2009 Computer-Aided Molecular Design, Zing Conferences, March 18 – 21, Antigua and Barbuda
- 2009 International Conference of the Quantum Bio-Informatics Research Center, ICQBIC2009 March 11 – 13, Chiba, Japan
- 2009 10<sup>th</sup> International Dahlem Symposium on “Signal Recognition and Transduction”, February 25 – 27, Berlin, Germany
- 2009 Clark Atlanta University Seminar Series, February 13, Atlanta, GA
- 2009 International Workshop in Memoriam of Angel Ramirez Ortiz: Structural Bioinformatics and Beyond, January 25 – 27, Madrid, Spain
- 2008 Department of Biochemistry Seminar Series and the Molecular Biophysics Discussion Group, The University of Texas Southwestern Medical Center at Dallas, November 11 – 14, Dallas, TX
- 2008 Frontiers in Multi-Scale Systems Biology Symposium, October 18 – 21, Atlanta, GA
- 2008 Twentieth Annual Harry Allen Symposium, Clark University, October 3<sup>rd</sup>, Worcester, MA
- 2008 6<sup>th</sup> Swiss National Center of Competence in Research (NCCR) – Symposium on New Trends in Structural Biology, September 8 – 9, Zurich, Switzerland
- 2008 236<sup>th</sup> American Chemical Society Meeting – “The Future of Structure-Based Drug Design for GPCR Targets”, August 20, Philadelphia, PA
- 2008 Genetic and Evolutionary Computation Conference (GECCO), July 14, Atlanta, GA
- 2008 Advanced Topics in Cell Model Systems - CMS<sup>3</sup>, June 10 – 14, Rome, Italy
- 2008 DE Shaw & Co. – Seminar Series, April 30, New York, NY
- 2008 3<sup>rd</sup> Annual Computational and Systems Biology Symposium, March 21, Athens, GA
- 2008 International Conference of the Quantum Bio-Informatics Research Center, ICQBIC2008 March 12 – 15, Chiba, Japan
- 2007 NIH Center for Scientific Review Open House Meeting, December 18, Bethesda, MD
- 2007 Joint Carnegie Mellon/University of Pittsburgh Ph.D. Program in Computational Biology Seminar Series, November 9, Pittsburgh, PA
- 2007 MPI 2007 – Modeling of Protein Interactions, September 30 – October 2, Lawrence, KS
- 2007 234<sup>th</sup> American Chemical Society National Meeting, August 19 – 23, Boston, MA
- 2007 Gordon Conference on Structural Functional & Evolutionary Genomics, July 28 – August 3, Hinxton, UK
- 2007 Canadian Proteomics Initiative - CPI 2007, June 17 – 19, Ottawa, Canada
- 2007 9<sup>th</sup> Northern European Bioinformatics Conference – Bioinformatics 2007, June 3 – 6, Umea, Sweden
- 2007 University of Kansas, Department of Molecular Biosciences Seminar Series, May 7, Lawrence, KS
- 2007 From Computational Biophysics to Systems Biology, CBSB07, May 1 – 4, Jülich, Germany
- 2007 47<sup>th</sup> Sanibel Symposium, February 21 – 25, St. Simons Island, FL
- 2007 5<sup>th</sup> European Conference on Computational Biology, January 21 – 25, Eilat, Israel
- 2006 Center for Computational Molecular Biology – Industrial Partners Program Symposium, December 6 – 8, Providence, RI
- 2006 7<sup>th</sup> Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, November 27 – 30, Pacific Grove, CA
- 2006 7<sup>th</sup> Spanish Symposium on Bioinformatics, November 19 – 22, Zaragoza, Spain
- 2006 Georgia Life Sciences Summit 2006, October 3 – 4, Atlanta, GA
- 2006 National Science Foundation – Workshop on Petascale Computing in the Biosciences, August 29 – 30, Arlington, VA
- 2006 6<sup>th</sup> Annual CCPN Meeting – Efficient and Rapid Structure Determination by NMR,

