

CURRICULUM VITAE

Name: Ruth Nussinov, Ph.D.

Education:

1964	Biology, Hebrew University, Jerusalem, Israel
1964-1966	B.Sc. (Microbiology), University of Washington, Seattle, Washington
1966-1967	M.Sc. (Biochemistry), Rutgers University, New Brunswick, New Jersey
1967-1975	Time off;
1975-1977	Ph.D. (Biochemistry), Rutgers University, New Brunswick, New Jersey

Brief Chronology of Employment:

1977-1980	Postdoctoral Fellow, Structural Chemistry Department, Weizmann Institute, Rehovot, Israel
1980-1981	Visiting Scientist, Chemistry Department, University of California at Berkeley, California
1981-1981	Visiting Scientist, Biochemistry Department, Harvard University, Cambridge, Massachusetts
1981-1981	Visiting Scientist, Chemistry Department, Cornell University, Ithaca, New York
1981-1983	Senior Lecturer, Dept. of Computer Sciences, School of Mathematics, Tel Aviv University, Tel Aviv, Israel
1983-1983	Visiting Scientist, Los Alamos National Laboratory, Los Alamos, New Mexico
1983-1984	Visiting Associate, NIH, National Child Health and Human Development, Bethesda, Maryland
1984-1990	Associate Professor, Sackler Institute of Molecular Medicine, Medical School, Tel Aviv University, Tel Aviv, Israel
1985-2001	Senior Scientist, SAIC, NCI-FCRDC, Frederick, Maryland
1990-2012	Professor of Biochemistry, Department of Human Genetics, Sackler Institute of Molecular Medicine, Medical School, Tel Aviv University, Tel Aviv, Israel
2001-2013	Senior Principal Scientist, SAIC, Computational Structural Biology Section, Nanobiology Program (formerly LECB), Center for Cancer Research, National Cancer Institute, National Institutes of Health, Frederick, MD
2002-2013	Senior Principal Investigator, Leidos Biomedical Research (formerly SAIC), Head, Computational Structural Biology Section, Nanobiology Program (formerly LECB), Center for Cancer Research, National Cancer Institute, National Institutes of Health, Frederick, MD

2012-Present	Professor Emeritus of Biochemistry, Department of Human Genetics, Sackler Institute of Molecular Medicine, Medical School, Tel Aviv University, Tel Aviv, Israel
2013-Present	Senior Principal Investigator, Leidos Biomedical Research, Head, Computational Structural Biology Section, Cancer and Inflammation Program, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Frederick, MD
2016-present	Adjunct Professor, Department of Chemistry & Biochemistry, University of Maryland, College Park
2018-present	Special Member of the Graduate Faculty, University of Maryland, College Park

Societies:

- Protein Society
- Biophysical Society
- American Chemical Society
- International Society for Computational Biology
- American Society for Biochemistry and Molecular Biology
- American Association for Cancer Research

Editor /Editorial Boards - Journals:

- Biophysical Journal (two terms)
- BMC Bioinformatics
- **Editor-in-Chief, PLOS Computational Biology**
Served in this role for many years. I stepped down in March 2019 to take over **PLOS Computational Biology** initiatives to promote pivotal emerging directions in Computational Biology

“Ruth Nussinov has been a leader of this journal for many years... exemplary and visionary leadership of the journal—past, present, and future”

- **Editor-in-Chief, Current Opinion in Structural Biology** (As of July 2019)
- Opinion in Structural Biology (formerly, Editorial Board)
- Journal of Biological Chemistry (JBC)
- Trends in the Pharmacological Sciences (TiPS)
- Journal of Molecular Recognition
- Physical Biology
- Proteins: Structure, Function and Bioinformatics
- Protein Engineering, Design and selectivity
- Intrinsically disordered proteins
- Guest Editor, Chemical Reviews, Special Issue on allostery and conformational ensembles
- Current Pharmaceutical Design

- Guest Editor, Seminars in Cell and Developmental Biology, Special Issue on Signaling in Cancer Initiation and Development
- ACS Medicinal Chemistry Letters Editorial Advisory Board
- F1000

Editor – Books/Issues:

- Methods in Molecular Biology Series: Protocols in Protein Folding (co-edit with Yawen Bai), Humana Press, Totowa, NJ, September 2006
- Methods in Molecular Biology Series: Protocols in Nano Structure Design (co-edit with Ehud Gazit), Humana Press, Totowa, NJ
- Computational Protein-Protein Interactions, CRC Series Press, Taylor and Francis Group (co-edit with Gideon Schreiber)
- Focus Issues in Physical Biology. Three issues:
 - Protein-protein Interactions
 - Nanobiology (with Carlos Aleman)
 - Protein Folding with (Rohit Pappu)
 - Molecular Crowding (with Giuseppe Foffi, Francesco Piazza, Annalisa Pastore)
- Reviews Editor, Frontiers in Molecular and Structural Endocrinology (area of allosteric Regulation)
- Chemical Reviews, Special issue on allostery and conformational ensembles (2015/2016)
- A Special Issue on "The free energy landscape: from folding to cellular function" Physical Chemistry Chemical Physics (PCCP), (co-edited with Peter Wolynes), 2013
- Invited by Tom Blundell to co-edit an issue in Progress in Biophysics and Molecular Biology on Structural Bioinformatics of Protein-Protein Interactions
- Guest Editor, Chemical Reviews, Special Issue "Protein Ensembles and Allostery", 2015
- Co-Editor, Current Opinion Structural Biology, Section of "Folding and Binding", 2016; Protein Nucleic Acid Interactions section, 2021
- Guest Editor, Seminars in Cell and Developmental Biology, 2016

Reviews:

Journals:

- Reviewer for Biochemistry, J. Molecular Biology, TIBS, Proceedings National Academy of Science (USA), Protein Science, Protein Engineering, JACS, Biopolymers, J. Biomolecular Structure and Dynamics, Structure, J. Theoretical Biology, Biophysical J., Proteins, Nucleic Acids Research, Bioinformatics, PLoS, J. Med. Chem., J. Physical Chemistry, J. Chemical Physics, Physical Biology, Trends in Biotechnology, FEBS Lett., PEDS, BMC Series Journals, Nature journals, Science, and many others.

Honors & Other Special Scientific Recognition:

- Scholarship, University of Washington, Seattle WA (1965)
- John Russel Scholarship, Rutgers University, New Brunswick, NJ (1976)

- Weizmann Fellowship (1977)
- On the Presidents' list of the Researchers Attaining the Most External Funding in Tel Aviv University
- Top CCR, NCI Science Advances (2009)
- Recommended by Faculty of 1000: Protein allostery, signal transmission and dynamics: A classification scheme of allosteric mechanisms "A way to categorize allosteric change is proposed on conformational change"
- Among the most highly downloaded PNAS paper (2010)
- Among the most highly downloaded review on the Mechanisms of transcription factor selectivity Trends in Genetics paper (2010)
- Member of the Center for Cancer Research, National Cancer Institute Advisory Board (advises the Scientific Director and the CCR Director)
- Voted unanimously "Distinguished Speaker" by the students of the Molecular Biophysics Program, Northwestern University (June 2010)
- **Voted A Fellow of the 2011 Biophysical Society "for her extraordinary contributions to advances in computational biology on both nucleic acids and proteins"**
- Lecture in the Institute Pasteur, Paris; a seminar series given by eminent scientists (2010)
- Invited by the Chairman of the Board of Directors of Forschungszentrum Jülich, and the Partnership for Advanced Computing in Europe, to Chair the External Overview the Genomic/Biocomputational initiative, Aachen, Germany (January 2011)
- The paper, "Allostery: absence of a change in shape does not imply that allostery is not at play", Tsai, C-J, del Sol, A., and Nussinov, R., J. Mol Biol. 378(1): 1-11, 2008, is among the top 10 cited JMB papers since 2008 (the year of its publication).
- The paper, "Comparing interfacial dynamics in protein-protein complexes: an elastic network approach", Zen, A., Micheletti, C., Keskin, O., and Nussinov, R., BMC Structural Biology, 10:26 (08 Aug 2010) is among the "Highly Accessed".
- Top ten most accessed articles in Molecular Biosystems: "Towards inferring time dimensionality in protein-protein interaction networks by integrating structures: the p53 example", Tuncbag, N., Kar, G., Gursoy, A., Keskin, O., and Nussinov, R., Mol. Biosyst. 5(10): 1770-1778, 2009.
- Citation in the Coordinator's Report for Technical and Management Report of the National Cancer Institute as "a recognized leader in the field and having exemplary record of accomplishments" and "for having a great record of training and mentoring", 2011
- Our paper, "Antimicrobial protegrin-1 forms amyloid-like fibrils with rapid kinetics suggestion a functional link", Biophysical Journal was selected for the "New and Notable" highlights, 2011
- Distinguished J. Clarence Karcher (Rosetta Barton) Lecturer in "Frontiers in Chemical Research", University of Oklahoma, 2011
- Fellow, Institute of Physics, London, UK, 2011
- Cited by SAIC, NCI-Frederick as being "Internationally recognized leader", 2011
- Author of one of the top 1% most highly cited papers in the field worldwide according to the Council of Canadian Academies letter, 2011

