

Curriculum Vitae

JEFFREY SKOLNICK, Ph.D.

ADDRESS: Center for the Study of Systems Biology
Georgia Institute of Technology
School of Biological Sciences
950 Atlantic Drive, NW, Room 2151
Atlanta, GA 30332-2000
(404) 407-8975 Voice
(404) 385-7478 Fax
skolnick@gatech.edu

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
2007-2018	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 & 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 & 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:

2018	Editorial Board Member, NIH Director's Early Independence Research Program
2018	Ad hoc Member, NIH BCMB Study Section
2018	Chair and Ad hoc Member, NIH MIRA for New and Early Stage Investigators Study Section
2018	Ad hoc Member, NIH Catalyst Award in Diabetes, Endocrinology and Metabolic Diseases Study Section
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 *in vivo* 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

2003-present Advisory Committee, Modeling of Protein Interactions Biennial Conference

2002-2005 Nominations Committee, Protein Society

2001-2004 Member, Scientific Advisory Board of the Proteome Society

2000-2004 Member, NIH BBKA 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 BBKA 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:

2018 Sigma Xi Sustained Research Award

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:

Sigma Xi, Georgia Tech Chapter
 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

GRADUATE STUDENTS AND POSTDOCTORAL SCHOLARS:

Total number of Post-docs: 58

S. Tonddast-Navaei	2014-2017	Data Scientist, Systematrix Solutions Inc.
B. Srinivasan	2012-2017	Marie Skłodowska-Curie Research Associate, Instituto Gulbenkian de Ciencia, Portugal
A. Roy	2012-2015	Research Scientist II, Data Strategy and Solutions, Vertex Pharmaceuticals
S. Chaudhury	2014-2015	Medical Communications (Oncology), Regulatory Submission Writer, Novartis
S. Mukherjee	2013-2015	Data Scientist, Novartis
A. Hussain	2012-2014	
J. Grahnen	2012-2013	Senior Data Scientist, Microsoft
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	Associate Professor, Louisiana State University
J. Borreguero	2005-2008	Scientific Software Engineer, Oakridge National Laboratory
Y. Huang	2005-2008	Senior Staff Scientist, Regeneron Pharmaceuticals
D. Ivankov	2007-2008	Postdoctoral Fellow, Institute of Science and Technology Austria
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 Software Architect, Stealth Startup
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	Computational Biologist, Neumann Institute for Computing
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 at Leidos Biomedical Research Adjunct Faculty - Bioinformatics at Hood College
P. Xavier	2002-2004	Senior Director - Computational Chemistry, Molecular and Materials Modeling, Alleesh Biosciences Labs Pvt. Ltd.
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	Computational Biologist, Morgridge Institute for Research
M. Betancourt	1999-2001	Assistant Professor, Borough of Manhattan Community College
M. Wojciechowski	1999-2001	Assistant Professor, Gdańsk University of Technology
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	Director of Computational Drug Discovery, 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:

2018	Modeling of Protein Interactions (MPI 2018), November 8-10, Lawrence, KS
2018	Seminar, Northern Illinois University, October 16, DeKalb, Illinois
2018	Keynote Lecture, LINXS Workshop on "Dynamics of Biological Macromolecules", June 4-6, Lund, Sweden
2018	Seminar, Sigma Xi Awards Banquet, April 9, Atlanta, GA
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, 6th 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 14th 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 66th 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 27th 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 90th 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 90th 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, AM³, November 11 – 14, Austin, TX
- 2009 Beckman Institute 20th 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 238th 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 10th 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 3rd, Worcester, MA
- 2008 6th Swiss National Center of Competence in Research (NCCR) – Symposium on New Trends in Structural Biology, September 8 – 9, Zurich, Switzerland
- 2008 236th 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 - CMS³, June 10 – 14, Rome, Italy
- 2008 DE Shaw & Co. – Seminar Series, April 30, New York, NY
- 2008 3rd 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 234th 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 9th 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 47th Sanibel Symposium, February 21 – 25, St. Simons Island, FL
- 2007 5th 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 7th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, November 27 – 30, Pacific Grove, CA
- 2006 7th 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 6th 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 32nd 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 6th Annual Bologna Winter School, February 16 – 19, 2005, Bologna, Italy
- 2005 49th 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 227th 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 4th 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 5th 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 80th 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 4th 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 3rd 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 15th American Peptide Symposium, Chair & Speaker, Design, Modeling, and Structure Session, June 18 – 19, Nashville, TN
- 1997 9th International Congress of Quantum Chemistry, Chemistry in Biology Satellite Symposium, June 3 – 5, Savannah, GA

- 1997 213th 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 9th 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.

Patent No. 9,920,058, issued 3/20/2018. Molecules with potent DHFR binding affinity and antibacterial activity. Bharath Srinivasan, Jeffrey Skolnick and Hongyi Zhou 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.
9. J. Skolnick and A.M. Holtzer. Effect of urea on the intrinsic viscosity of randomly coiled poly (α -L-glutamate). *Macromolecules* 1980: **13**: 1311-1313.
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.
15. E. Helfand, Z. Wasserman, T. Weber, J. Skolnick and J.H. Runnels. The kinetics bonds of conformational transitions: Effects of variation of bond angle bending and bond stretching force constants. *J Chem Phys* 1981: **75**: 4441.
16. J. Skolnick and A. Holtzer. Theory of helix-coil transitions of α -helical, two-chain, coiled coils. *Macromolecules* 1982: **15**: 303-314.

17. J. Skolnick and A. Holtzer. Theory of α -helix-to-random coil transitions of two-chain, coiled coils. Application to a synthetic analogue of tropomyosin. *Macromolecules* 1982: **15**: 812-821.
18. W. L. Mattice and J. Skolnick. Stability of the cross-linked tropomyosin dimer: Cross-link effect on the cooperativity of the ordering process and on the maximum in the helix probability profile. *Macromolecules* 1982: **15**: 1088-1093.
19. J. Skolnick and R. Yaris. Damped orientational diffusion model of polymer local main chain polymer motion. 1. General theory. *Macromolecules* 1982: **15**: 1041-1046.
20. J. Skolnick and R. Yaris. Damped orientational diffusion model of polymer local main-chain motion. 2. Application to poly (vinyl acetate). *Macromolecules* 1982: **15**: 1046-1051.
21. E. Helfand and J. Skolnick. Mechanism and rates of conformational transitions in heterogeneous polymers. *J Chem Phys* 1982: **77**: 5714-5724.
22. J. Skolnick. An order-disorder theory of stress-strain behavior of glassy polymers In: *Static and Dynamic Properties of the Polymeric Solid State*. Pethrick, A. and R.W. Richards, eds., Boston: D. Reidel Publishing Company, 1982: 459-460.
23. M. E. Holtzer, A. Holtzer and J. Skolnick. α -helix-to-random-coil transition of two-chain, coiled coils. Theory and experiments for thermal denaturation of α -tropomyosin. *Macromolecules* 1983: **16**: 173-180.
24. J. Skolnick and R. Yaris. Damped orientational diffusion model of polymer local main-chain motion. 3. Inclusion of chain-chain interactions. *Macromolecules* 1983: **16**: 266-272.
25. M. E. Holtzer, A. Holtzer and J. Skolnick. α -Helix to random coil transition of two-chain, coiled coils. Theory and experiments for thermal denaturation of α -tropomyosin at acidic pH. *Macromolecules* 1983: **16**: 462-465.
26. J. Skolnick. Effect of loop entropy on the helix-coil transition of α -helical, two-chain, coiled coils. *Macromolecules* 1983: **16**: 1069-1083.
27. D. Perchak, R. Yaris and J. Skolnick. Effects of topological solitons on autocorrelation functions for chains of coupled torsional oscillators. *J Chem Phys* 1983: **78**: 6914-6927.
28. J. Skolnick and A. Holtzer. Theory of α -helix-to-random-coil transitions of two-chain coiled coils. Application to the T1 and T2 fragments of α -tropomyosin. *Macromolecules* 1983: **16**: 1548-1550.
29. J. Skolnick. Effect of loop entropy on the helix-coil transition of α -helical, two-chain, coiled coils. 2. Supermatrix formulation of the perfect-matching model. *Macromolecules* 1983: **16**: 1763-1770.
30. J. Skolnick. Effect of loop entropy on the helix-coil transition of α -helical, two-chain, coiled coils. 3. Supermatrix formulation of the imperfect-matching model. *Macromolecules* 1984: **17**: 645-658.
31. J. Skolnick, D. Perchak and R. Yaris. Restricted internal segmental rotational diffusion model with segment-segment interactions. Application to ^{13}C NMR. *J Mag Reson* 1984: **57**: 204-220.
32. J. Skolnick. Theory of helix-coil transitions of α -helical, two-chain, coiled coils. Analytic treatment of the homopolymeric, neglect-loop-entropy model. *Macromolecules* 1984: **17**: 2153-2158.
33. J. Skolnick. Theory of the kinetics of the helix-coil transition in two-chain, coiled coils. 1. Infinite chain limit. *Macromolecules* 1984: **17**: 2158-2173.
34. J. Skolnick, D. Perchak, R. Yaris and J. Schaefer. Phenomenological model of the stress-strain behavior of glassy polymers. *Macromolecules* 1984: **17**: 2332-2336.
35. J. Skolnick. Theory of the kinetics of the helix-coil transition in two-chain, coiled coils. 2. The finite chain. *Macromolecules* 1985:**18**: 232-243.
36. B. Pant, J. Skolnick and R. Yaris. Damped orientational diffusion model of polymer local main chain motion. 4. Effects of probes and side chains. *Macromolecules* 1985: **18**: 253-259.