- June 29 – 31, Ambleside, UK
- 2006 NIH Seminar, June 20, Bethesda, MD
- 2006 The Innovative Imperative: IBM Life Sciences Symposium, June 6, La Jolla, CA
- 2006 32<sup>nd</sup> Steenbock Symposium: Dynamics of Protein and Macromolecular Assemblies, May 18 – 21, Madison, WI
- 2006 Between CASP 6.5 Meeting, May 1, New York, NY
- 2006 NIH NCBI BoSC Meeting, April 25, Bethesda, MD
- 2006 Cornell Theory Center Review, March 28 – 30, Ithaca, NY
- 2006 2006 Annual Retreat and Advisory Committee of the National Research Program for Genomic Medicine, March 3 – 6, Taipei, Taiwan
- 2005 Rice Theoretical and Computational Biology Symposium, December 9 – 10, Houston, TX
- 2005 University of California – Irvine, Distinguished Speaker Series – Institute for Genomics and Bioinformatics, October 27 – 29, Irvine, CA
- 2005 BIOINFO 2005, International Joint Conference of InCoB, AASBi, and KSBI, September 22 – 24, Busan, Korea
- 2005 Northeast Biodefense Center Annual Meeting, September 12 – 13, Cold Spring Harbor, NY
- 2005 Modeling of Protein Interactions in Genomics, June 26 – 28, Lawrence, KS
- 2005 Georgia Institute of Technology, Seminar Series, June 15 – 17, Atlanta, GA
- 2005 Flexibility in Biomolecules, May 16 – 19, Tempe, AZ
- 2005 Frontiers in Macromolecular Simulations, April 28 – 29, Atlanta, GA
- 2005 Lawrence Livermore National Laboratory, Seminar Series, April 10 – 13, Livermore, CA
- 2005 Florida State University, Seminar Series, April 5 – 7, Tallahassee, FL
- 2005 University of Maryland, Biophysics Seminar Series, March 20 – 21, College Park, MD
- 2005 Advisory Committee of the National Research Program for Genomic Medicine of Taiwan, February 25 – March 2, Taipei, Taiwan
- 2005 6<sup>th</sup> Annual Bologna Winter School, February 16 – 19, 2005, Bologna, Italy
- 2005 49<sup>th</sup> Annual Biophysical Society Meeting, February 14 – 15 Long Beach, CA
- 2004 CASP6, December 5, Gaeta, Italy
- 2004 Johns Hopkins University, Chemical Engineering Seminar Series, October 27, Baltimore, MD
- 2004 Genome Annotation Colloquium, July 19 – 20, Washington, DC
- 2004 Brooklyn Polytechnic, Biogeometry Workshop, June 12, New York, NY
- 2004 Columbia University, Biomedical Informatics Seminar, April 22, New York, NY
- 2004 Institute for Pure & Applied Mathematics, University of California - Los Angeles Proteomics Workshop III, May 9 – 14, Los Angeles, CA
- 2004 University of Illinois, Urbana-Champaign, Seminar Series, April 7 – 9, Urbana, IL
- 2004 227<sup>th</sup> American Chemical Society (ACS) National Meeting, March 28 – April 1, Anaheim, CA
- 2004 Bio-IT World Conference and Expo, March 30 – April 1, Boston, MA
- 2004 University of North Carolina Chapel Hill, Seminar, March 22 – 23, Chapel Hill, NC
- 2004 North Carolina State University, Seminar Series, March 17 – 18, Raleigh, NC
- 2004 Boston University, Seminar Series, February 4 – 5, Boston, MA
- 2004 Dartmouth College, Seminar Series, February 1 – 3, Hanover, NH
- 2004 University of Michigan, Seminar Series, January 29, Ann Arbor, MI
- 2003 US Army Medical Research and Material Command Bioinformatics Workshop, November 4-6, Frederick, MD
- 2003 International Symposium on Modern Computing, October 30 – November 1, Ames, IA
- 2003 Gordon Research Conference, Bioinformatics: From Predictive Models to Inference, August 24 – 29, Oxford University, UK