- Placed by Thomson Reuters in the top 5% of cited authors for journals in Biology and Chemistry, 2011
- Distinguished Ulam Scholar, The Center for Nonlinear Studies (CNLS), Los Alamos National labs, 2012
- Paper, “How do dynamic cellular signals travel long distances?” in Mol. Biosyst. has been selected as “Hot paper”, 2012
- Paper, “How do dynamic cellular signals travel long distances?” in Mol. Biosyst. is a top accessed paper, 2012
- Max Planck Institute for the Physics of Complex Systems, Institute Colloquium Speaker, Dresden, Germany, 2012
- Paper on, “Protein dynamics and conformational selection in bidirectional signal transduction”, in BMC Biology, has achieved a ‘Highly Accessed’ level, 2012
- Our Current Opinion in Structural Biology paper "Constructing structural networks of signaling pathways on the proteome scale" is among the most read/downloaded papers, 2012
- Nussinov R, Ma B: Protein dynamics and conformational selection in bidirectional signal transduction. BMC Biol; 2012; 10:2 PMID: 22277130 heads the top 20 articles in its domain in its domain in BioMedLib since its publication, 2012
- Our TiBS paper “Allosteric post-translational modification codes is among the most downloaded/read
- Identified by Thomson Reuters as “a scientist with prestigious publication history in biology and biochemistry
- The manuscript on Enriching the human apoptosis pathway by predicting the structures of protein-protein complexes was featured in Global Medical Discovery
- Nominated for the President of the Biophysical Society, narrowly losing to Jane Richardson
- The paper "Allosteric post-translational modification codes", Nussinov et al. TiBS, stood out as the outstanding winner among all winners of the STFC 2012 Publication Awards, NCI for" pointing the way to a body of new research, 2012
- **Elected Fellow of the International Society of Computational Biology (ISCB), for significant contributions to the fields of computational biology and biochemistry**, particularly through her work in the areas of protein alignment and docking, protein structure and function, and the proposition and development of the conformational selection and population shift model for binding, and allostery. Nussinov has authored over 450 scientific papers, and is highly cited, 2013
- Publication selected for Spotlight by the NCI- Basic Science Program: Nussinov R, Tsai C-J: Allostery in disease and in drug discovery. Cell 153(2): 293-305, 2013The article Allostery in disease and in drug discovery. Nussinov R, Tsai CJ: Cell 153: 293-305, 2013 highlighted in F1000 Structural Biology: "So far, allostery has been largely described as a molecular event that occurs in a population of a single-protein species. But, in this insightful review, Nussinov and Tsai suggest that the concept should be extended to explain the regulation of functional cellular networks in which multiple protein components participate. Another important take-home message is that the new concept can be a useful theoretical framework for drug-development strategies. The authors also nicely present the historical overview on the efforts to explain the allostery at a molecular

level. So, I strongly recommend this review to students in the wide areas such as biochemistry, biophysics, and pharmacology”, 2013

- The manuscript "Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection" in *Angewandte Chemie* has been designated a "Hot Paper", 2014
- Awarded the The Michael and Ada Anbar Lectureship in the Biophysical Sciences, Buffalo University, 2014
- The biophysical students in the Chemistry and Molecular Biophysics and Biochemistry Departments at Yale University voted an invitation as a “Student Invited Speaker to help keep this continuing BPTG tradition of prestigious speakers.” 2014
- Fellow Internationally recognized scientist, RWTH Aachen University, Institute for Advanced Simulation and Institute for Neuroscience and Medicine, Forschungszentrum Jülich, and German Research School for Simulation Sciences, 2015
- **Elected a Theodore von Kármán Fellow Award**, Germany, 2015
- **The 2015 Sarkar Lecturer**, Molecular Structure & Function Program, the Hospital for Sick Children (SickKids). The lecturer is selected each year by the Program's students and PDFs for “Distinguished Research”. Toronto, Canada, 2015.
- **Special Life Time Award**. The Israeli Society for Bioinformatics and Computational Biology (ISBCB), Tel Aviv University, Tel Aviv 2015
- **Computational Molecular Medicine: A minisymposium dedicated to Ruth Nussinov, Aachen, Germany, 2015**
- Invited Elected Senior Fellow, International Society for Computational Biology Keynote Speaker in the ISMB 2016. Orlando, Fl. 2016
- **Highly Cited Researcher**. “**Highly Cited Researcher represents some of world’s most influential scientific... About three thousand researchers earned this distinction by writing the greatest number of reports officially designated by Essential Science Indicators as Highly Cited Papers — ranking among the top 1% most cited for their subject field and year of publication, earning them the mark of exceptional impact.**” (<http://highlycited.com/> Thomson Reuters, December 2015). **Covering an 11-year period (and presenting a special subset of “hot” researchers whose very recent work has won distinction in the form of citations).**
- A special invitation from the Chemistry Department at Hamilton College: As part of a comprehensive assignment, to explore physical chemistry concepts and methods using the work of a Distinguished Scholar as a common thread: “course emphasizes molecular interactions and conformations, thermodynamics, and kinetics, and you have contributed new concepts that have changed the way biophysicists and structural biologists think about protein folding, protein-protein interactions, and ligand binding. (... can’t imagine a student graduating with a Biochemistry degree without knowing your research!)... Being exposed to the depth and breadth of your work, which includes applications relevant to health such as cancer and inflammation, would be tremendously beneficial and inspiring to [the students]”, 2015.
- The paper [Allostery without a conformational change? Revisiting the paradigm](#) is the most highly saved *Current Opinion in Structural Biology* paper in 2015.
- The paper [Structural Modeling of GR Interactions with the SWI/SNF Chromatin Remodeling Complex and C/EBP](#) by Muratcioglu S. et al. *Biophys J.* 2015 Sep 15;109(6):1227-39. doi: 10.1016/j.bpj.2015.06.044. is among the “Best of 2015 re-print issue of the Biophysical Journal”

- **Voted unanimously Adjunct Professor**, Department of Chemistry & Biochemistry, University of Maryland, College Park, 2016
- **Invited Speaker, Xingda Lecture Series**, the College of Chemistry and Molecular Engineering, Peking University, China, 2017
- **Our AACR 2015 paper “The Key Role of Calmodulin in KRAS-Driven Adenocarcinomas”**, was the most highly-cited in the journal (MCR) and selected by AACR to highlight in the 2017 AACR Annual Meeting, including a printed collection and a dynamic online edition of most-cited articles. <http://sm.aacr.org/BE1230aDESh> <http://cdn.coverstand.com/32673/393305/d2d497b517d1c188e426b6c5a65034dd55ab833a.6.pdf>
- The Best of the AACR Journals Collection: Author Profiles (2017) <http://aacrjournals.org/content/bestof-author-profiles#>
Four of our reviews on RAS as well as four of our research papers that we published on RAS signaling were flagged by the Web of Science as “As of November/December 2016, this [highly cited paper](#) received enough citations to place it in the top 1% of the academic field of Chemistry based on a highly cited threshold for the field and publication year” (Thomson Reuters, April 2017).
- JBC selected two of our papers for their special virtual issues (<http://www.jbc.org/site/vi/>): one for the Structural Biology issue (GTP Binding and Oncogenic Mutations May Attenuate Hypervariable Region (HVR)-Catalytic Domain Interactions in Small GTPase K-Ras4B, Exposing the Effector Binding Site. Lu S, Banerjee A, Jang H, Zhang J, Gaponenko V, Nussinov R. *J Biol Chem*. 2015 Nov 27;290(48):28887-900, where our Ras mutant paper was elected <http://www.jbc.org/content/290/48/28887.full.pdf>); the second for the Ion Channels (Allostery modulates the beat rate of a cardiac pacemaker. Tsai CJ, Nussinov R. *J Biol Chem*. 2017 Apr 14;292(15):6429-6430 (<http://www.jbc.org/content/292/15/6429.full.pdf>))
- Our [Phosphorylated Calmodulin Promotes PI3K Activation by Binding to the SH₂ Domains](#). Zhang M, Jang H, Gaponenko V, Nussinov R. *Biophys J*. 2017 Nov 7;113(9):1956-1967. doi: 10.1016/j.bpj.2017.09.008 selected to head the **Best of 2017** papers in a special issue of the *Biophysical J*.
- Our K-Ras4B/Calmodulin paper (Flexible-body motions of calmodulin and the farnesylated hypervariable region yield a high-affinity interaction enabling K-Ras4B membrane extraction. Jang H, Banerjee A, Chavan T, Gaponenko V, Nussinov R. *J Biol Chem*. 2017 Jul 28;292(30):12544-12559) was the first among two publications selected from all September 2017 published papers in *JBC* for highlighting.
- **KeyLab Award for outstanding achievements** in biomolecular simulations in Translational Medicine, **Ho Chi Minh City (Saigon), Vietnam**, 2018. The Award is by Vietnam/Germany (Forschungszentrum Jülich). The Award is by Vietnam/Germany (Forschungszentrum Jülich). This is the second year of the Award. First year’s prize was awarded to Michele Parrinello.
- **The ISCB 2018 Accomplishment Award by a Senior Scientist Award** <http://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1006138>
- **Highly Cited Researcher**. “Highly Cited Researcher represents some of world’s most influential scientific... About three thousand researchers earned this