37. J. Schaefer, E.O. Stejskal, D. Perchak, J. Skolnick and R. Yaris. Molecular mechanism of the ring-flip process in polycarbonate. *Macromolecules* 1985: **18**: 368-373.
38. D. Perchak, J. Skolnick and R. Yaris. Dynamics of rigid and flexible constraints for polymers. Effect of the Fixman potential. *Macromolecules* 1985: **18**: 519-525.
39. J. Skolnick. Theory of helix-coil transition in single chain polypeptides with interhelical contacts. The broken α -helical hairpin model. *Macromolecules* 1985: **18**: 1073-1083.
40. J. Skolnick and R. Yaris. Damped orientational diffusion model of polymer local main chain motion. 5. Comparison with three alternative models. *Macromolecules* 1985: **18**: 1635-1637.
41. J. Skolnick. Theory of the helix-coil transition in singly cross-linked, two-chain, coiled coils. *Macromolecules* 1985: **18**: 1535-1549.
42. J. Skolnick and A. Holtzer. Theory of α -helix-to-random coil transition of two-chain, coiled coils. Application of the augmented theory to thermal denaturation of tropomyosin. *Macromolecules* 1985: **18**: 1549-1559.
43. J. Skolnick. Theory of the helix-coil transition in two-chain, coiled coils. A globular protein folding model. 11th IMACS World Congress Proceedings 1985: **2**: 259.
44. J. Skolnick. Role of topological constraints in the all-or-none transition of a globular protein model. Theory of the helix-coil transition in doubly cross-linked, coiled coils. *Biochem Biophys Res Commun* 1985: **129**: 848-853.
45. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo dynamics of diamond-lattice multichain systems. Proceedings of the 1985 La Jolla Workshop on Polymer Flow Interaction. AIP Conference Proceedings, (Y. Rabin, ed.) 1985: **137**: 241-245.
46. C. L. Chen and J. Skolnick. Theory of the helix-coil transition in singly cross-linked, two-chain, coiled coils. II. Role of mismatched states. *Macromolecules* 1986: **19**: 242-243.
47. A. Kolinski, J. Skolnick and R. Yaris. On the short time dynamics of dense polymeric systems and the origin of the glass transition: A model system. *J Chem Phys* 1986: **84**: 1922-1931.
48. J. Skolnick. Theory of the helix-coil transition in doubly cross-linked, two-chain, coiled coils. A globular protein model. *Macromolecules* 1986: **19**: 1153-1166.
49. J. Skolnick and A. Holtzer. α -helix-to-random coil transitions of two-chain, coiled coils: A theoretical model for the "pretransition" in cysteine-190-cross-linked tropomyosin. *Biochemistry* 1986: **25**: 6192-6202.
50. A. Holtzer and J. Skolnick. Theory of α -helix to random coil transition of two-chain, coiled coils. Application of the augmented theory to thermal denaturation of α -tropomyosin. *Macromolecules* 1986: **19**: 1769-1770.
51. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo study of local orientational order in a semiflexible polymer melt model. *Macromolecules* 1986: **19**: 2550-2560.
52. A. Kolinski, J. Skolnick and R. Yaris. Order-disorder transitions in tetrahedral lattice polymer systems. *Macromolecules* 1986: **19**: 2560-2567.
53. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo simulations on an equilibrium globular protein folding model. *Proc Natl Acad Sci USA* 1986: **83**: 7267-7271.
54. A. Kolinski, J. Skolnick and R. Yaris. The collapse transition of semiflexible polymers. A Monte Carlo simulation of a model system. *J Chem Phys* 1986: **85**: 3585-3597.
55. P. Duffy, J. Skolnick and A. Holtzer. A theoretical model simulating the anomalous concentration dependence of the equilibrium thermal unfolding curve of non-cross-linked tropomyosin. *Biochem Biophys Res Commun* 1986: **141**: 394-398.
56. J. Skolnick. Theory of the helix-coil transition in doubly cross-linked, two-chain, coiled coils. A globular protein model. In: Eisenfeld, J. and M. Witten, eds. *Modelling of Biomedical Systems*. 1986: 167-172.
57. A. Kolinski, J. Skolnick and R. Yaris. Dynamic Monte Carlo study of the conformational properties of long flexible polymers. *Macromolecules* 1987: **20**: 438-440.
58. D. Perchak, J. Skolnick and R. Yaris. Computer simulations of simple models of the ring-flip process in polycarbonate. *Macromolecules* 1987: **20**: 121-129.

59. J. Skolnick. Possible role of helix-coil transitions in the microscopic mechanism of muscle contraction. *Biophys J* 1987: **51**: 227-243.
60. A. Kolinski, J. Skolnick and R. Yaris. Does reptation describe the dynamics of entangled finite length polymer systems? A model simulation. *J Chem Phys* 1987: **86**: 1567-1585.
61. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo studies on the long time dynamic properties of dense cubic lattice multichain systems. I. The homopolymeric melt. *J Chem Phys* 1987: **86**: 7164-7173.
62. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo studies on the long time dynamic properties of dense cubic lattice multichain systems. II. Probe polymer in a matrix of different degrees of polymerization. *J Chem Phys* 1987: **86**: 7174-7180.
63. A. Kolinski, J. Skolnick and R. Yaris. Monte Carlo studies on equilibrium globular protein folding. I. Homopolymeric lattice models of β -barrel proteins. *Biopolymers* 1987: **26**: 937-962.
64. J. Skolnick, A. Kolinski and R. Yaris. Monte Carlo studies of the long time dynamics of dense polymer systems. The failure of the reptation model. *Accts Chem Research* 1987: **20**: 350-356.
65. A. Holtzer and J. Skolnick. Application of the augmented theory of α -helix-to-random-coil transitions of two-chain, coiled coils to extant data on synthetic, tropomyosin-analog peptides. *Biopolymers* 1988: **27**: 87-96.
66. J. Skolnick, R. Yaris and A. Kolinski. Phenomenological theory of the dynamics of polymer melts. I. Analytic treatment of self-diffusion. *J Chem Phys* 1988: **88**: 1407-1417.
67. J. Skolnick and R. Yaris. Phenomenological theory of the dynamics of polymer melts. II. Viscoelastic properties. *J Chem Phys* 1988: **88**: 1418-1442.
68. A. J. Barrett and J. Skolnick. On the apparent radius of gyration of linear polymers and the experimental determination of the excluded volume parameter. *Macromolecules* 1988:**21**: 1141-1145.
69. J. Skolnick, A. Kolinski and R. Yaris. Monte Carlo simulations of the folding of β -barrel globular proteins. *Proc Natl Acad Sci USA* 1988: **85**: 5057-5061.
70. J. Skolnick, R. Yaris, and A. Kolinski. Phenomenological theory of polymer melt dynamics. *Int J Mod Phys* 1989: **3**: 33-64.
71. A. T. Yeates, J. Skolnick and R. Yaris. Fit of a nonreptative model of polymer melt dynamics to experimental melt diffusion constant measurements. *J Poly Sci Poly Phys Ed* 1989: **27**: 151-154 (1989).
72. J. Skolnick, A. Kolinski and R. Yaris. Monte Carlo studies on equilibrium globular protein folding. II. β -barrel globular protein models. *Biopolymers* 1989: **28**: 1059-1095.
73. A. Sikorski and J. Skolnick. Monte Carlo studies on equilibrium globular protein folding. III. The four helix bundle. *Biopolymers* 1989: **28**: 1097-1113.
74. J. Skolnick, A. Kolinski and R. Yaris. Dynamic Monte Carlo study of the folding of a six stranded Greek key globular protein. *Proc Natl Acad Sci* 1989: **86**: 1229-1233.
75. A. Sikorski and J. Skolnick. Monte Carlo simulation of equilibrium globular protein folding: α -helical bundles with long loops. *Proc Natl Acad Sci USA* 1989: **86**: 2668-2672.
76. J. Skolnick, A. Kolinski, A. Sikorski and R. Yaris. Dynamic Monte Carlo simulation of a melt of ring polymers. *Polymer Preprints* 1989: **30**: 70-73.
77. J. Skolnick. Dynamics of dense polymer systems. Dynamic Monte Carlo simulation results and analytic theory. In: *Reactive and Flexible Molecules Liquids*. Dorfmueller, T., ed., Klumer Academic Publishers, 1989: **291**: 199-220.
78. J. Skolnick and A. Kolinski. Computer simulations of globular protein folding and tertiary structure. *Annu Rev Phys Chem* 1989: **40**: 207-235.
79. A. Holtzer, M.E. Holtzer and J. Skolnick. Does the unfolding transition of two-chain, coiled coil proteins involve a continuum of intermediates? *AAAS Seminar Volume on The Protein Folding Problem* (1990).
80. J. Skolnick and A. Kolinski. Dynamics of dense polymer systems: Computer simulations and analytic theories. *Advances in Chemical Physics* 1990: **77**: 223-278.

81. J. Skolnick and A. Kolinski. Dynamic Monte Carlo simulations of globular protein folding/unfolding pathways. I. Six member, Greek key β -barrels. *J Mol Biol* 1990: **212**: 787-817.
82. A. Sikorski and J. Skolnick. Dynamic Monte Carlo simulations of globular protein folding/unfolding pathways. II. α -helical motifs. *J Mol Biol* 1990: **212**: 819-836.
83. A. Sikorski and J. Skolnick. Dynamic Monte Carlo simulations of globular protein folding. Model studies of *in vivo* assembly of four helix bundles and four member β -barrels. *J Mol Biol* 1990: **215**: 183-198.
84. J. Skolnick, A. Kolinski and A. Sikorski. Dynamic Monte Carlo simulations of globular protein folding, structure and dynamics. *Comments on Mol. & Cell. Biol* 1990: **6**: 223-247.
85. J. Skolnick, A. Kolinski and A. Sikorski. Dynamic Monte Carlo simulations of globular protein and structure. *Chemical Design Automation News* 1990: **5**: 1-20.
86. M. Milik, A. Kolinski and J. Skolnick. Monte Carlo dynamics of a dense system of chain molecules constrained to lie near an interface. A simplified membrane model. *J. Chem. Phys* 1990: **93**: 4440-4446.
87. J. Skolnick and A. Kolinski. Simulations of the folding of a globular protein. *Science* 1990: **250**: 1121-1125.
88. K. L. Ngai and J. Skolnick. Correspondence between coupling model predictions and computer simulations: Diffusion of a probe polymer in a matrix having different degrees of polymerization. *Macromolecules* 1991: **24**: 1561-1566.
89. A. Kolinski, M. Milik and J. Skolnick. Static and dynamic properties of a new lattice model of polypeptide chains. *J Chem Phys* 1991: **94**: 3978-3985.
90. J. Skolnick and A. Kolinski. Dynamic Monte Carlo simulations of a new lattice model of globular protein folding, structure, and dynamics. *J Mol Biol* 1991: **221**: 499-531.
91. Y. Levine, A. Kolinski and J. Skolnick. Monte Carlo dynamics study of motions in CIS-unsaturated hydrocarbon chains. *J Chem Phys* 1991: **95**: 3826-3834.
92. A. Rey and J. Skolnick. Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α -helical hairpins. *Chemical Physics* 1991: **158**: 199-219.
93. A. Godzik, J. Skolnick and A. Kolinski. Simulations of the folding pathway of triose phosphate isomerase-type α/β barrel proteins. *Proc Natl Acad Sci USA* 1992: **89**: 2629-2633.
94. A. Rey and J. Skolnick. Efficient algorithm for the reconstruction of a protein backbone from the α -carbon coordinates. *J Comput Chem* 1992: **13**: 443-456.
95. M. Milik, J. Skolnick and A. Kolinski. Monte Carlo studies of an idealized model of a lipid-water system. *J Phys Chem* 1992: **96**: 4015-4022.
96. A. Godzik, J. Skolnick and A. Kolinski. A topology fingerprint approach to the inverse protein folding problem. *J Mol Biol* 1992: **227**: 227-238.
97. M. Milik and J. Skolnick. Spontaneous insertion of polypeptide chains into membranes: A Monte Carlo model. *Proc Natl Acad Sci USA* 1992: **89**: 9391-9395.
98. A. Rey, A. Kolinski, J. Skolnick and Y. Levine. Effect of double bonds on the dynamics of hydrocarbon chains. *J Chem Phys* 1992: **97**: 1240-1249.
99. M. Vieth, A. Kolinski, J. Skolnick and A. Sikorski. Prediction of protein secondary structure by neural networks: Encoding short and long range patterns of amino acid packing. *Acta Biochimica Polonica* 1992: **39**: 369-392.
100. A. Kolinski and J. Skolnick. Discretized model of proteins. I. Monte Carlo study of cooperativity in homopolypeptides. *J Chem Phys* 1992: **97**: 9412-9426.
101. A. Godzik and J. Skolnick. Sequence-structure matching in globular proteins: Application to supersecondary and tertiary structure determination. *Proc Natl Acad Sci USA* 1992: **89**: 12098-12102.
102. K. L. Ngai, S. L. Peng and J. Skolnick. Generalized Fokker-Planck approach to the coupling model and comparison with computer simulation. *Macromolecules* 1992: **25**: 2184-2191.