- 2003 US Department of Energy, Genomes to Life: Computational Protein Structure Prediction, July 24, Gaithersburg, MD
- 2003 University of Texas Medical Branch, Symposium on Structural Biology, May 2 – 4, Galveston, TX
- 2003 4<sup>th</sup> Bologna Winter School 2003, Hot Topics in Structural Genomics, February 10, Bologna, Italy
- 2003 Keystone Conference, Frontiers of NMR in Molecular Biology VII, February 5, Taos, NM
- 2002 5<sup>th</sup> Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, December 1 – 5, Pacific Grove, CA
- 2002 American Institute of Chemical Engineers Annual Meeting 2002, November 5, Indianapolis, IN
- 2002 Dow Agrosiences Seminar, November 4, Indianapolis, IN
- 2002 Keystone Symposia, Structural Genomics: From Gene Sequence to Function, January 5 – 11, Breckenridge, CO
- 2001 International Conference on Sequence, Structure, and Function in Membrane Protein Systems, November 4 – 8, Zichron Ya'acov, Israel
- 2001 Harold Scheraga 80<sup>th</sup> Birthday Symposium, October 25 – 27, Cornell University
- 2001 CABM Symposium on Structural Genomics and Pharmaceutical Design, October 24-25, Princeton, NJ
- 2001 Annual International Meeting of the Molecular Graphics and Modeling Society, September 17 – 21, Erlangen, Germany
- 2001 Summer School on Parallel Computing in Biomolecular Simulations, September 1 – 3, Gdansk, Poland
- 2001 ORNL and University of Tennessee Mini-Symposium, August 17, Oak Ridge
- 2001 Participating in the Telluride Summer Research Center, July 15 – 29 in Telluride, CO
- 2001 AIST Waterfront Symposium – Ring of Sciences, July 11 – 13, Tokyo, Japan
- 2001 Conference on “Modeling of Protein Interactions in Genomes,” June 17 – 20, Charleston, SC
- 2001 International Workshop on Protein Folding and Design, June 11 – 22, Trieste, Italy
- 2001 IBC Proteomics Seminar, May 14 – 17, Philadelphia, PA
- 2001 ACS symposium "Energy Landscapes of Proteins, Glasses and Clusters: Dynamics, Folding, Function and Prediction," April 1 – 5 San Diego, CA
- 2001 DIMACS Workshop on Protein Structure and Structural Genomics: Prediction, Determination, Technology, and Algorithms, March 8 – 9, Rutgers University.
- 2001 Cologne Spring Meeting, Evolutionary Genomics and Bioinformatics, Feb 28 – March 2, Cologne, Germany
- 2001 Winter School at KIAS, Seoul, Korea
- 2000 The Annual Meeting of the Society of Molecular Biology of Japan, “Approach to Structural Genomics from Computational Bioinformatics,” December 13 – 16, Japan
- 2000 4<sup>th</sup> Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, Asilomar Conference Center, December 3 – 7, Pacific Grove, CA
- 2000 International Meeting on Sequence Structure and Function of Membrane Proteins, November 5 – 9, Israel
- 2000 Keck 2000 Symposium, W.M. Keck Center for Computational Biology, October 16 – 17, Houston, TX
- 2000 International Workshop on Methods for Macromolecular Modeling, October 12 – 14, Courant Institute.
- 2000 SIAM Conference on Computational Science and Engineering, September 21 – 24, Washington, DC
- 2000 Conformation of Peptides, Proteins and Nucleic Acids, August 29 – September 2, Debrzyno by Gdansk, Poland