distinction by writing the greatest number of reports officially designated by Essential Science Indicators as Highly Cited Papers — ranking among the top 1% most cited for their subject field and year of publication, earning them the mark of exceptional impact.” (<http://highlycited.com/> Thomson Reuters, December 2018). Covering an 11-year period (and presenting a special subset of “hot” researchers whose very recent work has won distinction in the form of citations).

- Our publication on the ramification of ubiquitination of Ras’ hypervariable region (HVR) to amplification of MAPK signalling and rasopathy (Science, Dec 2018) was highlighted by CCR (https://ccr.cancer.gov/news/article/protein-mutations-lead-to-human-disease-by-altering-a-cancer-promoting-pathway?cid=eb_govdel)
- Invited by AACR President (and agreed) to serve as **Chairperson of the AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee** (2018-2019)
- Our article “Unraveling the molecular mechanism of interactions of the Rho GTPases Cdc42 and Rac1 with the scaffolding protein IQGAP2” has been selected as the representative ‘Computational biology’ article for our 2018 retrospective collection called “The year in JBC: 2018.” <http://www.jbc.org/site/vi/2018/>
- Special Member of the Graduate Faculty, University of Maryland, College Park, 2018
- Scientific Council, Forschungszentrum Juelich GmbH, Germany, 2019
- Organizing Committee, Workshops on evolutionary medicine, Institute for Mathematics and its Applications (IMA), at the University of Minnesota during the Spring 2021

Committees and Boards:

Advisory committee reviewing the Department of Bioinformatics in Bergen, Norway; Site visit committee of DCRT (Division of Computing Resources and Technology, NIH); Site visit committee GMD Institute of Algorithms, Bonn, Germany; NCI Steering Committee for Bioinformatics and Computational Biology NCI; NCI Steering Committee for Systems Biology; NCI Immunology Center of Excellence; Program Committee, Intelligent Systems in Molecular Biology Brazil, 2006; Program Committee, Intelligent Systems in Molecular Biology-ECCB, Vienna, 2007; Advisory Committee Modeling Protein Interactions; Numerous tenure and promotion committees and evaluations; Chair, Graduate Studies in Bioinformatics; Organized the NIH-INRIA (France) Workshop; Program Committee, Intelligent Systems in Molecular Biology; External Review Committee for the Science Focus Area for Basic Energy Research, Los Alamos National Laboratory to assess LANL capability to address Gene Function Discovery; PC Member of Bioinformatics Track, 2008; Tenure/Tenure Track Committee at the NIH, 2008; Site Visitor, Biomolecular Modeling Laboratory, Cancer Research UK London Research Institute, 2009; Chair, NIH-wide Earl Stadtman Investigator in Computational Biology, 2009/2010; Program Committee, ECCB, Protein and Nucleotide Structure, 2010; Member, Earl Stadtman NIH-wide tenure-track Investigator Search Committee, 2010, 2011; Invitation, Earl Stadtman NIH-wide tenure-track Investigator Search Committee, 2011, 2012; NSF external advisory board of the University of Chicago, multiscale theory and simulation for bimolecular systems, 2011-2013; Assisted in many other meeting organizations; Organizing Committee, Modeling of Protein Interactions, November 2012; Faculty Committee, Uppsala University,

February 2013; National Academy of Sciences, Molecular Dynamics ANTON Award Committee (2013); The NIH Stadtman Investigator Search Committee in Computational Biology, 2013/2014; Review Committee, Universite' de Toulouse, LAAS, CNRS, Toulouse, France, April, 2014; Site Visit Committee, Quinquennial Review, London Cancer Research Institute, London, UK, 2009; Invited to Site Visit the theory group, Los Alamos, 2010; Invited by AERES (Agence d'Evaluation de la Recherche et des etablissements d'Enseignement Superieur) to Site Visit CEA Saclay in Paris, 2010; Site Visit Committee, RWTH Aachen University and the Forschungszentrum Julich, German Research School, responsible for the Laboratory of Computational Biophysics, 2011; Site Visit Committee, Chair, Site visit of the German Research School for Simulation Science, FZ-Julich and RWTH Aachen, 2011; NSF Advisory Board, University of Chicago, 2013; Advisory Board, responding to the recommendation "Thought Leaders from the Various Structural Biology Disciplines..." to overview "the future of structural biology is hybrid" in the Protein Data Bank (PDB). UK, 2014; Scientific Advisory Board and Management of Heidelberg Institute for Theoretical Studies, Heidelberg, Germany, 2015; International Scientific Advisory Board, Center for Computer-Aided Drug Design, China Pharmaceutical University, Nanjing, China, 2015; Biophysical Society Fellows Committee, 2017; AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee, 2018-2019; NCI, Tenure Search Committee Cancer Data Science Lab (CDSL), 2018; Chairperson of the AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee (2018-2019); Scientific Council, Forschungszentrum Juelich GmbH, Germany, 2019; Organizing Committee, Workshops on evolutionary medicine, Institute for Mathematics and its Applications (IMA), at the University of Minnesota during the Spring 2021; AACR Innovation Summit October 2019

Numerous various other Committees and Boards (also listed below)

Community Activities:

- Advisory Committee to Modeling of Protein Interactions since its inception in 2001
- IEEE Computer Soc. Bioinformatics, Stanford Program Committee, 2003
- Elected Member to the Council of the Biophysical Society
- IEEE Computer Soc. Stanford, Program Committee, 2005
- Elected Council Member, Biophysical Society (2005-2008)
- Biophysical Society, Abstract Sort and Speaker Assignment, many times
- INRIA-NIH; Organized on behalf of NIH together with French Embassy, 2007
- NCI Steering Committee in Bioinformatics and Computational Biology
- NCI Steering Committee in Systems Biology
- NCI Faculty of Structural and Chemical Biology
- Supervisor, SAIC, NCI-Frederick
- Organizer in Gordon Research Conference on Protein Interaction Dynamics: Theory, Methods, and Practice, January 2008
- Search Committee for the Editor of Proteins
- Serves on the NCI/CCR Site Visit Team to UMD to Foster Collaborations
- Ad hoc Member of the CSR Molecular Structure and Function Study Section (Computational Biophysics Panel)