103. A. Rey and J. Skolnick. Computer modeling and folding of four-helix bundles. *Proteins* 1993: **16**: 8-28.
104. M. Milik and J. Skolnick. Insertion of peptide chains into lipid membranes: An off-lattice Monte Carlo dynamics model. *Proteins* 1993: **15**: 10-25.
105. A. Kolinski and J. Skolnick. Comment on local knot model of entangled polymer chains. *J Phys Chem* 1993: **97**: 3450.
106. Y. Levine, A. Kolinski and J. Skolnick. A lattice dynamics study of a Langmuir monolayer of monounsaturated fatty acids. *J Chem Phys* 1993: **98**: 7581-7587.
107. A. Kolinski, A. Godzik and J. Skolnick. A general method for the prediction of the three dimensional structure and folding pathway of globular proteins. Application to designed helical proteins. *J Chem Phys* 1993: **98**: 7420-7433.
108. J. Skolnick, A. Kolinski and A. Godzik. From independent modules to molten globules: Observations on the nature of protein folding intermediates. *Commentary in Proc Natl Acad Sci USA* 1993: **90**: 2099-2100.
109. M. Baginski, L. Piela and J. Skolnick. The ethylene group as a peptide bond mimicking unit: A theoretical conformational analysis. *J Comput Chem* 1993: **14**: 471-477.
110. A. Godzik, A. Kolinski and J. Skolnick. De novo and inverse folding predictions of protein structure and dynamics. *J Comput-Aided Mol Design* 1993: **7**: 397-438.
111. J. Skolnick, A. Kolinski, C. L. Brooks, III, A. Godzik and A. Rey. A method for predicting protein structure from sequence. *Current Biology* 1993: **3**: 414-423.
112. A. Godzik, J. Skolnick and A. Kolinski. Regularities in interaction patterns of globular proteins. *Protein Eng* 1993: **6**: 801-810.
113. A. Godzik, A. Kolinski and J. Skolnick. Lattice representation of globular proteins: How good are they? *J Comput Chem* 1994: **14**: 1194-1202.
114. M. Vieth, A. Kolinski, C. L. Brooks, III and J. Skolnick. Prediction of the folding pathways and structure of the GCN4 "leucine zipper." *J Mol Biol* 1994: **237**: 361-367.
115. A. Rey and J. Skolnick. Computer simulation of the folding of coiled coils. *J Chem Phys* 1994: **100**: 2267-2276.
116. A. Kolinski and J. Skolnick. Monte Carlo simulations of protein folding. I. Lattice model and interaction scheme. *Proteins* 1994: **18**: 338-352.
117. A. Kolinski and J. Skolnick. Monte Carlo simulations of protein folding. II. Application to protein A, ROP, and crambin. *Proteins* 1994: **18**: 353-366.
118. A. Godzik and J. Skolnick. Flexible algorithm for direct multiple alignment of protein structures and sequences. *CABIOS* 1994: **10**: 587-596.
119. J. Skolnick and A. Kolinski. De novo prediction of protein tertiary structure. *Polymer Preprints* 1994: **35**: 82-83.
120. A. Sikorski, A. Kolinski and J. Skolnick. Dynamics of star branched polymers in a matrix of linear chains. A Monte Carlo study. *Macromolecular Theory and Simulations* 1994: **3**: 715-719.
121. M. Milik, A. Kolinski and J. Skolnick. Neural network system for the evaluation of side-chain packing in protein structures. *Protein Eng* 1995: **8**: 225-236.
122. M. Vieth, A. Kolinski and J. Skolnick. A simple technique to estimate partition functions and equilibrium constants from Monte Carlo simulations. *J Chem Phys* 1995: **102**: 6189-6193.
123. M. Vieth, A. Kolinski, C. L. Brooks III and J. Skolnick. Prediction of the quaternary structure of coiled coils. Application to mutants of the GCN4 leucine zipper. *J Mol Biol* 1995: **251**: 448-467.
124. J. Skolnick, M. Vieth, A. Kolinski and C. Brooks III. De novo simulations of the folding of GCN4 and its mutants. In: *Modeling of Biomolecular Structures and Mechanisms*. A. Pullman, et al., Eds., Kluwer Acad./Netherlands 1995: **8**: 95-98.
125. M. Milik and J. Skolnick. An object oriented environment for artificial evolution of protein sequences: The example of rational design of transmembrane sequences. *Evolutionary Conference* (1995).

126. A. Baumgärtner and J. Skolnick. Spontaneous translocation of a polymer across a curved membrane. *Phys Rev Letters* 1995: **74**: 2142-2145.
127. A. Kolinski, M. Milik, J. Rycobel and J. Skolnick. A reduced model of short range interactions in polypeptide chains. *J Chem Phys* 1995: **103**: 4312-4323.
128. A. Kolinski, W. Galazka and J. Skolnick. Computer design of idealized β -motifs. *J Chem Phys* 1995: **103**: 10286-10297.
129. A. Baumgärtner and J. Skolnick. Polymer electrophoresis across a model membrane. *J Phys Chem* 1995: **98**: 10655-10658.
130. M. Milik and J. Skolnick. A Monte Carlo model of fd and Pf1 coat proteins in lipid membranes. *Biophys J* 1995: **69**: 1382-1386.
131. A. Godzik, A. Kolinski and J. Skolnick. Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets. *Protein Sci* 1995: **4**: 2107-2117.
132. J. Skolnick and M. Milik. Monte Carlo Models of Spontaneous Insertion of Peptides into Lipid Membranes. In: *Membrane Structures & Dynamics*. Merz, K., B. Roux, Eds. Boston: Birkhauser, 1996: 535-554.
133. K. Olszewski, A. Kolinski and J. Skolnick. Folding simulations and computer redesign of protein A three-helix bundle motifs. *Proteins* 1996: **25**: 286-299.
134. M. Vieth, A. Kolinski, C. L. Brooks III, and J. Skolnick. A hierarchical approach to the prediction of the quaternary structure of GCN4 and its mutants. *DIMACS* 1996:**23**: 233-236.
135. M. Vieth, A. Kolinski and J. Skolnick. Method for predicting the state of association of discretized protein models. Application to leucine zippers. *Biochemistry* 1996: **35**: 955-967.
136. S. DeBolt and J. Skolnick. Evaluation of atomic level mean force potentials via inverse folding and inverse refinement of protein structures: Atomic burial position and pairwise non-bonded Interactions. *Protein Eng* 1996: **9**: 637-655.
137. K. Olszewski, A. Kolinski and J. Skolnick. Does a backwardly read protein sequence have a unique native state? *Protein Eng* 1996: **9**: 5-14.
138. A. Kolinski, W. Galazka and J. Skolnick. On the origin of the cooperativity of protein folding: Implications from model simulations. *Proteins* 1996: **26**: 271-287.
139. A. Kolinski and J. Skolnick. *Lattice Models of Protein Folding, Dynamics and Thermodynamics*. Austin: R.G. Landes Company, 1996: 202.
140. J. Hirst, M. Vieth, J. Skolnick and C. L. Brooks III. Predicting leucine zipper structures from sequence. *Protein Eng* 1996: **9**: 657-662.
141. A. Kolinski, J. Skolnick and A. Godzik. An algorithm for prediction of structural elements in small proteins. *Proc. Pacific Symposium on Biocomputing (PSB-96)*. Hunter, L., T. Klein, Eds. World Scientific, Singapore, 1996: 446-460.
142. M. Vieth, A. Kolinski, C. Brooks, III and J. Skolnick. Prediction of the quaternary structure of coiled coils: GCN4 leucine zipper and its mutants. *Proc. Pacific Symposium on Biocomputing (PSB-96)*. Hunter, L., T. Klein, Eds. World Scientific, Singapore, 1996: 653-662 (1996).
143. J. Skolnick and A. Kolinski. Monte Carlo Lattice Dynamics and the Prediction of Protein Folds. *Computer Simulations of Biomolecular Systems*. In: *Theoretical and Experimental Studies*. van Gunsteren, W. F., P.K. Weiner and A. J. Wilkinson, eds. Leiden, The Netherlands: ESCOM Science, 1997: 395-429.
144. J. Skolnick and A. Kolinski. Protein Modeling. In: Schleyer, P. and P. Kollman, eds. *Encyclopedia of Computational Chemistry*. Sussex, England: John Wiley & Sons, 1998: 2200-2211.
145. M. Milik, A. Kolinski and J. Skolnick. Algorithm for rapid reconstruction of a protein backbone from alpha carbon coordinates. *J Comput Chem* 1997:**18**: 80-85.
146. J. Skolnick and M. Milik. Modeling of Membrane Proteins and Peptides. In: *Membrane Proteins Assembly, Part IV. Modeling and Simulation*, von Heijne, G., ed. Austin: R.G. Landes Company, 1997:201-220.