- 2000 Zerner Conference, International Society of Quantum Biology and Pharmacology, August 17 – 19, University of New Orleans
- 2000 Protein Flexibility and Folding, August 13 – 17, Michigan State University
- 2000 Fourth Annual Gene Functional Analysis Conference, March 2 – 3, San Francisco, CA
- 1999 Seventh Conference on Small Genomes, November 13 – 17, Arlington, VA
- 1999 Pioneer Hi-Bred Symposium, "Challenges Beyond the Genome," November 4 – 5, Johnston, IA
- 1999 Cornell University, "Intersections of Structural Biology and Genomics," October 14, Ithaca, NY
- 1999 Workshop on "Overcoming Broken Ergodicity in Simulations of Condensed Matter Systems," September 27 – 29, Lyon, France
- 1999 International Scientific Conference on Folding of Soluble and Membrane Proteins, June 14 – 17, Gambloux, Belgium
- 1999 American Society for Biochemistry and Molecular Biology, Computational Biology Session, May 20, San Francisco, CA
- 1999 Functional Genomics: Technology Development & Research Applications Conference, April 25 – 28, Banbury Center, Cold Spring Harbor, NY
- 1999 ACS Hirshman Award Symposium for Harold Scheraga, March 23, Anaheim, CA,
- 1999 IMS International Workshop on Protein Stability/Folding,
- 1999 Opportunities in Molecular Biomedicine in the Era of Teraflop Computing, March 3, Rockville, MD
- 1999 3rd Annual Gene Functional Analysis Conference, Chairman of the Structural Genomics Session, March 4, San Francisco, CA
- 1999 3rd Annual conference on Microbial Genomes, January 29 – February 1, Chantilly, VA
- 1999 3rd International Lake Tahoe Symposium on Molecular Diversity, January 24 – 29, Lake Tahoe, NV
- 1998 3<sup>rd</sup> Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, (CASP3), December 13 – 17, Asilomar Conference Center
- 1998 Advanced Study Institute at Hebrew University on Protein Folding, November 14 – 21.
- 1998 After the Genome IV (ATG IV) Meeting, October 10 – 14, Jackson Hole, WY
- 1998 Rutgers University Center for Advanced Biotechnology and Medicine, Structure-Based Functional Genomics Meeting, October 4 – 7, Avalon, NJ.
- 1998 American Chemical Society Fall Meeting, August 23 – 27, Boston, MA
- 1998 Gordon Conference on Biopolymers, June 14 – 19, Newport, RI
- 1998 Tripos Inc. User Meeting, May 17 – 19, Somerset, NJ
- 1998 Pacific Symposium on Biocomputing III, January, Maui, Hawaii
- 1997 Howard Hughes Medical Institute Workshop on Protein Function from Primary Sequence, September 9 – 10, Chevy Chase, MD
- 1997 15<sup>th</sup> American Peptide Symposium, Chair & Speaker, Design, Modeling, and Structure Session, June 18 – 19, Nashville, TN
- 1997 9<sup>th</sup> International Congress of Quantum Chemistry, Chemistry in Biology Satellite Symposium, June 3 – 5, Savannah, GA
- 1997 213<sup>th</sup> American Chemical Society National Meeting, Symposium on Polymer Modeling, April 13 – 15, San Francisco, CA
- 1997 Sanibel Symposium, Quantum Theory Project, March 4 – 8, St. Augustine, FL
- 1997 Protons and Membranes Gordon Conference, Membrane Protein Folding and Assembly session, February 23-28, Ventura, CA
- 1997 Pacific Symposium on Biocomputing II, January, Maui, Hawaii
- 1996 The Protein Folding Problem: Analysis and Prediction of Protein Structure Symposium, University of North Carolina, Chapel Hill, December 14, Chapel Hill, NC