- Program Committee ECCB08
- Co-Chair: Protein Structure and Allosteric Communication, 52nd Biophysical Society Meeting & 16th IUPAB Biophysics Congress
- Invited to Serve as a Member of the Macromolecular Structure and Function D Study Section for the Center for Scientific Review, NIH
- External Review Committee for the Science Focus Area for Basic Energy Research, Los Alamos National Laboratory, to assess LANL capability to address Gene Function Discovery
- Evaluation panel Ghent University, 2008
- Reviewer for the GRC Board of Trustees, 2009, 2009
- Site Visit Committee, Quinquennial Review, London Research Institute, London, UK, 2009
- Responded to the request to assist in the review of the NIH American Recovery and Reinvestment Act (ARRA) Challenge Grant RFA, 2009
- Assisted the NIGMS Grant Opportunity (GO grants, RC2 mechanism) Award Program, 2009
- MSFD NIH Study Section, 2009
- Committee Chair for Trans-NIH Tenured or Tenure Track Recruitment in Systems Biology, and Earl Stadtman Investigators, for top-tier tenure-track candidates to become “NIH Earl Stadtman Investigators” in Computational Biology.
- MSFD NIH Study Section, Long Term Member, 2009-2015
- Member of the Center for Cancer Research, National Cancer Institute Advisory Board
- Invited to serve on the reviewing committee in CEA Saclay, Agence d’Evaluation de la Recherche et des etablissement d’Enseignement Superieur, Paris, France, March 2010
- Graduate School Committee, Computational Biophysics, German Research School for Simulation Sciences GmbH, GmbH, Aachen, Germany, January 2011
- External Reviewer of Computational, Genomics and Systems Biology in GmbH, Aachen, Germany, 2011
- NSF external advisory board of the University of Chicago, multiscale theory and simulation for biomolecular systems, 2011
- NSF-Structural Biochemistry Review Panel, 2011
- NSF external advisory board of the University of Chicago, multiscale theory and simulation for bimolecular systems, 2011- to date
- Editor-in-Chief, PLoS Computational Biology
- Editor/Editorial Boards: Physical Biology; Proteins; JBC; BMC Bioinformatics; Intrinsically disordered proteins; Critical Opinion in Structural Biology, and more
- Review Committee, Universite' de Toulouse, LAAS, CNRS, Toulouse, France, April, 2014
- Advisory Board, responding to the recommendation "Thought Leaders from the Various Structural Biology Disciplines..." to overview "the future of structural biology is hybrid" in the Protein Data Bank (PDB). UK, 2014
- International Scientific Advisory Board, Center for Computer-Aided Drug Design, China Pharmaceutical University, Nanjing, China, 2015
- Biophysical Society Fellows Committee, 2018-2021

- **AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee (2018)**
- Chair, search committee to identify multiple tenure track/tenure eligible investigators for the Cancer Data Science Laboratory (CDSL), at the CCR, NCI, 2018.
- **Chairperson of the AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee (2019)**. The Award is for outstanding, novel, and significant chemistry research, which has led to important contributions to the fields of basic cancer research; translational cancer research; cancer diagnosis; the prevention of cancer; or the treatment of patients with cancer (2019)
- Scientific Council, Forschungszentrum Juelich GmbH, Germany, 2019
- Organizing Committee, Workshops on evolutionary medicine, Institute for Mathematics and its Applications (IMA), at the University of Minnesota, during the Spring 2021
- Asked to serve as Advisor to initiate and lead research projects in the Institute of Bioinformatics and Medical Engineering, Jiangsu University of Technology, 2019-to date
- Invited to serve on the **AACR Innovation Summit** panel “to bring together ... a small group of individuals (45 total) ... (leaders in the fields of emerging technologies, big data, artificial intelligence, systems and computational biology, and their application to cancer research and care) ... to discuss emerging technologies and methodologies that are uncovering new cancer pathways. The primary goal is ... to attack the cancer problem, to determine the challenges in integrating these diverse disciplines, and to identify new opportunities for the AACR to further address these challenges”, October 2019
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Reviews:

Journals:

- Reviewer for Biochemistry, J. Molecular Biology, TIBS, Proceedings National Academy of Science (USA), Protein Science, Protein Engineering, JACS, Biopolymers, J. Biomolecular Structure and Dynamics, Structure, J. Theoretical Biology, Biophysical J., Proteins, Nucleic Acids Research, Bioinformatics, PLoS, J. Med. Chem., J. Physical Chemistry, J. Chemical Physics, Physical Biology, Trends in Biotechnology, FEBS Lett., PEDS, BMC Series Journals, Nature journals, and many others.

Grants:

- Welcome Trust Funds (Britain), Australian Grant system, Austria, Canadian grants (Research Council of Canada), NSF, Israel Academy of Science, Special advisor to GIF (German - Israel Funds); BSF (US-Israel Binational Science Foundation); CPA II, Center of Excellence Academy of Science; U.S. Army; NSF; NIH Project Grants; NSF Cancer Development Award; DOE; Netherland Science Foundation; Petroleum Research Fund; NIAID; Science Center Programs of the U.S. Department of State; Cyprus Grant System, and numerous others.

Students:

- About 70 current and past advised and co-advised graduate students since 1990

Grants - at Tel Aviv University, and at the NCI:

- Center of Excellence (funded by the Israel Academy of Science)
- U.S. Army
- Tel Aviv Research Foundation
- Da'at Consortium – Industry Development Grant
- Adams Brain Center
- U.S. Army (to Tel Aviv Univ.)
- Binational Science Foundation
- Israel Academy of Science
- Ministry of Science
- ADMET Consortium for Drug Design Joint with Industry
- NIAID (Renewed July 2007 for 3 years)
- U.S. Army (to the NCI)
- PI NCI – Nano Alliance (with Barcelona; extended 2009)
- NCI Nanotechnology Alliance for Cancer (2006-2008). Collaboration with Polytechnic University of Catalonia
- Our student received the UMD-NCI Fellowship (2017, 2018)
- With our help our young collaborator won a K99 (2017-)
- We have co-collaborated on several submitted/funded NIH grants (no cost for us)

Invited Talks (Since 2004):

26. Invited Speaker, Special Symposium in Quantum Bioinformatics in Kyoto Hall, Kyoto, Japan, 2004.
27. Invited Speaker, University of Tokyo, Japan, 2004.
28. Invited Speaker, Kyushu Technical University, Kyushu, Japan, 2004.
29. Invited Speaker, Biophysical Society Meeting, Baltimore, MD, 2004.
30. Organizer and Invited Speaker, Protein Interactions, Philadelphia, PA, 2004.
31. Invited Speaker, Program Committee of the Third IEEE Computer Society Bioinformatics Conference, Stanford, CA, 2004.
32. Invited Speaker, From Structural Genomics to Drug Design, Palma, Italy, 2004.

33. Invited Speaker, Frontiers in Computational Biophysics and Drug Design, organized by the U.S. Army, Frederick, MD, 2004.
34. Invited Speaker, DARPA Workshop on Protein Stability and Preservation, Fairfax, VA, 2005.
35. Invited Speaker, Biophysical Society Meeting, Long Beach, CA, 2005.
36. Invited Speaker, Bologna Winter School, Bologna, Italy, 2005.
37. Invited Speaker, ACS Meeting, San Diego, CA, 2005.
38. Invited Speaker, Biodefense Workshop, Frederick, MD, 2005.
39. Invited Speaker, DIMACS Workshop on Systems Biology, 2005.
40. Organizer and Invited Speaker, Protein Society Meeting, Barcelona, Spain, 2005.
41. Invited Speaker and Organizer, Protein Flexibility, Tempe, AZ, 2005.
42. Invited Speaker 14th Conversation Biomolecular Stereodynamics, Albany, NY, 2005.
43. Invited Speaker and on Organizing Committee, Protein Interactions, Lawrence, KS, 2005.
44. Invited Speaker, IEEE Computer Society Bioinformatics Conference, Program Committee, Stanford, Palo Alto, CA, 2005.
45. Featured Speaker, JCIS Meeting, Salt Lake City, UT, 2005.
46. Invited Speaker, Biophysics Program, Opening the Seminar Year, University of Wisconsin, Madison, WI, 2005.
47. Invited Talk, Laboratory of Structural Biology Research, NIH, Bethesda, MD, 2005.
48. Invited Speaker, Hebrew University, Jerusalem, Israel, 2005.
49. Featured Speaker, Annual Molecular Biophysics Symposium, University of Michigan, Ann Arbor, MI, 2006.
50. Invited Speaker, CCP4 (Collaborative Computational Project 4) Synchrotron Radiation Department, Leeds, United Kingdom, 2006.
51. Invited Speaker, Biochemistry and Molecular Biophysics, Washington University, St. Louis, MO, 2006.