147. J. Skolnick, A. Kolinski and A. Ortiz. MONSSTER: A method for folding globular proteins with a small number of distance restraints. *J Mol Biol* 1997: **265**: 217-241.
148. A. Kolinski, J. Skolnick, A. Godzik and W-P Hu. A method for the prediction of surface "U"-turns and transglobular connections in small proteins. *Proteins* 1997: **27**: 290-308.
149. W-P.Hu, A. Godzik and J. Skolnick. Sequence-structure specificity-how does an inverse folding approach work? *Protein Eng* 1997: **10**: 317-331.
150. A. Kolinski and J. Skolnick. High coordination lattice models of protein structure, dynamics and thermodynamics. *Acta Biochimica Polonica (Review)* 1997: **44**: 389-422.
151. J. Skolnick. A Monte Carlo model of fd and Pf1 coat proteins in membranes. *Chemtracts* 1997: **10**: 242-245.
152. J. Skolnick, L. Jaroszewski, A. Kolinski and A. Godzik. Derivation and testing of pair potentials for protein folding. When is the quasichemical approximation correct? *Protein Sci* 1997: **6**: 676-688.
153. A. Kolinski and J. Skolnick. Determinants of secondary structure of polypeptide chains: interplay between short range and burial interactions. *J Chem Physics* 1997:**107**: 953-964.
154. C. Keasar, R. Elber and J. Skolnick. Simultaneous and coupled energy optimization of homologous proteins: A new tool for structure prediction. *Folding & Design* 1997: **2**: 247-259.
155. A.Sikorski, A. Kolinski and J. Skolnick. Computer simulations of de novo designed helical proteins. *Biophys J* 1998: **75**: 92-105.
156. A. Ortiz, A. Kolinski and J. Skolnick. Fold assembly of small proteins using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. *J Mol Biol* 1998: **277**: 419-448.
157. W-P. Hu, A. Kolinski and J. Skolnick. Improved method for the prediction of the protein backbone U-turn positions and the major secondary structures between the U-turns. *Proteins* 1997: **29**: 443-460.
158. B. Reva, A. Finkelstein, M. Sanner, A. Olson and J. Skolnick. Recognition of protein structure on coarse lattices with residue-residue energy functions. *Protein Eng* 1997: **10**: 1123-1130.
159. J. Skolnick and A. Kolinski. Monte Carlo approaches to the protein folding problem. In: Ferguson, D., J.I. Siepmann, D.G. Truhlar, eds. *Monte Carlo Methods in Chemical Physics. Advances in Chemical Physics Series.* John Wiley & Sons, 1998: 203-242.
160. L. Zhang and J. Skolnick. How do potentials derived from structural databases relate to "true" potentials? *Protein Sci* 1998: **7**: 112-122.
161. A. Ortiz, W-P. Hu, A. Kolinski and J. Skolnick. Method for low resolution prediction of small protein tertiary structure. *Proceedings of the Pacific Symposium on Biocomputing 1997.* R.B. Altman, A.K. Dunker, L. Hunter, T.E. Klein, eds. Singapore: World Scientific Pub., 1997: 316-327.
162. A. Ortiz, A. Kolinski and J. Skolnick. Tertiary structure prediction of the KIX domain of CBP using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. *Proteins* 1998: **30**: 287-294.
163. A. Kolinski and J. Skolnick. Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model. *Proteins* 1998: **32**: 475-494.
164. A. Ortiz, A. Kolinski and J. Skolnick. Combined multiple sequence reduced protein model approach to predict the tertiary structure of small proteins. *Proceedings of the Pacific Symposium on Biocomputing (PSB-98).* Altman, R., A.K. Dunker, L. Hunter and T.E. Klein, eds. Singapore: World Scientific Pub. 1998: 377-388.
165. A. Kolinski, W.Galazka and J. Skolnick. Monte Carlo studies of the thermodynamics and kinetics of reduced protein models. Application to small helical, α/β and β proteins. *J Chem Physics* 1998: **108**: 2608-2617.
166. M. Milik, D. Sauer, A. Brunmark, M. Jackson, P. Peterson, J. Skolnick and C. Glass. Application of an artificial neural network to predict specific Class I MHC binding peptide sequences. *Nature Biotech* 1998: **16**: 753-56.

167. A. Kolinski, L. Jaroszewski, P. Rotkiewicz and J. Skolnick. An efficient Monte Carlo model of protein chains. Modeling the short-range correlations between side group centers of mass. *J Phys Chem* 1998: **102**: 4628-4637.
168. A. Ortiz, A. Kolinski and J. Skolnick. Nativelike topology assembly of small proteins using predicted restraints in Monte Carlo folding simulations. *Proc Natl Acad Sci USA* 1998: **95**: 1020-1025.
169. L. Zhang and J. Skolnick. What should the Z-score of native protein structures be? *Protein Sci* 1998: **7**: 1201-1207.
170. J. S. Fetrow and J. Skolnick. Method for prediction of protein function from sequence using the sequence-to-structure-to-function paradigm with application to glutaredoxins/thioredoxins and T1 ribonucleases. *J Mol Biol* 1998: **281**: 949-968.
171. B. Reva, A.V. Finkelstein and J. Skolnick. What is the probability of a chance prediction of a protein structure with an RMSD of 6 Å? *Folding & Design* 1998: **3**: 141-147.
172. J. Fetrow, A. Godzik and J. Skolnick. Functional analysis of the *Escherichia coli* genome using the sequence-to-structure-to-function paradigm: Identification of proteins exhibiting the glutaredoxin/thioredoxin disulfide oxidoreductase activity. *J Mol Biol* 1998: **282**: 703-711.
173. B. Reva, A. Finkelstein and J. Skolnick. Derivation and testing residue-residue mean force potentials for use in protein structure recognition. In: Webster, D. M. ed. *Protein Structure Prediction Methods and Protocols*. Methods in Molecular Biology series. Bath, U.K.: Humana Press, 1999.
174. B. Reva, A. Finkelstein and J. Skolnick. A self-consistent field optimization approach to build energetically and geometrically correct lattice models of proteins. *Proceedings of the Second Annual International Conference on Computational Molecular Biology (RECOMB98) and J Comput Biol Special Issue*, 1998.
175. A. Kolinski, P. Rotkiewicz and J. Skolnick. Application of a high coordination lattice model in protein structure prediction. *Proceedings of the Workshop on Monte Carlo Approach to Biopolymers and Protein Folding*. Singapore: World Scientific, 1998: 377-388.
176. B. Reva, A.V. Finkelstein and J. Skolnick. Optimization of protein structure on lattices using a self-consistent field approach. *J Comput Biol* 1998: **5**: 531-538.
177. J. Skolnick, A. Kolinski and A. Ortiz. Application of reduced models to protein structure prediction. In: *Computational Molecular Biology, Theoretical Computational Chemistry*. Leszczynski, J., ed. Amsterdam: Elsevier, 1999: 397-440.
178. A. Kolinski, A. Godzik and J. Skolnick. Contact maps. In: Creighton, T.E., ed. *The Encyclopedia of Molecular Biology*. New York: John Wiley & Sons, 1999: 567-71.
179. K. Witte, J. Skolnick and C-H. Wong. A synthetic retrotransition (backwards reading) sequence of the right handed three-helix bundle domain B (10-53) of protein A shows similarity in conformation as predicted by computation. *J Amer Chem Soc* 1999: **120**: 13042-13045.
180. C. Simmerling, M. Lee, A.R. Ortiz, A. Kolinski, J. Skolnick and P.A. Kollman. Combining MONSSTER and LES/PME to predict protein structure from amino acid sequence: application to the small protein CMTI-1. *J Amer Chem Soc* 2000: **122**(35): 8392-8402.
181. B. Reva, J. Skolnick and A.V. Finkelstein. Averaging interaction energies over homologs improves protein fold recognition in gapless threading. *Proteins* 1999:**35**: 353-359.
182. J. Skolnick, A. Kolinski and A. Ortiz. Reduced protein models and their application to the protein folding problem. *J Biomolec Structure & Dynamics* 1998: **16**: 381-396.
183. J. Skolnick, A. Kolinski and D. Mohanty. De novo predictions of the quaternary structure of leucine zippers and other coiled coils. *Int'l J Quantum Chem* 1999: **75**: 165-176.
184. L. Zhang, A. Godzik, J. Skolnick and J. Fetrow. Functional analysis of *Escherichia coli* proteins for members of the α/β hydrolase family. *Folding & Design* 1998: **3**: 535-548.
185. D. Mohanty, A. Kolinski and J. Skolnick. De novo simulations of the folding thermodynamics of the GCN4 leucine zipper. *Biophysical J* 1999: **77**: 54-69.

186. D.C. Rapaport, J.E. Johnson and J. Skolnick. Supramolecular self-assembly: Molecular dynamics modeling of polyhedral shell formation. *Computer Physics Commun* 1999: **121-122**: 231-235.
187. A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick. A method for the improvement of threading-based protein models. *Proteins* 1999: **37**: 593-610.
188. D. Mohanty, B. Dominy, A. Kolinski, C.L. Brooks III and J. Skolnick. Correlation between knowledge-based and detailed atomic potentials for GCN4-Iz unfolding. *Proteins* 1999:**35**: 447-452.
189. C. Keasar, D. Tobi, R. Elber and J. Skolnick. Coupling the folding of homologous proteins. *Proc Natl Acad Sci USA* 1998: **95**: 5880-5883.
190. J. Skolnick, J. Fetrow, A.R. Ortiz and A. Kolinski. The role of computational biology in the genomics revolution. *Proceedings of the National Research Council's Chemical Sciences Roundtable Workshop on the Impact of Advances in Computing and Communications Technologies on Chemical Sciences and Technology*.
191. B. Zhang, L. Rychlewski, K. Pawlowski, J. Fetrow, J. Skolnick and A. Godzik. From fold predictions to function predictions: Automation of functional site conservation analysis for functional genome predictions. *Protein Science* 1999: **8**: 1104-1115.
192. J.S. Fetrow, N. Siew and J. Skolnick. Structure-based functional motif identifies a potential disulfide oxidoreductase active site in the serine-threonine protein phosphatase-1 subfamily. *FASEB J* 1999: **13**: 1866-1874.
193. A.R. Ortiz, A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick. CASP3 Proceedings: *Ab initio* folding of proteins using restraints derived from evolutionary information. *Proteins Suppl* 1999: **3**: 177-185.
194. A. Sikorski, A. Kolinski and J. Skolnick. Computer simulations of the properties of the α_2 , α_2C and α_2D de novo designed helical proteins. *Proteins* 2000: **38**: 17-28.
195. A.R. Ortiz and J. Skolnick. Sequence evolution and the mechanism of protein folding. *Biophys J* 1999: **79**: 1787-1799.
196. A. Kolinski, B. Ilkowski and J. Skolnick. Dynamics and thermodynamics of β -hairpin assembly: Insight from various simulation techniques. *Biophys J* 1999: **77**: 2942-52.
197. J. Skolnick and J.S. Fetrow. From genes to protein structure and function: Novel applications of computational approaches in the genomic era. *TIBTECH* 2000: **18**: 34-9.
198. J. Skolnick, A. Kolinski and A. Ortiz. Derivation of protein-specific pair potentials based on weak sequence fragment similarity. *Proteins* 2000: **38**: 3-16.
199. J. Skolnick, J. S. Fetrow and A. Kolinski. Structural genomics and its importance for gene function analysis. *Nature Biotechnology* 2000: **18**: 283-7.
200. A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick. Protein folding: Flexible lattice models. *Prog. Theor. Phys.* 2000: **138**: 292-300.
201. B. Ilkowski, J. Skolnick and A. Kolinski. Helix-coil and beta sheet-coil transitions in a simplified, yet realistic protein model. *Macromolecular Theory and Simulations* 2000: **9**: 523-533.
202. J. Fetrow, N. Siew, M. Yamout, J. Dyson, P. Wright and J. Skolnick. Genomic-scale comparison of sequence- and structure-based methods of function prediction: Does structure provide additional insight. *Protein Science* 2001: **10**: 1005-1014.
203. J. Skolnick and D. Kihara. Defrosting the frozen approximation: PROSPECTOR: A new approach to threading. *Proteins* 2001: **42**: 319-31.
204. M. Feig, P. Rotkiewicz, A. Kolinski, J. Skolnick and C. Brooks. Accurate reconstruction of all-atom protein representations from side chain based low-resolution models. *Proteins* 2000: **41**: 86-97.
205. D. Gront A. Kolinski and J. Skolnick. Comparison of three Monte Carlo conformational search strategies for protein-like polymer models: Identification of low energy structures and folding thermodynamics. *J Chem Phys* 2000: **113**(12): 5065-5071.
206. A.V. Finkelstein, D.S. Rykunov, M. Yu. Lobanov, A. Ya. Badretdinov, B.A. Reva, J. Skolnick, L.A. Mirny and E.I. Shakhnovich. Overcoming the crudeness of energy