- 1996 75th Birthday Symposium Honoring Harold Scheraga, Cornell University, October 1996, Ithaca, NY
- 1996 Fourth World Congress of Theoretically Oriented Chemists - WATOC '96, July, Jerusalem
- 1996 International Symposium on Theoretical and Experimental Aspects of Protein Folding, June 13 – 20, San Luis, Argentina
- 1996 Molecular Graphics and Modelling Society 15th International Conference and AGM, Molecular Interactions, University of York, April 13, UK
- 1995 Workshop on Nonlinear Dynamics and Molecular Evolution and Engineering, University of California - Los Angeles, November 10, Los Angeles, CA
- 1995 International Conference on Molecular Structural Biology, September 9 – 14, Bundeswirtschafts-kammer, Vienna
- 1995 ACS National Meeting, Frontiers in Biophysical Chemistry, August 20, Chicago, IL
- 1995 9<sup>th</sup> Symposium of the Protein Society in the Stein and Moore Symposium, July 22, Boston, MA
- 1995 Research Conference on Protein Folding and Stability, April 10, Barcelona, Spain
- 1995 DIMACS Conference, Global Minimization of Nonconvex Energy Functions: Molecular Conformation and Protein Folding, Rutgers University, March 25, NJ
- 1994 Molecular Modeling Conference 1994, Fundamentals and Applications for the Pharmaceutical Industry, October 27, NJ
- 1994 Symposium on Computation in Biophysical Chemistry, Cornell University, Ithaca, NY
- 1994 Advances in Protein Folding '94 Symposium, Protein Design/Folding at The Banbury Center, Cold Spring Harbor Laboratory, October 13
- 1994 SYBYL and TRIPOS/Europe User Group Meetings to demonstrate MatchMaker, September 20, Dresden, Germany
- 1994 Genes, Proteins and Computers: An International Conference on Bio-Informatics, Networking and Computing in Molecular Biology, September 10, Daresbury Laboratory, England
- 1994 American Chemical Society National Meeting, August 11 – 15, Washington, DC
- 1994 Gordon Conference on Computational Chemistry, July 24, Boston, MA
- 1994 Technical University of Wroclaw and University of Wroclaw, Poland, "Computers in Chemistry," June, 17 – 22, Wroclaw, Poland
- 1994 27th Jerusalem Symposium in Quantum Chemistry and Biochemistry; May, The Israel Academy of Science and Humanities
- 1993 ACS Midwest Regional Meeting, Structure and Dynamics of Biological Macromolecules, November, Columbia, MO
- 1993 Institute for Theoretical Physics, University of California, January, Santa Barbara, CA
- 1993 Drug Information Association, 7th Biennial Meeting, January, Orlando, FL
- 1993 Protein Dynamics and Thermodynamics, The Hebrew University, The Institute for Advanced Studies, March, Givat, Israel
- 1992 High Performance Computing and Grand Challenges in Structural Biology, The Florida State University, January, Tallahassee, FL
- 1992 1992 ASBMB/Biophysical Society Meeting, February, Houston, TX
- 1992 Pittsburgh Supercomputing Center, "Computational Challenges for the Future." March, San Juan, Puerto Rico
- 1992 The Dow Chemical Company, Polymer Modeling Symposium - ACS National Meeting, April, San Francisco, CA
- 1992 The Karolinska Institute Center for Structural Biochemistry - Understanding Protein Folding, August, Stockholm, Sweden
- 1992 The Second International Conference and Exhibition on Computer Applications to Materials and Molecular Science and Engineering, September, Yokohama, Japan
- 1991 Biophysical Society 35th Annual Meeting, February, San Francisco, CA
- 1991 Protein Structure and Design Symposium, University of Rochester, Medical Center, April, Rochester, NY

- 1991 Second Annual Symposium in Computational Chemistry, "Emerging Methods in Computational Chemistry," Cray Research, Inc., May, North Carolina
- 1991 Molecular Modeling Symposium, The R. W. Johnson Pharmaceutical Research Institute, May, Raritan, NJ
- 1991 The 3rd International Conference on Computational Physics, June, San Jose, CA
- 1991 American Chemical Society Symposium, October, New York, NY
- 1991 FACSS/Pacific Conference/ACS Western Regional Meeting, September, Anaheim, CA
- 1990 University of New Orleans, Mardi Gras Symposium, February, New Orleans, LA
- 1990 "International Discussion Meeting on Relaxations in Complex Systems." Speaker and Committee Member, June, Heraklion, Crete, Greece
- 1990 IUPAC International Symposium on Macromolecules, July
- 1990 "Converging Approaches to Computational Biology," Rensselaerville Institute, September, Rensselaerville, NY
- 1990 Colorado State University, Guest Speaker in Honor of Dr. Marshall Fixman's 60th Birthday. October, CO
- 1990 Banbury Center, Cold Springs Harbor Laboratory, December, Cold Springs, NY
- 1989 AAAS Annual Meeting "The Process of Protein Folding" Chaired by Jane Richardson and Irwin Kuntz. January, San Francisco, CA
- 1989 ACS Symposium on Molecular Theology, April, Dallas, TX
- 1989 ACS Symposium on Computational Modeling, April, Dallas, TX
- 1989 ACS Symposium on Computer Simulations of Polymers, September, Miami Beach, FL
- 1988 Session Chairman, Gordon Research Conference on Polymer Physics, July 1988
- 1988 Summer Gordon Research Conference on Biopolymers, June 1988.
- 1988 NATO Advanced Study Institute on "Reactive And Flexible Molecules in Liquids," September 23 – October 2, Nauplion, Greece
- 1987 Conference on Polymer Dynamics at the Michigan Molecular Institute, August 1987
- 1987 NRC Workshop on "Advanced Computation and Simulation of Complex Materials Phenomena," Seminar Entitled: "Current State of Computations in Polymer Physics," March 1987
- 1986 Summer Gordon Research Conference on Polymer Physics, July 1986
- 1985 11th World Congress of the International Association for Mathematics and Computers in Simulation, August 5 – 9, Oslo, Norway
- 1984 Symposium at Dartmouth College in Honor of Walter Stockmayer's 70th Birthday, July 13 – 14, Hanover, NH
- 1984 International Association of Mathematics and Computers Simulation Symposium on Biomedical Modeling, NIH, August 6 – 10
- 1982 Summer Gordon Research Conference on Polymer Physics, July 1982
- 1981 NATO Advanced Study Institute, Static and Dynamic Properties of the Polymeric Solid State, Glasgow, Scotland