52. Chair and Invited Speaker, Biophysical Society Meeting, Symposium on Nanobiology, Salt Lake City, UT, 2006.
53. Invited Speaker, CECAM Workshop on Self Assembly and Aggregation, Lyon, France, 2006.
54. Invited Speaker, Nanobiology, Barcelona, Spain, 2006.
55. Invited Speaker, Joint SIAM Conference on the Life Sciences, Raleigh, NC, 2006.
56. Invited Speaker, Gordon Conference on Cellular Systems Biology, Mt. Holyoke College, South Hadley, MA, 2006.
57. Invited Speaker, Virginia Tech, Blacksburg, VA, 2006.
58. Invited Speaker, Purdue University, Washington, DC, 2006.
59. Invited Featured Keynote Speaker, Keck Center, Houston, TX, 2006.
60. Invited Speaker, Polytechnique de Catalonia, Barcelona, Spain, 2006.
61. Invited Speaker, Koc University, Istanbul, Turkey, 2007.
62. Invited Speaker, Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel, 2007.
63. Invited Speaker, Center for Non-Linear Studies: Biosystems, Biophysics and Soft Matter Seminar Series, Los Alamos, 2007.
64. Chair and Speaker, Biophysical Society, Baltimore, MD, 2007.
65. Invited Speaker, Two Decades to the Launching of the Human Genome Project, Boston, MA, 2007.
66. Organizer and Chair, INRIA (French Institute for Computational Sciences)/NIH Workshop on Biomedical and Life Science Computing, Bethesda, MD, 2007.
67. Invited Speaker, EMBO Workshop on Disordered Proteins, Budapest, Hungary, 2007.
68. Invited Speaker, Workshop on Structure and Dynamics in Soft Matter and Macromolecules: From Single Molecules to Ensembles, the International Center for Theoretical Physics, Trieste, Italy, 2007.
69. Invited Speaker, 234th ACS Meeting, Boston, MA, 2007.
70. Invited Speaker, GTCbio First Protein Discovery and Development Summit, Washington, DC, 2007.

71. Invited Speaker, NIH Systems Biology Interest Group, NIH, Bethesda, MD, 2007.
72. Invited Speaker, Program in Structural and Computational Biology and Molecular Biophysics, Baylor College of Medicine, Houston, TX, 2007.
73. Invited Speaker, Modeling Protein Interactions, Kansas City, MO, 2007.
74. Invited Speaker, Workshop on RNA in Biology, Bioengineering and Nanotechnology, Minneapolis, MN, 2007.
75. Invited Participant, Nanotechnology Alliance Meeting, Chapel Hill, NC, 2007.
76. Invited to Serve on the NCI/CCR Site Visit Team to UMD and Present Open Collaborative Areas, 2007.
77. Invited Talk, Dahlem Colloquia in Molecular Genetics, Berlin, Germany, 2007.
78. Invited Speaker, Polymer Research Center and Chemical Engineering Department, Bogazici University, Istanbul, Turkey, 2007.
79. Invited Speaker, Sabanci University, Istanbul, Turkey, 2007.
80. Chair and Session Organizer, Gordon Research Conference, Protein Interaction Dynamics: Theory, Methods, Practice, Ventura, CA, 2008.
81. Invited Talk, Albert Einstein College of Medicine, Bronx, NY, 2008.
82. Invited to Chair a Session in the Biophysical Society Meeting, Long Beach, CA, 2008.
83. Invited Keynote Speaker, International Symposium on Health Informatics and Bioinformatics, Istanbul, Turkey, 2008.
84. Invited Panelist, Bio-Geometry and Computational Chemistry, ACM Symposium (Association for Computing Machinery, Solid and Physical Modeling, Stonybrook, NY, 2008.
85. Invited Speaker, 2nd International Conference on Molecular Perspectives on Protein-protein Interactions, Dubrovnic, Croatia, 2008.
86. Invited Plenary Talk, 2008 President's Meeting of the International Society of Quantum Biology and Pharmacology (ISQBP). Pushing the Boundaries of Biomolecular Simulation. Centro Stefano Franscini, Ascona, Switzerland, 2008.
87. Invited Speaker, Telluride Workshop on Characterizing Landscape: From Biomolecules to Cellular Networks, Telluride, CO, 2008.

88. Chair, Organizer and Invited Speaker, Gordon Conference on Macromolecular Organisation and Cell Function, Oxford, England, 2008.
89. Invited Speaker, American Chemical Society, Protein Folding Session, Philadelphia, PA, 2008.
90. Invited Talk, American Chemical Society Meeting, Symposium Combining Computational Chemistry with Sequence-based Bioinformatics for Structure-Function-Activity Relationships, Philadelphia, PA, 2008.
91. Invited Talk, GTBio, Protein-Protein Interactions, San Diego, CA, 2008.
92. Invited Talk, Protein Structure and Mechanics Symposium, Shanghai, China, 2008.
93. Invited Talk, Department of Chemistry, University of Miami, Miami, FL, 2008.
94. Invited Distinguished Lecturer, Molecular Basis of Disease Program, Georgia State University, Atlanta, GA, 2008.
95. Invited Talk, Gibbs Conference, Carbondale, IL, 2008.
96. Invited Talk, University of Missouri-Columbia, Columbia, MO, 2008.
97. Invited to give Lectures, International Course on Computational Structural Biology, Brno, Czech Republic, 2008.
98. Plenary BigRoc* Lecture, Weizmann Institute, Israel, 2008.
99. Invited Talk, Indiana University School of Medicine, Indianapolis, IN, 2008.
100. Invited Talk, Biowulf Symposium, Bethesda, MD, 2009.
101. Invited Talk, Johns Hopkins, Baltimore, MD, 2009.
102. Invited Talk, Symposium, Biophysical Society Meeting, Boston, MA, 2009.
103. Invited Keynote Speaker, 9th Swedish Bioinformatics Workshop, Umea, Sweden, 2009.
104. Invited Talk, Technion, A Workshop on RNA, DNA, and Protein Structure Prediction, Haifa, Israel, 2009.
105. Invited Talk, Chemistry Department, Penn State, University Park, PA, April 2009.
106. Invited Speaker, International Jacques Monod Conference, Centre Paul Langevin in Aussois (Savoie), France, 2009.

107. Invited Lecturer (three 2-hr lectures), The International School for Advanced Studies SISSA, Trieste, Italy, 2009.
108. Invited Talk, CECAM Workshop, Frontiers in Bio-molecular Aggregation, Dublin, Ireland, 2009.
109. Organizer and Chair, Biomolecular Structure and Dynamics, Albany, NY, 2009.
110. Organizer, NIH-INRIA Meeting on Biomedical Computing, Paris, France, 2009.
111. Invited Talk, Hebrew University, Jerusalem, Israel, 2009.
112. Invited Talk, 2nd Conference on Drug Development for the Third World: From Computational Molecular Biology to Experimental Approaches ICTP, Trieste, Italy, 2009.
113. Invited Talk, Telluride Workshop on Method Development for Protein Structure Prediction, Telluride, CO, 2009.
114. Invited Talk, Kavli Institute of Theoretical Physics in China (KITPC), a sister site to the KITP in Santa Barbara, CA, Beijing, China, 2009.
115. Invited Talk, International Symposium on Multi-Scale Dynamics of Protein Complex Formation, Tokyo, 2009.
116. Invited Talk, ACS Meeting, Washington, DC, 2009.
117. Invited Talk, CECAM Workshop, Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly, Lausanne, Switzerland, 2009.
118. Invited Talk, University of Akron, Chemical and Biomolecular Engineering, Akron, OH, 2009.
119. Invited Talk, Hebrew University, Jerusalem, Israel, 2009.
120. Invited Talk, Integrative Genomics and Department of Chemical Engineering, Princeton University, Washington, DC, 2009.
121. Invited Talk and Session Chair, Keystone Symposia on Biomolecular Interaction Networks: Function and Disease, Quebec, Canada, 2010.
122. Invited Talk, National Natural Science Foundation of China (NSFC), Theoretical and Experimental Approaches to Drug Design, Changzhou, China, 2010.

123. Invited Speaker, Biological Interfaces: A TYC Computational Modelling Workshop, King's College London, London, UK, 2010.
124. Invited Speaker, Proteins: Dynamics, Folding and Function Symposium, University of Maryland, MD, 2010.
125. Invited to give main lecture, First International Conference on Molecular Recognition under the auspices of Aegean Conferences, Crete, 2010.
126. Distinguished Speaker, Inaugural Annual Biophysics Symposium, Molecular Biophysics Training Program at Northwestern University, Evanston, IL, 2010.
127. Invited Speaker, Telluride, CO, 2010.
128. Invited Talk, CIPSM Lecture (Center of Integrated Protein Science Munich) and Physical Chemistry Series, Munich, Germany, 2010.
129. Invited Talk, 240th American Chemical Society National Meeting and Exposition, Boston, MA, 2010.
130. Invited Speaker, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA, 2010.
131. Invited Talk, Korean Protein Society, 10th International Conference on Protein Structure, Dynamics and Function, Seoul, Korea, 2010.
132. Invited Talks (two) & Keynote Speaker, Conference on Molecular Aspects of Cell Biology: A Perspective from Computational Physics, ICTP. Trieste, Italy, 2010
133. Invited Speaker, Modeling Protein Interactions, Lawrence, KS, 2010.
134. Invited Talk, Faculty of Agriculture, Hebrew University, Rehovoth, Israel, 2010.
135. Invited Speaker, Southeast/Southwest Regional ACS Meeting, New Orleans, 2010.
136. Invited Keynote Speaker, 2010 IEEE International Conference on Bioinformatics & Biomedicine (BIBM2010), Hong Kong, 2010.
137. Invited talk, Computational Biophysics, German Research School for Simulation Sciences GmbH, GmbH, Aachen, Germany, 2011.
138. Invited Speaker, Macromolecular Complexes & Interactions, ILANIT Conference, Eilat, 2011.
139. Invited talk, George Washington University, Biochemistry and Molecular Biology Department, Washington, DC, 2011.