- estimates in protein 3D structure prediction by homologs: The when and the how. *Biophysica* 1999: **44**(6): 980-91.
207. M. Betancourt and J. Skolnick. Finding the needle in a haystack: Educing native folds from ambiguous *ab initio* protein structure prediction. *J. Comput. Chem.* 2001: **22**(3): 339-353.
 208. Y. Bukhman and J. Skolnick. BioMolQuest: A new search engine for the integrated database-based retrieval of protein structural and functional information. *Bioinformatics.* 2001: **17**(5): 468-478.
 209. J. Skolnick and A. Kolinski. A unified approach to the prediction of protein structure and function. *Advances in Chemical Physics* 2002: **120**: 131-192.
 210. H. Lu and J. Skolnick. A distance-dependent atomic knowledge-based potential for protein structure selection. *Proteins* 2001: **44**: 223-32.
 211. A. Kolinski, M.R. Betancourt, D. Kihara, P. Rotkiewicz and J. Skolnick. Generalized Comparative Modeling (GENECOMP): A combination of sequence comparison, threading, and lattice modeling for protein structure prediction and refinement. *Proteins* 2001: **44**: 133-149.
 212. D. Gront, A. Kolinski and J. Skolnick. A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. *Journal of Chemical Physics* 2001: **115**(3): 1569-1574.
 213. J. Di Gennaro, N. Siew, B. Hoffman, L. Zhang, J. Skolnick, L. Neilson and J. Fetrow. Enhanced functional annotation of protein sequences via the use of structural descriptors. *Journal of Structural Biology* 2001: **134**: 232-245.
 214. M.R. Betancourt, J. Skolnick. Universal similarity measure for comparing protein structures. *Biopolymers.* 2001: **59**: 305-309.
 215. J. Skolnick, A. Kolinski, D. Kihara, M.R. Betancourt, P. Rotkiewicz and M. Boniecki. *Ab initio* protein structure prediction via a combination of threading, lattice folding, clustering, and structure refinement. *Proteins Special Issue* 2001: **5**: 149-156.
 216. A. Kolinski, P. Rotkiewicz and J. Skolnick. Structure of proteins: New approach to molecular modeling. *Polish J. Chem.* 2000: **75**: 587-599.
 217. M. Wojciechowski and J. Skolnick. Docking of small ligands to low-resolution and theoretically predicted receptor structures. *Journal of Computational Physics Special Issue* 2002: **23**: 189-197.
 218. D. Kihara, H. Lu, A. Kolinski and J. Skolnick. TOUCHSTONE: An *ab initio* protein structure prediction method that uses threading-based tertiary restraints. *Proc Natl Acad Sci.* 2001: **98**(18): 10125-10130.
 219. Y. Zhang and J. Skolnick. Parallel-hat tempering: A Monte Carlo search scheme for the identification of low-energy structures. *J Chem Phys.* 2001: **115**: 5027-5032.
 220. J. Skolnick and A. Kolinski. Computational studies of protein folding. *CISE* 2001: **3**: 40-48.
 221. D. Kihara, Y. Zhang, A. Kolinski and J. Skolnick. *Ab initio* protein structure prediction on a genomic scale: Application to the *Mycoplasma genitalium* genome. *Proc Natl Acad Sci.* 2002: **30**: 5993-5998.
 222. L. Lu, H. Lu and J. Skolnick. MULTIPROSPECTOR: An algorithm for the prediction of protein-protein interactions by multimeric threading. *Proteins* 2002: **49**: 350-64.
 223. J. Skolnick, Y. Zhang and D. Kihara. Local energy landscape flattening: parallel hyperbolic Monte Carlo sampling of protein folding. *Proteins* 2002: **48**: 192-201.
 224. J. S. Fetrow, A. Giammona, A. Kolinski and J. Skolnick. The protein folding problem: A biophysical enigma. *Current Pharmaceutical Biotechnology* 2002: **3**(4): 329-47.
 225. J. Viñals, A. Kolinski and J. Skolnick. Numerical study of the entropy loss of dimerization and the folding thermodynamics of the GCN4 leucine zipper. *Biophysical Journal* 2002: **83**(5): 2801-11.
 226. H. Lu, and J. Skolnick. Application of statistical potentials to protein structure refinement from low resolution *ab initio* models. *Biopolymers* 2003: **70**(4): 575-84.
 227. P. Pokarowski, A. Kolinski and J. Skolnick. A minimal physically realistic protein-like lattice model: Designing an energy landscape that ensures all-or-none folding to a unique native state. *Biophysical Journal.* 2003: **84**(3): 1518-26.

228. T. Haliloglu, A. Kolinski and J. Skolnick. Use of residual dipolar couplings as restraints in *ab initio* protein structure prediction. *Biopolymers* 2003: **70**(4): 548-62.
229. A. Sikorski, A. Kolinski and J. Skolnick. Computer simulation of protein folding with a small number of distance restraints. *Acta Biochimica Polonica* 2002: **49**: 683-692.
230. H. Lu, L. Lu and J. Skolnick. Development of unified statistical potentials describing protein-protein interactions. *Biophysical Journal*. 2002: **84**(3): 1895-901.
231. D. Kihara and J. Skolnick. The PDB is a covering set of small protein structures. *Journal of Molecular Biology* 2003: **333**: 393-802.
232. J. Skolnick, Y. Zhang, A. K. Arakaki, M. Betancourt, A. Szilagy and D. Kihara. Touchstone: A unified approach to protein structure prediction. *Proteins CASP5 Special Issue* 2003: **53**: 469-479.
233. Y. Zhang, A. Kolinski and J. Skolnick. Touchstone II: A new approach to *ab initio* protein structure prediction. *Biophysical Journal* 2003: **85**: 1145-1164.
234. L. Lu, A. K. Arakaki, H. Lu and J. Skolnick. Multimeric threading based prediction of protein interactions on a genomic scale: Application to the *Saccharomyces Cerevisiae* proteome. *Genome Research* 2003: **13**: 1146-1154.
235. A. Kolinski, P. Klein, P. Romiszowski and J. Skolnick. Unfolding of globular proteins: Monte Carlo dynamics of a realistic reduced model. *Biophysical Journal*. 2003: **85**: 3271-3278.
236. W. Li, Y. Zhang, D. Kihara, Y. Huang, D. Zheng, G. Montelione, A. Kolinski and J. Skolnick. Touchstonex: Protein structure prediction using sparse NMR data. *Proteins* 2003: **53**(2): 290-306.
237. J. Skolnick, Y. Zhang and A. Kolinski. *Ab Initio* modeling. In: A. Edwards, M. Norin and M. Sundstrom, Eds. *Structural Genomics and High Throughput Structural Biology*. CRC/Taylor & Francis, Boca Raton, FL, Chapter VIII, p 137-162, 2005.
238. W. Tian and J. Skolnick. How well is enzyme function conserved? *Journal of Molecular Biology* 2003: **333**: 863-882.
239. M. Boniecki, P. Rotkiewicz, J. Skolnick and A. Kolinski. Protein fragment reconstruction using various modeling techniques. *J. Computer Aided Molecular Design* 2003: **17**: 725-738.
240. A. Kolinski and J. Skolnick. Reduced models of proteins and their applications. *Polymer* 2004: **45**(2): 511-524.
241. A. Kolinski, D. Gront, P. Pokarowski and J. Skolnick. A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. *Biopolymers* 2003: **69**: 339-405.
242. D. Kihara and J. Skolnick. Microbial genomes have over 72% structure assignment by the threading algorithm PROSPECTOR_Q. *Proteins* 2004: **55**: 464-473.
243. J. Skolnick, D. Kihara and Y. Zhang. Development and testing of the **PROSPECTOR 3.0** threading algorithm. *Proteins* 2004: **56**: 502-518.
244. A. K. Arakaki, Y. Zhang and J. Skolnick. Large-scale assessment of the utility of low resolution protein structures for biochemical assignment. *Bioinformatics* 2004: **20**: 1087-1096.
245. Y. Zhang and J. Skolnick. Automated structure prediction of weakly homologous proteins on a genomic scale. *Proc Natl Acad Science* 2004: **101**: 7594-7599.
246. J. Skolnick. What practical use is protein structure prediction to drug discovery? *BioIT World*, Commentary, October 10, 2003.
247. Y. Zhang and J. Skolnick. *SPICKER*: A clustering approach to identify near-native protein folds. *J. Comput Chem*. 2004: **25**: 865-871.
248. Y. Zhang and J. Skolnick. The protein structure prediction problem could be solved using the current PDB library. *Proc Natl Acad Science* 2005: **102**(4): 1029-1034. PMID: PMC545829.
249. Y. Zhang and J. Skolnick. A scoring function for the automated assessment of protein structure template quality. *Proteins* 2004: **57**: 702-710.
250. M. Betancourt and J. Skolnick. Local propensities and statistical potentials of backbone dihedral angles in proteins. *Journal of Molecular Biology* 2004: **342**: 635-649.