## PATENTS

Patent No. 5,265,030 issued 11/23/1993. System and method for determining three-dimensional structures of proteins. Jeffrey Skolnick and Andrzej Kolinski Inventors.

Patent No. 5,933,819 issued 8/3/1999. Prediction of relative binding motifs of biologically active peptides and peptide mimetics. Jeffrey Skolnick, Mariusz Milik and Andrzej Kolinski Inventors.

Patent No. 6,631,332, issued 10/7/2003. Methods for using functional site descriptors and predicting protein function. Jeffrey Skolnick and Jacquelyn S. Fetrow Inventors.

**PUBLICATIONS**

1. J. Skolnick and M. Fixman. Electrostatic persistence length of a wormlike polyelectrolyte. *Macromolecules* 1977: **10**: 944-948.
2. J. Skolnick. Investigations on a rod-like polyelectrolyte model. Ph.D. Thesis. Yale University (1978).
3. M. Fixman and J. Skolnick. Polyelectrolyte excluded volume paradox. *Macromolecules* 1978: **11**: 863-867.
4. J. Skolnick and M. Fixman. Charge interactions in cylindrical polyelectrolytes. *Macromolecules*. 1978: **11**: 867.
5. J. Skolnick and M. Fixman. Screened coulomb interactions on a dielectric cylinder. *Polym Preprints* 1978: **19**: 247.
6. J. Skolnick. Colligative properties of helical polyelectrolytes. *Macromolecules* 1979: **12**: 515-521.
7. J. Skolnick and E.K. Grimmelman. A preliminary examination of end effects in polyelectrolyte theory: The potential of a line segment of charge. *Macromolecules* 1980:**13**: 335-338.
8. J. Skolnick and E. Helfand. Kinetics of conformational transitions in chain molecules. *J Chem Phys* 1980: **72**: 5489-5500.
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10. J. Skolnick and W.L. Mattice. Rates of conformational transitions in branched chain molecules. *Macromolecules*. 1981: **14**: 292-299.
11. J. Skolnick. Kinetics of conformational transitions in polymers containing skeletal double bonds. *Macromolecules* 1981: **14**: 646-654.
12. W. L. Mattice and J. Skolnick. Conformational properties of bolaform electrolytes. *Macromolecules*. 1981: **14**: 863-867.
13. D. K. Carpenter and J. Skolnick. Depolarized light scattering from macromolecules: Effects of torsional oscillations, conformational transitions and overall rotations. *Macromolecules*. 1981: **14**: 1284-1290.
14. W. L. Mattice and J. Skolnick. Trans placements, expansion and asymmetry of star like polyethylenes bearing similarly charged ends. *Macromolecules* 1981: **14**: 1463-1468.
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