140. Invited Speaker, Program Frontiers in Genomics 2011 of the National University of Mexico, the Center for Genomic Sciences (CCG), the Institute of Biotechnology (IBT) and the Undergraduate Program of Genomic Sciences of the National University of Mexico and the Mexican Society of Genomic Sciences, Cuernavaca, Mexico, 2011.
141. Invited committee member and talk in the Department of Biology, University of Copenhagen, Denmark, 2011.
142. Invited talk, Howard Hughes Medical Institute, Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX, 2011.
143. Invited talk, ACS Meeting, Anaheim, CA, 2011.
144. Invited talk, Mini Workshop on Modeling Electrostatics in Molecular Biology, Clemson, SC, 2011.
145. Invited Teacher, University of Copenhagen Summer School on Protein Science, Spetses Island, Greece, 2011.
146. Invited talk, FASEB 2011 Summer Research Conference entitled: "The Basic Origins and Medical Consequences of Protein Aggregation", Snowmass, CO, 2011.
147. Invited Keynote Lecture at 3DSig, Vienna, ISMB, 2011.
148. Invited Speaker, Semmelweis University, School of Medicine, Department of Medical Chemistry, Budapest, Hungary, 2011.
149. Invited talk, International Conference on Mathematical Biology, Bangalore, India, 2011.
150. Invited talk, Biological & Soft Matter Physics Seminar, Arizona State University, Phoenix, AZ, 2011.
151. Invited talk, Biochemistry and Biomedical Sciences' Seminar Series, McMaster University, Hamilton, Ontario, Canada, 2011.
152. Invited talk, Barcelona Biomed Conference on Macromolecular Dynamics (BBCMD), Barcelona, Spain, 2011.
153. Invited talk, University of Massachusetts at Boston, 2011.
154. Session Chair, Macromolecular Dynamics Conference, Barcelona, 2011.
155. Invited Plenary speaker, Protein and RNA Structure Prediction Conference, Cancun, Mexico, 2011.

156. Invited talk, Gordon Research Conference, Ventura, CA, 2012.
157. Invited talk, University of Colorado at Boulder, Boulder, CO, 2012.
158. Invited talk, Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ, 2012.
159. Invited talk, Symposium in American Physical Society (APS) Meeting, Austin, TX, 2012.
160. Invited talk, Iowa State University, Ames, IA, 2012.
161. Invited talk, Addex, Geneva, Switzerland, 2012.
162. Invited Distinguished J. Clarence Karcher (Rosetta Barton) Lecturer in "Frontiers in Chemical Research", University of Oklahoma, 2012.
163. Invited talk, Anchoring simulations to experiments: challenges for understanding and treating Alzheimer's disease, Cecam Meeting, Paris, 2012.
164. Invited talk, the Department of Experimental Therapeutics and the Center for Targeted Therapy, Univ. Texas M.D. Anderson Cancer Center, 2012.
165. Invited talk at the ACS Mid-Atlantic Regional Meeting, Frontiers in the Application of Computational Chemistry to Biological Systems, Maryland, 2012.
166. Invited talk, Gordon Research Conference, Biopolymers, Salve Regina, Newport, RI, 2012.
167. Session Chair, Gordon Research Conference, Biopolymers, Salve Regina, Newport, RI 2012.
168. Invited speaker, international conference on Molecular Crowding: Chemistry and Physics meet Biology, ETHZ Monte Verita Congress center at Ascona, Switzerland, 2012.
169. Colloquium, Distinguished Ulam Scholar, The Center for Nonlinear Studies (CNLS), Los Alamos National Labs, 2012.
170. Invited talk, Conference on protein plasticity in allostery, evolution, and self-assembly, Dresden, 2012.
171. Invited Plenary Speaker and Special Max Planck Institute for the Physics of Complex Systems, Institute Colloquium Speaker Conference on protein plasticity in allostery, evolution, and self-assembly, Dresden, 2012.
172. Invited talk, q-bio seminar, Los Alamos, 2012.

173. Organizer, Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, 2012.
174. Invited talk, ACS Symposium on "Continuum Solvation Modeling in Biological Systems: Developments and Applications", Philadelphia, 2012.
175. Invited talk, ACS Symposium on "multi-scale modeling of biological systems", Philadelphia, 2012.
176. Invited Speaker, CNIO Frontiers Meetings: Allosteric Regulation of Cell Signaling, Madrid, 2012.
177. Invited Keynote Speaker in the German Conference on Bioinformatics, Jena, Germany, 2012.
178. Invited talk, Exploring Protein Interactions through Theory and Experiments, Cecam, Lausanne, Switzerland, 2012.
179. Invited Speaker, Cecam, "Signalling pathways: interplay between microscopic changes and global behaviour of biological systems", Ecole Normale Supérieure de Cachan, France, 2012.
180. Invited lectures (2), at the School in Biological Physics of Protein Folding and Conformational Diseases, Rio de Janeiro, Brazil, 2012.
181. Invited talk, Department of Chemistry and Biochemistry, University of Notre Dame, Indiana, 2012.
182. Invited talk, Department of Computational Medicine and Bioinformatics seminar, University of Michigan, Ann Arbor, 2012.
183. Invited speaker, Biophysics seminar, University of Michigan, Ann Arbor, 2012.
184. Invited talk, Modeling of Protein Interactions, Lawrence, Kansas, 2012.
185. Invited Colloquium speaker, Chemistry Graduate Students Association, Northeastern University, 2012.
186. Invited speaker, Department of Bioengineering, University of Maryland, 2012.
187. Invited Plenary Speaker, Mathematical and Computational Medicine Conference, Zing Conference, Occidental Grand Xcaret, Mexico, 2012.
188. Invited speaker, King's College London, London, UK, 2013.
189. Invited talk, Biological Sector, Department of Chemistry, University of Cambridge,

- Cambridge, UK, 2013.
190. Invited Plenary talk, Royal Society of Chemistry, Protein-protein Interaction Meeting, London, UK, 2013.
 191. Invited speaker, Department of Biology, Copenhagen Biocenter, University of Copenhagen, Copenhagen, Denmark, 2013
 192. Invited seminar speaker, Chemistry Department, Drexel University, Philadelphia, PA, 2013.
 193. Invited Distinguished Speaker, College of Medicine, University of South Florida, Tampa, 2013.
 194. Invited speaker, Uppsala University, Sweden, 2013.
 195. Invited Talk, CSIR-Indian Institute of Chemical Biology, Transcription and Chromatin Conference, 2013.
 196. Invited to participate in a Speaker panel at the American Physical Society meeting, Baltimore, MD, 2013
 197. Invited seminar speaker, Department of Bioinformatics and Genomics, University of North Carolina at Charlotte, Charlotte, NC, 2013.
 198. Plenary speaker at the CCP-BioSim Conference: Frontiers of Biomolecular Simulation 2013, the University of Nottingham, UK, 2013.
 199. Invited seminar speaker, Chemistry Department, University of Cincinnati, April 2013.
 200. Invited speaker, Protein Dynamics Conference, Durham, UK, 2013.
 201. Invited speaker, Department of Chemistry at Bowling Green State University in Ohio, 2013.
 202. Invited Speaker, "Computational Biology: Then and Now" Weizmann Institute of Science, Rehovoth, Israel, 2013.
 203. Invited talk, Department of Pharmaceutical Sciences at the University of Maryland, Baltimore, 2013.
 204. Invited talk, Cancer and Inflammation Symposium, National Cancer Institute, Bethesda, 2013.
 205. Invited talk, Clinical Genomics Unit, Head and Neck Surgery Branch, NIDCD, National Cancer Institute, Bethesda, MD, 2013.