251. W. Li, Y. Zhang and J. Skolnick. Application of sparse NMR restraints to large-scale protein structure prediction. *Biophysical Journal* 2004: **87**: 241-1248.
252. Y. Zhang and J. Skolnick. Tertiary structure predictions on a comprehensive benchmark of medium to large size proteins. *Biophysical Journal* 2004: **87**: 2647-2655. PMID: PMC1304683.
253. E. Bindewald and J. Skolnick. A scoring function for docking ligands to low-resolution protein structures. *Journal of Computational Chemistry* 2005: **26**: 374-383.
254. J. Skolnick and Y. Zhang. Protein Structure Prediction, in: *Systems Biology*, I. Rigoutsos and G. Stephanopoulos, Editors. 2007, Oxford University Press: Oxford; New York. p. 187-218.
255. W. Tian, A. K. Arakaki and J. Skolnick. EFICAZ: a comprehensive approach to accurate genome-scale enzyme function inference. *Nucleic Acids Research* 2004: **32**: 6226-6239. PMID: PMC535665.
256. A. Szilagyi, V. Grimm, A. K. Arakaki and J. Skolnick. Prediction of physical protein-protein interactions. *Physical Biology* 2005: **(2)**: S1-S16.
257. J. Skolnick. Putting the pathway back into protein folding. *Proc Natl Acad Science* 2005: **102**(7): 2265-2266. PMID: PMC549015.
258. Y. Zhang and J. Skolnick. TM-align: A protein structure alignment algorithm based on the TM-score. *Nucleic Acids Research* 2005: **33**: 2302-2309. PMID: PMC1084323.
259. Y. Zhang, A. K. Arakaki and J. Skolnick. TASSER: An automated method for the prediction of protein tertiary structures in CASP6. *Proteins* 2005: **61**(S7): 91-98.
260. Y. Zhang, M. E. DeVries and J. Skolnick. Structure modeling of all identified G protein-coupled receptors in the human genome. *PLoS Computational Biology* 2006: **2**(2): 88-99. PMID: PMC1364505.
261. V. Grimm, Y. Zhang and J. Skolnick. Benchmarking of dimeric threading and structure refinement. *Proteins* 2006: **63**: 457-465.
262. Y. Zhang, I. A. Hubner, A. K. Arakaki, E. Shakhnovich and J. Skolnick. On the origin and completeness of single domain structures. *Proc Natl Acad Science* 2006: **103**: 2605-2610. PMID: PMC1413790.
263. J. Yang, W. Chen, J. Skolnick and E. Shakhnovich. All-atom ab initio folding of a diverse set of protein structures. *Structure* 2007: **15**: 53-63.
264. S. Lee, Y. Zhang and J. Skolnick. TASSER-based refinement of NMR structures. *Proteins* 2006: **63**: 451-456.
265. A. Szilagyi and J. Skolnick. Efficient prediction of nucleic acid binding function from low-resolution protein structures. *J Mol Biol* 2006: **358**: 922-933.
266. S. B. Pandit, Y. Zhang and J. Skolnick. *TASSER-Lite*: An automated tool for protein comparative modeling. *Biophysical Journal* 2006: **91**: 4180-4190. PMID: PMC1635668.
267. J. Skolnick. In quest of an empirical potential for protein structure prediction. *Current Opinion in Structural Biology* 2006: **16**: 166-171.
268. A. K. Arakaki, W. Tian, and J. Skolnick. High accuracy multi-genome scale reannotation of enzyme function by EFICAZ. *BMC Genomics* 2006: **7**: 315. PMID: PMC1764738.
269. A. Jagielska and J. Skolnick. Origin of intrinsic helix versus strand stability in homopolypeptides and its implications for the accuracy of the Amber force field. *Journal of Computational Chemistry* 2007: **28**(10): 1648-1657.
270. J. Borreguero and J. Skolnick. Benchmarking of TASSER in the *ab initio* limit. *Proteins* 2007: **68**: 48-56.
271. Z. Ding, H. Wang, X. Liang, E. Morris, F. Gallazzi, S. B. Pandit, J. Skolnick, J. C. Walker, and S. R. Van Doren. Phosphoprotein and Phosphopeptide Interactions with the FHA Domain from Kinase-Associated Protein Phosphatase. *Biochemistry* 2007: **46**(10): 2684-2696.
272. S. Lee and J. Skolnick. Development and benchmarking of TASSER^{iter} for the iterative improvement of protein structure predictions. *Proteins* 2007: **68**: 39-47.
273. M. Brylinski and J. Skolnick. What is the relationship between the global structures of apo and holo proteins? *Proteins* 2007: **70**(2): 363-377.

274. L. Wroblewska and J. Skolnick. Can a physics-based, all-atom potential find a protein's native structure among misfolded structures? I. Large scale AMBER benchmarking. *Journal of Computational Chemistry* 2007: **28**(12): 2059-2066.
275. J. Skolnick. Protein Structure Prediction, in: *The Encyclopedia of Life Sciences (ELS)*, John Wiley & Sons, Ltd: Chichester. DOI: 10.1002/9780470015902.a0003031.
276. S. Wu, J. Skolnick and Y. Zhang. Ab initio modeling of small proteins by iterative TASSER simulations. *BMC Biology* 2007: **5**: 17. PMID: PMC1878469.
277. R. Kim and J. Skolnick. Assessment of Programs for Ligand Binding Affinity Prediction. *Journal of Computational Chemistry* 2008: **29**: 1316-1331. PMID: PMC2702145.
278. R. J. Martinez, M. J. Beazley, M. Taillefert, A. K. Arakaki, J. Skolnick, and P. A. Sobecky. Aerobic Uranium(VI) BioPrecipitation by Metal Resistant Bacteria Isolated from Radionuclide- and Metal-Contaminated Subsurface Soils. *Environmental Microbiology* 2007: **9**(12): 3122-3133.
279. H. Zhou, S. B. Pandit, S. Lee, J. Borreguerro, H. Chen, L. Wroblewska and J. Skolnick. Analysis of TASSER based CASP7 protein structure prediction results. *Proteins* 2007: **69**(S8): 90-97.
280. H. Zhou and J. Skolnick. *Ab initio* protein structure prediction using chunk-TASSER. *Biophysical Journal* 2007: **93**: 1510-1518. PMID: PMC1948038.
281. H. Zhou and J. Skolnick. Protein model quality assessment prediction by combining fragment comparisons and a consensus C_α contact potential. *Proteins* 2007: **71**: 1211-1218. PMID: PMC2725406.
282. H. Chen and J. Skolnick. M-TASSER: An Algorithm for Protein Quaternary Structure Prediction. *Biophysical Journal* 2008: **94**(3): 918-928. PMID: PMC2186260.
283. M. Brylinski and J. Skolnick. FINDSITE: A threading-based method for ligand-binding site prediction and functional annotation. *Proc Natl Acad Science* 2008: **105**: 129-134. PMID: PMC2224172.
284. M. Brylinski and J. Skolnick. Q-Dock: Low-resolution flexible ligand docking with pocket-specific threading restraints. *Journal of Computational Chemistry* 2008: **29**(10): 1574-1588. PMID: PMC2726574.
285. L. Wroblewska, A. Jagielska, and J. Skolnick. Development of a physics-based force field for the scoring and refinement of protein models. *Biophysical Journal* 2008: **94**(8): 3227-3240. PMID: PMC2275715.
286. P. Rotkiewicz and J. Skolnick. Fast procedure for reconstruction of all-atom protein models from reduced representations. *Journal of Computational Chemistry* 2008: **29**(9): 1460-1465. PMID: PMC2692024.
287. A. K. Arakaki, R. Mezencev, N. Bowen, Y. Huang, J. McDonald and J. Skolnick. Identification of metabolites with anticancer properties by Computational Metabolomics. *Molecular Cancer* 2008: **7**: 57. PMID: PMC2453147.
288. S. Lee and J. Skolnick. Benchmarking of TASSER_2.0: An improved protein structure prediction algorithm with more accurate predicted contact restraints. *Biophysical Journal* 2008: **95**(4): 1956-1964. PMID: PMC2483784.
289. J. A. Somarelli, S. Lee, J. Skolnick, and R. J. Herrera. Structure-based classification of 45 FK506-binding proteins. *Proteins* 2008: **72**(1): 197-208. PMID: PMC2694576.
290. S. H. Thomas, R. D. Wagner, A. K. Arakaki, J. Skolnick, J. R. Kirby, L. J. Shimkets, R. A. Sanford, and F. E. Löffler. The mosaic genome of *Anaeromyxobacter dehalogenans* strain 2CP-C suggests an aerobic common ancestor to the delta-Proteobacteria. *PLoS ONE* 2008: **3**(5): e2103. PMID: PMC2330069.
291. A. Jagielska, L. Wroblewska and J. Skolnick. Protein model refinement using an optimized physic-based all atom force field. *Proc Natl Acad Science* 2008: **105**(24): 8268-8273. PMID: PMC2448826.
292. M. Gao and J. Skolnick. DBD-Hunter: A knowledge-based method for the prediction of DNA-protein interactions. *Nucleic Acids Research* 2008: **36**(12): 3978-3992. PMID: PMC2475642.

293. S. B. Pandit and J. Skolnick. Fr-TM-align: A new protein structural alignment method based on fragment alignments and the TM-score. *BMC Bioinformatics* 2008: **9**: 531. PMID: PMC2628391.
294. H. Zhou and J. Skolnick. Protein structure prediction by pro-sp3-TASSER. *Biophysical Journal* 2009: **96**(6): 2119-2127. PMID: PMC2717286.
295. M. Gao and J. Skolnick. From nonspecific DNA-protein encounter complexes to the prediction of DNA-protein interactions. *PLoS Computational Biology* 2009: **5**(3): e1000341. doi:10.1371/journal.pcbi.1000341 PMID: PMC2659451.
296. A. K. Arakaki, J. F. McDonald and J. Skolnick. Marker metabolites can be therapeutic targets as well. *Nature* 2008: **456**(7221): 443. NIHMSID: 165613
297. A. K. Arakaki, Y. Huang and J. Skolnick. EFICAZ²: Enzyme Function Inference by a Combined Approach enhanced by machine learning. *BMC Bioinformatics* 2009: (10): 107. PMID: PMC2670841.
298. M. Brylinski and J. Skolnick. FINDSITE^{LHM}: A threading-based approach to ligand homology modeling. *PLoS Computational Biology* 2009: **5**(6): e1000405. doi:10.1371/journal.pcbi.1000405. PMID: PMC2685473.
299. S. B. Pandit, H. Zhou and J. Skolnick. TASSER-based protein structure prediction, in *Introduction to Protein Structure Prediction: Methods and Algorithms*, H. Rangwala and G. Karypis, Editors. 2010, John Wiley & Sons, Inc.: Hoboken, New Jersey. p. 219-242.
300. J. Skolnick and M. Brylinski. FINDSITE: A combined evolution/structure-based approach to protein function prediction. *Briefings in Bioinformatics* 2009: doi: 10.1093/bib/bbp017. PMID: PMC2691936.
301. H. Zhou, S. B. Pandit and J. Skolnick. Performance of the Pro-sp3-TASSER Server in CASP8. *Proteins* 2009: **77**(S9): 123-127. PMID: PMC2785221.
302. J. Skolnick, A. K. Arakaki, S. Lee and M. Brylinski. The continuity of protein structure space is an intrinsic property of proteins. *Proc Natl Acad Science* 2009:**106**(37): 15609-15695. PMID: PMC2747181.
303. M. Brylinski and J. Skolnick. Comparison of structure- and threading-based approaches to protein functional annotation. *Proteins* 2009: **78**(1): 118-134. PMID: PMC2804779.
304. J. Skolnick and R. A. Friesner. Theory and simulation. *Current Opinion in Structural Biology* 2009: **19**: 117-119. PMID: PMC2692031.
305. M. Gao and J. Skolnick. A threading-based method for the prediction of DNA-binding proteins with application to the human genome. *PLoS Computational Biology* 2009:**5**(11): e1000567. doi:10.1371/journal.pcbi.1000567. PMID: PMC2770119.
306. M. Brylinski and J. Skolnick. Q-Dock^{LHM}: Low-resolution refinement for ligand comparative modeling. *Journal of Computational Chemistry* 2009: **31**(5):1093-1105. PMID: PMC2823986.
307. J. Skolnick and M. Brylinski. Novel computational approaches to drug discovery. *Proceedings of the International Conference of the Quantum Bio-Informatics III*, eds. L Accardi, W. Freudenberg & M. Ohya, 2010 World Scientific Publishing (327-336).
308. S. B. Pandit, M. Brylinski, H. Zhou, M. Gao, A. K. Arakaki and J. Skolnick. PSiFR: An integrated resource for prediction of protein structure and function. *Bioinformatics* 2010: **26**(5): 687-688. PMID: PMC2828114.
309. J. Skolnick, M. Brylinski and S. Y. Lee. Reply to Zimmerman et al.: The space of single domain protein structures is continuous and highly connected. *Proc Natl Acad Science* 2009: **106**:E138. PMID: PMC2799847.
310. H. Zhou and J. Skolnick. Improving threading algorithms for remote homology modeling by combining fragment and template comparisons. *Proteins* 2010:**78**(9): 2041-2048. doi: 10.1002/prot.22717. PMID: PMC2868272.
311. S. B. Pandit and J. Skolnick. TASSER_low-zsc: An approach to improve structure prediction using low z-score ranked templates. *Proteins* 2010:**78**(13): 2769-2080. PMID: PMC2927721.
312. M. Gao and J. Skolnick. iAlign: A method for the structural comparison of protein-protein interfaces. *Bioinformatics* 2010:**26**(18): 2259-2265. PMID: PMC2935406.

313. M. Brylinski and J. Skolnick. Comprehensive structural and functional characterization of the human kinome by protein structure modeling and ligand virtual screening. *Journal of Chemical Information and Modeling* 2010: **50**(10): 1839-1854. PMID: PMC2963673.
314. M. Brylinski, S. Lee, H. Zhou and J. Skolnick. The utility of geometrical and chemical restraint information extracted from predicted ligand binding sites in protein structure refinement. *Journal of Structural Biology* 2011: **173**(3): 558-569. PMID: PMC3036769.
315. T. Ando and J. Skolnick. Brownian dynamics simulation of macromolecule diffusion in a protocell. *Proceedings of the International Conference of the Quantum Bio-Informatics IV* 2011: **28**: 413-426. PMID: PMC4295211.
316. T. Ando and J. Skolnick. Crowding and hydrodynamic interactions likely dominate *in vivo* macromolecular motion. *Proc Natl Acad Science* 2010: **107**: 18457-18462. PMID: PMC2973006.
317. S. Lee and J. Skolnick. TASSER_WT: A protein structure prediction algorithm with accurate predicted contact restraints for difficult protein targets. *Biophysical Journal* 2010: **99**(9): 3066-3075. PMID: PMC2966002.
318. M. Brylinski and J. Skolnick. FINDSITE-metal: Integrating evolutionary information and machine learning for structure-based metal binding site prediction at the proteome level. *Proteins* 2010: **79**(3): 735-751. PMID: PMC3060289.
319. M. Gao and J. Skolnick. Structural space of protein-protein interfaces is degenerate, close to complete, and highly connected. *Proc Natl Acad Science* 2010: **107**(52): 22517-22522. doi: 10.1073/pnas.1012820107. PMID: PMC3012513.
320. M. Brylinski and J. Skolnick. Cross-reactivity virtual profiling of the human kinome by X-React^{KIN} – a Chemical Systems Biology approach. *Molecular Pharmaceutics* 2010: **7**(6): 2324-2333. PMID: PMC2997910.
321. M. Gao and J. Skolnick. New benchmark metrics for protein-protein docking methods. *Proteins* 2011: **79**(5): 1623-34. PMID: PMC3076516.
322. J. Skolnick and R. Friesner. Theory and simulation. Editorial overview. *Current Opinion in Structural Biology* 2011: **21**: 147-149. PMID: PMC2692031.
323. M. Brylinski, M. Gao and J. Skolnick. Why not consider a spherical protein? Implications of backbone hydrogen bonding for protein structure and function. *Physical Chemistry Chemical Physics* 2011: **13**(38): 17044-17055. PMID: PMC3289135.
324. H. Zhou and J. Skolnick. Template-based protein structure modeling using TASSER^{VMT}. *Proteins* 2012: **80**(2): 352-361. PMID: PMC3291807.
325. T. Ando and J. Skolnick. Importance of excluded volume and hydrodynamic interactions on macromolecular diffusion *in vivo*. *Proceedings of the International Conference of the Quantum Bio-Informatics IV* 2013: **30**: 375-387. PMID: PMC4295833.
326. H. Zhou and J. Skolnick. GOAP: A generalized orientation-dependent, all-atom statistical potential for protein structure prediction. *Biophysical Journal* 2011: **101**(8): 2043-2052. PMID: PMC3192975.
327. M. Gao and J. Skolnick. The distribution of ligand-binding pockets around protein-protein interfaces suggests a general mechanism for pocket formation. *Proc Natl Acad Science* 2012: **109**(10): 3784-3789. PMID: PMC3309739.
328. H. Zhou and J. Skolnick. FINDSITE^X: A structure based, small molecule virtual screening approach with application to all identified human GPCRs. *Molecular Pharmaceutics* 2012: **9**(6): 1775-1784. PMID: PMC3396429.
329. J. Skolnick, H. Zhou and M. Brylinski. Further evidence for the likely completeness of the library of solved single domain protein structures. *Journal of Physical Chemistry, B* 2012: **116**(23): 6654-6664. PMID: PMC3351587.
330. W. Guan, A. Ozakin, A. Gray, J. Borreguero, S. B. Pandit, A. Jagielska, L. Wroblewska and J. Skolnick. Learning Protein Folding Energy Functions. *IEEE 11th International Conference on Data Mining (ICDM) 2011 IEEE 11th International Conference on Data Mining*. 2011: 1062-1067. PMID: PMC4192713.

331. N. Kumar and J. Skolnick. EFICAZ^{2,5}: Application of a high-precision enzyme function predictor to 396 proteomes. *Bioinformatics* 2012: **28**(20): 2687-2688. PMID: PMC3467752.
332. T. Ando and J. Skolnick. On the Importance of Hydrodynamic Interactions in Lipid Membrane Formation. *Biophysical Journal* 2013: **104**(1): 96-105. PMID: PMC3540244.
333. T. Ando, E. Chow, Y. Saad and J. Skolnick. Krylov subspace methods for computing hydrodynamic interactions in Brownian dynamics simulations. *The Journal of Chemical Physics* 2012: **137**(6): 064106. PMID: PMC3427343.
334. G. G. Hammes and J. Skolnick. Career Accomplishments of Harold A. Scheraga. *Journal of Physical Chemistry, B* 2012: **116**(23): 6569-6571.
335. G. G. Hammes and J. Skolnick. Biography of Harold A. Scheraga. *Journal of Physical Chemistry, B* 2012: **116**(23): 6572-6572.
336. M. Gao and J. Skolnick. APoc: Large scale identification of similar protein pockets. *Bioinformatics* 2013: **29**(5): 597-604. PMID: PMC3582269.
337. H. Zhou and J. Skolnick. FINDSITE^{comb}: A threading/structure-based, proteomic-scale virtual ligand screening approach. *Journal of Chemical Information and Modeling* 2013: **53**(1): 230-240. PMID: PMC3557555.
338. S. Jo, H.S. Lee, J. Skolnick and W. Im. Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. *PLOS Computational Biology* 2013: **9**(3): e1002946. PMID: PMC3597548.
339. Y. Zhang and J. Skolnick. Segment assembly, structure alignment and iterative simulation in protein structure prediction. *BMC Biology* 2013: **11**(1): 44. PMID: PMC3626933.
340. J. Skolnick, H. Zhou and M. Gao. Are predicted protein structures of any value for binding site prediction and virtual ligand screening? *Current Opinion in Structural Biology* 2013: **23**(2): 191-7. PMID: PMC3659186.
341. T. Ando, E. Chow and J. Skolnick. Dynamic simulation of concentrated macromolecular solutions with screened long-range hydrodynamic interactions: Algorithm and limitations. *Journal of Chemical Physics* 2013: **139**(12): 121922. PMID: PMC3758360.
342. J. Skolnick and M. Gao. Interplay of physics and evolution in the likely origin of protein biochemical function. *Proc Natl Acad Science* 2013: **110**(23): 9344-9. PMID: PMC3677488.
343. M. Gao and J. Skolnick. A comprehensive survey of small-molecule binding pockets in proteins. *PLOS Computational Biology* 2013: **9**(10): e1003302. PMID: PMC3812058.
344. B. Srinivasan, H. Zhou, J. Kubanek and J. Skolnick. Experimental validation of FINDSITE^{comb} virtual ligand screening results for eight proteins yields novel nanomolar and picomolar binders. *Journal of Cheminformatics* 2014: **6**:16. PMID: PMC4038399.
345. J. Skolnick, M. Gao and H. Zhou. On the role of physics and evolution in dictating protein structure and function. *Israel Journal of Chemistry* 2014: **54**(8-9): 1176-1188. PMID: PMC4255337.
346. G. A. Khoury, A. Liwo, F. Khatib, H. Zhou, G. Chopra, J. Bacardit, L. O. Bortot, R. A. Faccioli, X. Deng, Y. He, P. Krupa, J. Li, M. A. Mozolewska, A. K. Sieradzan, J. Smadbeck, T. Wirecki, S. Cooper, J. Flatten, K. Xu, D. Baker, J. Cheng, A. C. B. Delbem, C. A. Floudas, C. Keasar, M. Levitt, Z. Popović, H. A. Scheraga, J. Skolnick, S. N. Crivelli and Foldit Players. WeFold: A Coopetition for Protein Structure Prediction. *Proteins* 2014: **82**(9): 1850-68. PMID: PMC4249725.
347. A. Roy and J. Skolnick. LIGSIFT: An open-source tool for ligand structural alignment and virtual screening. *Bioinformatics* 2015: **31**(4): 539-44. PMID: PMC4325547.
348. T. Ando and J. Skolnick. Sliding of Proteins Non-Specifically Bound to DNA: Brownian Dynamics Studies with Coarse-Grained Protein and DNA Models. *PLOS Computational Biology* 2014: **10**(12): e1003990. PMID: PMC4263368.
349. I. Kufareva, M. Rueda, V. Katritch, Participants of GPCR of Dock 2013*, R.C. Stevens and R. Abagyan. Advances in GPCR Modeling Evaluated by GPCR Dock 2013 Assessment: Meeting New Challenges. *Structure* 2014: **22**: 1120-1139. PMID: PMC4126895.