206. Invited Keynote Speaker, SNP-SIG: Identification and annotation of SNPs in the context of structure, function, and disease, ISMB, Berlin, Germany, 2013.
207. Invited talk, American Chemical Society (ACS) Symposium, Indianapolis, IN, 2013.
208. Invited keynote lecture, the 2013 ACM Conference on Bioinformatics, Computational Biology, and Biomedicine (ACM BCB 2013), Washington, DC 2013.
209. Keynote speaker, Computational Structural Bioinformatics Workshop, ACM Conference On Bioinformatics, Computational Biology and Biomedical Informatics, Bethesda, MD, 2013.
210. Invited colloquium in the Center for Structural Biology, University of Florida, Gainesville, FL, 2013.
211. Invited speaker, Annual Anbar Lecture, honoring and endowed by the Chair of Biophysics, Neuroscience Program, University at Buffalo, NY, 2013.
212. Keynote talk, PLOS Computational Biology Board meeting, Washington, DC, 2013.
213. Invited Speaker, International Structure Biology and Functional Genomics (SBFG) Conference: Five Facets of Human Genome Function, National University of Singapore, Singapore, 2013.
214. Invited Keynote speaker, Basel Chemical Society, Symposium on Targeting Protein-Protein Interactions, Basel, Switzerland, 2013.
215. Invited keynote speaker, Special Symposium on Protein-DNA Modeling, Bioscience and Bioinformatics, Graduate School of Computer Science and Systems Engineering, Kyushu Institute of Technology, Iizuka, Fukuoka, Japan, 2014.
216. Invited speaker, Molecular Modeling and Simulation, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Kyoto, Japan, 2014.
217. Invited speaker, Laboratory for Integrated Cellular Systems, RIKEN Center for Integrated Medical Sciences, Yokohama, Japan, 2014.
218. Invited speaker, Molecular Biology and Genetics, Virginia Commonwealth University VCU, Richmond, VA, 2014.
219. The Michael and Ada Anbar Award Lecture in the Biophysical Sciences, Buffalo University, 2014.
220. Invited speaker, Ras Symposium, NCI, Shady Grove, MD, 2014.

221. Invited Speaker, EMBO Workshop on Magnetic Resonance for Cellular Structural Biology, Fattoria La Principina, Principina Terra, Grosseto, Italy, 2014.
222. Invited Speaker, The Nobel Swedish Structural Biology Meeting, Tallberg, Sweden, 2014.
223. Invited Speaker, Protein Folding, Misfolding, Aggregation & Diseases, 8th IUPAP International Conference on Biological Physics, Beijing, China, 2014.
224. Invited lecturer, FEBS advanced course, Ligand-binding theory and practice, Nove' Hradý, the South Bohemian Region of the Czech Republic, 2014.
225. Invited Keynote Speaker, Gordon Research Conference on Intrinsically Disordered Proteins, Stonehill College, Easton, MA, 2014.
226. Discussion Leader, Gordon Research Conference Human Single Nucleotide Polymorphisms & Disease. Stonehill College, Easton, MA, 2014.
227. Invited Speaker, ACS Symposium, Modeling the Effects of Water and Solvation in Biological Systems: Developments and Applications, San Francisco, CA, 2014.
228. Invited Speaker, Special Symposium on Modeling of Protein Kinases and Phosphorylation: Protein Dynamics, Regulation, Function and Signal Transduction, San Francisco, CA, 2014.
229. Invited Speaker, the Biophysical Society Thematic Meeting "Modeling of Biomolecular Systems Dynamics, Allostery and regulation: Bridging Experiment and Computations", Istanbul, Turkey, 2014.
230. Invited wWPDB "The future of structural biology is hybrid", European Bioinformatics Institute (EBI), Hinxton, UK, 2014.
231. Invited Speaker, Modeling of Protein Interactions. Lawrence, Kansas, 2014.
232. Chair, 40+ Years of Protein Structure Analysis. Symposium. NIH, Bethesda, MD, 2014.
233. Invited Speaker, University of Maryland Department of Chemistry, 2014.
234. Invited Speaker, the Cancer: Research, Discovery and Therapeutics BioConference Live, 2014.
235. Invited Speaker, Koc University, Istanbul, December 2014
236. Invited Speaker, University of Florida, 2015.

237. Invited Speaker, Physics of Proteins Focus Session, the American Physical Society meeting, San Antonio, Texas, 2015.
238. Invited Speaker, The CCB (Chemistry and Chemical Biology Graduate Program)/iPQB (Integrative Program in Quantitative Biology, encompassing Biophysics, Bioinformatics and Systems Biology) Seminar, University of California San Francisco, 2015.
239. Invited Speaker, ACS Symposium on Membranes and Amyloids, Denver, Colorado, March, 2015.
240. Invited Speaker, ACS Symposium on Progress and Challenges in Molecular Simulations of Biomolecules, Denver, Colorado, 2015.
241. Invited Speaker, Biophysical Properties and Biological Significance of Amyloid- β Assemblies, Cold Spring Harbor Laboratory symposium, Banbury Center, Cold Spring Harbor Laboratory, 2015
242. Invited Speaker, **The 2015 Sarkar Lecturer**, Molecular Structure & Function Program, the Hospital for Sick Children (SickKids). The lecturer is selected each year by the Program's students and PDFs for "Distinguished Research". Toronto, Canada, 2015.
243. Yale University, The Biophysical Students in the Chemistry and Molecular Biophysics and Biochemistry Departments voted invitation as the "Student Invited Speaker to help keep this continuing BPTG tradition of prestigious speakers", 2015.
244. Invited Speaker, Dept. of Chemistry and Biochemistry, University of Maryland, 2015
245. Invited Speaker, Department of Chemistry and Biochemistry, University of Oklahoma, 2015
246. Invited Keynote Speaker, From Computational Biophysics to Systems Biology (CBSB2015), Oklahoma, 2015.
247. Invited Speaker, Special Life Time Award talk. The Israeli Society for Bioinformatics and Computational Biology (ISBCB), Tel Aviv University, Tel Aviv 2015
248. Invited Speaker, Workshop on the physical properties of viral RNA, Trieste, Italy, 2015
249. Invited keynote speaker, symposium on Structural Bioinformatics, 98th Canadian Chemistry Conference, Ottawa, 2015
250. Invited keynote speaker, ISMB, ISCB Student Council Symposium, Dublin, 2015
251. Invited Speaker, Shanghai International Symposium on Computational Chemistry, sponsored by the NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai, 2015

252. Invited Speaker, Physics Department, Fudan University, Shanghai, China, 2015
253. Invited Speaker, Medicinal Bioinformatics Center, Shanghai Jiaotong University Jiantao University, Shanghai, 2015
254. Invited Speaker, Queenstown Molecular Biology Meeting, Computational Genomics satellite, Queenstown, New Zealand, September 2015
255. Invited Speaker, ComBio 2015, Australian Society for Biochemistry and Molecular Biology, Australia and New Zealand Society for Cell and Developmental Biology, New Zealand Society for Biochemistry and Molecular Biology and New Zealand Society of Plant Biologists. Melbourne, Victoria, 2015
256. Theodore von Kármán Award Lecture, and Seminar, Aachen, Germany, 2015
257. Invited Speaker, Department of Organic Chemistry, Aachen University, Aachen, Germany, 2016
258. Computational Molecular Medicine: **A minisymposium dedicated to Ruth Nussinov**, Aachen, Germany, 2015
259. Invited Speaker, Biomolecular Interactions, The National Centre for Biological Sciences (NCBS), Bangalore, India, 2015
260. Invited Speaker, Workshop 4: Mathematical Challenges in Drug and Protein Design. The Mathematical Biosciences Institute (MBI). Columbus, Ohio, 2015.
261. Invited Speaker, American Chemical Society Pacificchem Symposium “Metal ions and protein function: theoretical models and applications”. Hawaii, 2015
262. Invited Speaker, Koc University, Istanbul, Turkey, 2016
263. Invited Speaker, Chemistry Department, University of Cincinnati, OH, 2016
264. Invited Speaker, American Society for Biochemistry & Molecular Biology (ASBMB), special symposium on Small Molecule Modulators in genomic Reprogramming, co-organized by the CSIR-Institute of Genomics and Integrative Biology, New Delhi, India, 2016
265. Invited teacher as part of a comprehensive student assignment to explore physical chemistry concepts and methods using the work of a Distinguished Scholar as a common thread, where the work is explored over the entire semester. Department of Chemistry, Hamilton College, 2016