350. I. Kufareva, M. Rueda, V. Katriitch, GPCR Dock Participants*, R.C. Stevens and R. Abagyan. Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. *Structure* 2011: **19**: 1108-1126. PMID: PMC3154726.
351. B. Srinivasan and J. Skolnick. Insights into the slow-onset tight-binding inhibition of *Escherichia coli* dihydrofolate reductase: detailed mechanistic characterization of pyrrolo [3, 2-f] quinazoline-1, 3-diamine and its derivatives as novel tight-binding inhibitors. *FEBS Journal* 2015: **282**(10): 1922-1938. PMID: PMC4445455.
352. H. Zhou, M. Gao and J. Skolnick. ENTPRISE: An algorithm for predicting human disease-associated amino acid mutations from sequence entropy and predicted protein structures. *PLOS ONE* 2016: **11**(3): e0150965. PMID: PMC4794227.
353. H. Lee, S. Jo, S. Mukherjee, S-J. Park, J. Skolnick, J. Lee and W. Im. GS-align for Glycan Structure Alignment and Similarity Measurement. *Bioinformatics* 2015: **31**(16): 2653-2659. PMID: PMC4528633.
354. H. Zhou, M. Gao and J. Skolnick. Comprehensive prediction of drug-protein interactions and side effects for the human proteome. *Nature Scientific Reports* 2015: **5**: 11090. PMID: PMC4603786.
355. M. Gao, H. Zhou and J. Skolnick. Insights into disease-associated mutations in the human proteome through protein structural analysis. *Structure* 2015: **23**(7): 1362-1369. PMID: PMC4497952.
356. J. Skolnick, M. Gao, A. Roy, B. Srinivasan and H. Zhou. Implications of the small number of distinct ligand binding pockets in proteins for drug discovery, evolution and biochemical function. *BMCL Digests* 2015: **25**: 1163-1170. PMID: PMC4593502.
357. S. Dhakshinamoorthy, N. Dinh, J. Skolnick, and M. P. Styczynski. Metabolomics identifies the intersection of phosphoethanolamine with menaquinone-triggered apoptosis in an *in vitro* model of leukemia. *Molecular BioSystems* 2015: **11**(9): 2406-2416. PMID: PMC4534331.
358. R. Boles, H. A. Hornung, A. E. Moody, T. B. Ortiz, S. A. Wong, J. M. Eggington, M. Gao, H. Zhou, S. McLaughlin, A. S. Zare, K. M. Sheldon and J. Skolnick. Hurt, tired, and queasy: Specific variants in the ATPase domain of the TRAP1 mitochondrial chaperone are associated with common, chronic "functional" symptomatology including pain, fatigue and gastrointestinal dysmotility. *Mitochondrion* 2015: **23**: 64-70. PMID: PMC4586064.
359. A. Roy, B. Srinivasan and J. Skolnick. *PoLi*: A virtual screening pipeline based on template pocket and ligand similarity. *Journal of Chemical Information and Modeling* 2015: **55**(8): 1757-1770. PMID: PMC4593500.
360. B. Srinivasan, S. Tonddast-Navaei and J. Skolnick. Ligand binding studies, preliminary structure-activity relationships and detailed mechanistic characterization of 1-phenyl-6,6-dimethyl-1,3,5-triazine-2,4-diamine derivatives as inhibitors of *Escherichia coli* dihydrofolate reductase. *European Journal of Medicinal Chemistry* 2015: **103**: 600-614. PMID: PMC4610388.
361. E. Chow and J. Skolnick. Effects of confinement on models of intracellular macromolecular dynamics. *Proc Natl Acad Science* 2015: **112**(48): 14846-14851. PMID: PMC4672785.
362. S. Tonddast-Navaei and J. Skolnick. Are protein-protein interfaces special regions on a protein's surface? *Journal of Chemical Physics* 2015: **143**(24): 243149. PMID: PMC4684567.
363. J. Skolnick, M. Gao and H. Zhou. How special is the biochemical function of native proteins? *F1000Research* 2016: **5**(F1000 Faculty Rev): 207. PMID: PMC4765716.
364. H. Zhou and J. Skolnick. A knowledge-based approach for predicting gene-disease associations. *Bioinformatics* 2016: **32**(18): 2831-8. PMID: PMC5018378.
365. B. Srinivasan, H. Marks, S. Mitra, D. Smalley and J. Skolnick. Catalytic and substrate promiscuity: Distinct multiple chemistries catalyzed by the phosphatase domain of receptor protein tyrosine phosphatase. *Biochemical Journal* 2016: **473**: 2165-2177. PMID: PMC5049700.
366. T. Snell, R. Johnson, B. Srinivasan, H. Zhou, M. Gao and J. Skolnick. Repurposing FDA-

- approved drugs for anti-aging therapies. *Biogerontology* 2016: **17**(5-6): 907-920. PMID: PMC5065615.
367. B. Srinivasan, H. Zhou, S. Mitra and J. Skolnick. Novel small molecule binders of human N-glycanase 1, a key player in the endoplasmic reticulum associated degradation pathway. *Bioorganic and Medicinal Chemistry* 2016: **24**(19): 4750-4758. PMID: PMC5015769.
368. J. Skolnick. Perspective: On the importance of hydrodynamic interactions in the subcellular dynamics of macromolecules. *The Journal of Chemical Physics* 2016: **145**(10): 100901. PMID: PMC5018002.
369. S. Tonddast-Navaei, B. Srinivasan and J. Skolnick. On the importance of COmposite Protein multiple LIgand (COLIG) Interactions in Protein Pockets. *Journal of Computational Chemistry* 2017: **38**(15): 1252-1259. doi: 10.1002/jcc.24523. PMID: PMC5403588.
370. J. Skolnick and H. Zhou. Why is there a glass ceiling for threading-based structure prediction methods? *Journal of Physical Chemistry B* 2017: **121**(15): 3546-3554 doi: 10.1021/acs.jpcc.6b09517. PMID: PMC5398921.
371. B. Srinivasan, J. Rodrigues, E. Shakhnovich and J. Skolnick. Rational design of novel allosteric dihydrofolate reductase inhibitors showing antibacterial effects on drug resistant *E. coli* escape variants. *ACS Chemical Biology* 2017: **12**(7): 1848-1857. PMID: PMC5819740.
372. E. Chow and J. Skolnick. DNA internal motion likely accelerates protein target search in a packed nucleoid. *Biophysical Journal* 2017: **112**(11): 2261-2270 doi: 10.1016/j.bpj.2017.04.049. PMID: PMC5474843.
373. P. M. Eimon, M. Ghannad-Rezaie, G. De Rienzo, A. Allalou, Y. Wu, M. Gao, A. Roy, J. Skolnick and M. F. Yanik. Brain activity patterns in high-throughput *in vivo* electrophysiology screen predict the true efficacy of compounds. *Nature Communications* 2018: **9**: 219. PMID: PMC5768723.
374. B. Srinivasan, S. Tonddast-Navaei and J. Skolnick. Pocket detection and interaction-weighted ligand-similarity search yields novel high-affinity binders for Myocilin-OLF, a protein implicated in glaucoma. *Bioorganic Medicinal Chemistry Letters* 2017: **27**(17): 4133-4139. PMID: PMC5568477.
375. H. Zhou, M. Gao and J. Skolnick. ENTPRISE-X: Predicting disease-associated frameshift and nonsense mutations. *PlosOne* 2018: **13**(5): e0196849. doi: 10.1371/journal.pone.0196849. PMID: PMC5933770.
376. T. Snell, R. Johnson, A. B. Matthews, H. Zhou, M. Gao and J. Skolnick. Repurposed FDA-approved drugs targeting genes influencing aging can extend lifespan and healthspan in rotifers. *Biogerontology* 2018: <https://doi.org/10.1007/s10522-018-9745-9>. PMID: PMC5834582.
377. J. Skolnick. Editorial: Integrating the whole from the sum of the parts: Vignettes in Computational Biology. *Emerging Topics in Life Sciences* 2017: **1**(3): 241-243.
378. B. Srinivasan, S. Tonddast-Navaei, A. Roy, H. Zhou, J. Skolnick. Chemical Space of *Escherichia coli* Dihydrofolate Reductase Inhibitors: New Approaches for Discovering Novel Drugs for Old Bugs. *Medicinal Research Reviews* 2018: 1-22. <https://doi.org/10.1002/med.21538>. NIHMSID: 990685.
379. H. Cao, M. Gao, J. Skolnick and H. Zhou. The crystal structure of a tetrahydrofolate-bound dihydrofolate reductase reveals the origin of slow product release. *Communications Biology* 2018: **1**:226: <https://doi.org/10.1038/s42003-018-0236-y>. PMID: PMC6290769.
380. H. Zhou, H. Cao and J. Skolnick. FINDSITE^{comb2.0}: A New Approach for Virtual Ligand Screening of Proteins and Virtual Target Screening of Biomolecules. *Journal of Chemical Information and Modeling* 2018: **58**(11): 2343-2354. <https://doi.org/10.1021/acs.jcim.8b00309>. NIHMSID: 1009560.
381. M. Gao, H. Zhou and J. Skolnick. DESTINI: A deep-learning approach to protein structure prediction. (Submitted).
382. H. Cao and J. Skolnick. Time resolved x-ray crystallography capture of a slow reaction tetrahydrofolate intermediate. (Submitted).