266. Invited Speaker, Symposium on Landscapes, Pathways, and Kinetics in Biomolecular Simulations (retitled: Computer Simulations of Thermodynamics and Long Time Kinetics of Molecular Events), ACS meeting, Denver, CO, 2016
267. Invited Speaker, Symposium on peptide for protein-protein interruption. ACS meeting, Denver, CO 2016
268. Keynote Speaker, Gordon Research Conference "Human Single Nucleotide Polymorphisms & Disease: Understanding the Mechanisms of Variant Effects in the Era of Genome Sequencing", Mount Holyoke College, South Hadley, MA, 2016
269. Invited Plenary Speaker to the 2nd edition of the Protein Engineering Canada (PEC) Conference, Ottawa, Canada, 2016
270. Invited Keynote Speaker in the ISMB 2016, as ISCB Fellow. Orlando, FL. 2016
271. Invited Plenary Speaker, CECAM Workshop on "Multiscale modeling of biomolecular aggregation and protein-membrane interactions in amyloid diseases". Universite della Svizzera Italiana (USI), Lugano, Switzerland, 2016
272. Invited talk, FEBS advanced course "Ligand-binding theory and practice", South Bohemia, Czech Republic, 2016
273. Invited Speaker, ACS meeting, Philadelphia, PA, 2016
274. Invited Plenary Speaker, and organizer. PLOS Computational Biology Symposium. NIH, Bethesda, MD, 2016
275. Invited Speaker, University of St. Louis, MO, 2016
276. Invited talk, Department of Laboratory Medicine, NIH Clinical Center, America's Research Hospital, 2016
277. Featured Speaker, International Conference on Cancer Research and Targeted Therapy, Baltimore, MD, 2016
278. Invited Speaker, New York Academy of Sciences Symposium. Chemical Biology: Identifying, Characterizing and Validating Targets for Drug Discovery. New York, 2016
279. Invited Speaker, Modeling Protein Interactions, Lawrence, Kansas, 2016
280. Invited Speaker, Relay Therapeutics, Boston, MA, 2016.
281. Invited Speaker, Mathematical Challenges in Drug and Protein Design, Columbus, OH, 2015

282. Invited Keynote Address at the ISCB-Latin America in Buenos Aires. Buenos Aires, Argentina, 2016
283. Keynote Speaker, the 2nd Latin American Student Council Symposium (LA-SCS), Buenos Aires, Argentina, 2016
284. Invited Plenary talk in a Symposium titled: Advances in Enzymology: Implications in Health, Disease, and Therapeutics. Mumbai, India, 2017.
285. Invited Speaker, da Vinci Convergence Symposium: A Scientific Summit on Computational Modeling Across the Scales, aiming to image the whole body at the atomic scale. Santa Monica, 2017
286. Invited Speaker, Copenhagen Bioscience Conference 2017, in the series of biannual highprofile conferences in Copenhagen "Data-driven Biotechnology" - the use of big biological data and models in health-related and industrial biotechnology. The conference is organized by the Novo Nordisk Foundation together with The Novo Nordisk Foundation Center for Biosustainability, Copenhagen, Denmark, 2017
287. Invited Speaker, NCI-Frederick faculty seminar series, 2017.
288. Invited seminar speaker, Laboratory of Cell Biology, NIH. Bethesda, MD, 2017
289. Invited Speaker, ACS meeting, session on Allostery, San Francisco, CA, 2017
290. Invited Speaker, 9th IUPAP International Conference on Biological Physics (ICBP2017), Rio de Janeiro, Brazil, 2017.
291. Invited Speaker. Computational Aspects of Biomolecular NMR Gordon Research Conference. Sunday River, Maine, 2017
292. Invited Speaker, International Conference on Biological Physics (ICBP2017), Symposium on Protein Folding, Misfolding and Structural Prediction Rio de Janeiro, Brazil
293. Invited Plenary Speaker, Interdisciplinary Signalling Workshop, Visegrad, Hungary, 2017
294. Invited Speaker, International Symposium on Protein Misfolding Diseases, University of Catania, Catania, Sicily, Italy, 2017
295. Invited Speaker, ACS Symposium "Molecular recognition: Revealing the effects associated with receptor-ligand binding", Washington DC, 2017
296. Invited talk, Chemistry Department, Peking University, Beijing, China, 2017
297. **Invited Speaker, Xingda Lecture Series**, the College of Chemistry and Molecular Engineering, Peking University, Beijing, China, 2017

298. Invited Distinguished Speaker, Computer Science Department, Virginia Tech, Blacksburg, Virginia 2017
299. Keynote talk, Brazilian Bioinformatics and Computational Biology Association, San Paulo, Brazil, 2017
300. Invited Speaker, Laboratory of Metabolism seminar series, NIH, Bethesda MD 2017
301. Invited Speaker, “Computational approaches to investigating allostery, Lausanne, Switzerland, 2017
302. Invited Speaker, Heidelberg International Chronic Inflammation Workshop, Heidelberg, Germany, 2017
303. Invited Speaker, Biophysical Society Meeting, San Francisco, CA, 2018
304. Invited talk, American Chemical Society Meeting, Insights into Structure, Function, Dynamics and Evolution of Enzymatic Mechanisms from Computational Simulation. New Orleans, Louisiana, 2018
305. Invited Speaker, Towards a Unified Approach to the Analysis and Design of Allostery, Lausanne, Switzerland, 2018
306. Invited Keynote **KeyLab Award** Lecture, workshop on “Recent computational and experimental advances in molecular medicine”. Ho Chi Minh City, Vietnam, 2018
307. The ISCB 2018 Accomplishment Award by a Senior Scientist Award Keynote talk, Chicago, IL, 2018
308. Invited Keynote Speaker, Neurological Disorders, Dead Sea, Israel, 2018
309. Invited Speaker, Cold Spring Harbor Asia Conference entitled “Frontiers in Computational Biology and Bioinformatics 2018.” Dushu Lake Hotel and Conference Center, Suzhou, China
310. Invited Speaker, Multiscale simulations of allosteric regulatory mechanisms in cancer-associated proteins and signaling protein networks, Lugano, Switzerland, 2018
311. Invited speaker, Univ of Maryland-NCI Partnership Symposium, Univ. of Maryland, College Park, 2018
312. Invited Speaker, Modeling Protein Interactions, Lawrence, Kansas, 2018
313. Invited Speaker, Pathomechanisms of Amyloid Diseases, Miami, FL, 2018

314. Invited Speaker, Koc University, Istanbul, 2019
315. Invited Speaker, Biophysics Seminar series, MARYLAND BIOPHYSICS PROGRAM. The College of Computer, Mathematical, and Natural Sciences, University of Maryland, College Park, 2019
316. Invited Speaker, ACS meeting, Orlando, Florida, 2019
317. Invited Speaker, BME faculty seminar series featuring prominent nationwide and international scientists, Oregon Health & Science University (OHSU) Biomedical Engineering, Portland, Oregon, 2019
318. Invited Speaker, MIT, Spring at the MIT Math & MIT's Computer Science and Artificial Intelligence Laboratory Seminar, 2019
319. Invited talk Jiangsu University of Technology, Changzhou, China, 2019
320. Invited Speaker, ACS meeting, San Diego, 2019
321. Invited Speaker, Cleveland Clinic, Lerner College of Medicine, Case Western Reserve University, Cleveland, 2019
322. Invited Speaker, Annual Symposium of the Center of Excellence in Immunology at the National Cancer Institute, Bethesda, 2019
323. Keynote Speaker, the IV International Conference on Cancer Research & drug Development, Baltimore, 2019
324. Invited Speaker, FAST Foundation (<https://fast.foundation/>) meeting, Armenia, 2019 (could not attend)
325. Invited Speaker, Biochemistry Department Colloquium, the University of Wisconsin-Madison. 2019
326. Invited Commencement MolTag (Molecular Targets) Doctoral Program Opening Event Speaker, University of Vienna, 2019
327. Invited Speaker, Pathomechanisms of Amyloid Diseases, Miami Beach, Florida, 2019
328. Keynote Speaker (following dinner following dinner), 2020 Protein Folding Dynamics Gordon Research Conference, Galveston, Texas, 2020
329. Invited Speaker, ACS meeting, Philadelphia, 2020
330. Invited Speaker, Trieste/Sissa, Italy, 2020

331. Invited Distinguished Speaker, Forschungszentrum Juelich GmbH, Germany, 2020

BIBLIOGRAPHY

Published:

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