

## 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
- American Physical Society

Editor /Editorial Boards - Journals:

- *Biophysical Journal* (two terms)
- *BMC Bioinformatics* Editorial Board
- **Editor-in-Chief, PLOS Computational Biology**  
Served in this role for close to a decade; stepped down in 2019 to take up Editor-in-Chief of *Current Opinion in Structural Biology*.  
“Ruth Nussinov has been a leader of this journal for many years... exemplary and visionary leadership of the journal—past, present, and future” (Subsequent PLOS CB Editorial)
- **Editor-in-Chief, Current Opinion in Structural Biology** (As of July 2019)
- *Current Opinion in Structural Biology* (formerly, Editorial Board)
- *Journal of Biological Chemistry* (JBC)
- *Trends in the Pharmacological Sciences* (TiPS)
- *Structure* Editorial Advisory Board (Cell Press)
- Journal of Molecular Recognition Editorial Board
- *Physical Biology* Editorial Board
- *Proteins: Structure, Function and Bioinformatics*, Editorial Board
- *Protein Engineering, Design and selectivity* (PEDS) Editorial Board
- *Chemical Reviews*, Guest Editor, Special Issue on allostery and conformational ensembles
- Current Pharmaceutical Design

- Seminars in Cell and Developmental Biology, Special Issue on Signaling in Cancer Initiation and Development, Guest Editor
- *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 SH<sub>2</sub> 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](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
- Invited to serve and 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”, and to speak, October 2019
- **A 3.5 Day symposium in honor of Ruth Nussinov ACS Fall 2020 meeting “Dynamic ensembles, cell signaling and drug discovery: A symposium in honor of Ruth Nussinov” ACS Fall 2020 meeting, San Francisco, August 2020**

“Ruth Nussinov is a computational biologist who has made extraordinary contributions to advances in the understanding of structure and function of biomacromolecules. Early on she proposed the first algorithm for the prediction of RNA secondary structure, which is still the leading algorithm today. She was also a pioneer of DNA sequence analysis. Especially, she proposed the “Conformational Selection and Population Shift” as an alternative to the textbook “Induced-Fit” model in molecular recognition, a paradigm of vast importance in signaling and drug discovery. She further proposed that energy landscapes are dynamic with the shifts in the conformational ensembles following perturbation events the basis of allostery under normal conditions and in disease. Building on these concepts, recently she has been studying Ras signaling in cancer. The symposium will invite scientists from academia, industries, and national labs who have worked on these topics or collaborated with Ruth Nussinov in the areas of conformational ensembles, allostery in signaling and drug discovery, Ras and oncogenic signaling, etc. Speakers are by invitation only.”



- **A Festschrift Special Issue in honor of Ruth Nussinov Achievements, ACS, Journal of Physical Chemistry, 2021**
- Special Achievement Award of the Frederick National Laboratory for cancer Research with the following citation: “Dr. Ruth Nussinov received the highest score possible on a recent site visit and has received numerous international awards and honors. Dr. Nussinov’s work reaches a level of mechanistic detail that is hard for experimental or big data strategies alone to attain, leading to deeper understanding and innovative ideas. Dr. Nussinov is recognized world-wide as having made significant contributions to the area of protein dynamics and function and the intramural research program benefits greatly from her expertise and insights.”
- Annual Achievement Award Frederick National Laboratory for Cancer Research, 2020 “... The NCI Intramural Research Program benefits greatly from her expertise and insight. ... Her ability to conceive ideas and influence the research community to adopt and follow them is a testament to her scientific leadership. Dr. Nussinov’s work reaches a level of mechanistic detail that other strategies struggle to attain alone. Her efforts have expanded scientists’ knowledge and inspired new ideas....”
- Elected Fellow of the American Physical Society (APS) “For extraordinary advancements in the understanding of the structure and function of biomacromolecules, an algorithm for predicting RNA secondary structure, and the Conformational Selection and Population Shift concept as an alternative to the Induced-Fit model in molecular recognition.” APS Division of Biological Physics, 2020
- Highlighted by the Frederick National Laboratory for Cancer Research (2020) <https://frederick.cancer.gov/news/ruth-nussinov-elected-fellow-american-physical-society>
- Elected Fellow, American Institute for Medical and Biological Engineering (AIMBE) College of Fellows (2021)
- Featured as the woman in science in Women’s History by ISCB (2021)
- Plenary Speaker, CRD, Cancer Research and Drug Development, 2021; along with Ethan Dmitrovsky, Director, Frederick National Laboratory for Cancer Research, President, Leidos Biomedical Research, Eric B. Kmiec, Director, Gene Editing Institute, Helen F. Graham Cancer Center & Research Institute, ChristianaCare DE, and Robert A. Weinberg, MIT Director, MIT Ludwig Center for Molecular Oncology, MA, <https://cancerresearchconference.org/plenary-keynote>
- **Biophysical Chemistry, special issue in honor of Professor Ruth Nussinov (2022). Computational Data-Driven Design and Modeling of Biomolecules and Biomimetics.** Guest Editors: Professor Jie Zheng, Department of Chemical, Biomolecular, and Corrosion Engineering, University of Akron, OH, USA; Professor Nurit Haspel, Computer Science, University of Massachusetts, Boston, MA, USA; Professor Liqun Zhang, Chemical Engineering, Tennessee Tech, Cookeville, TN, USA.
- Two of our publications were selected by *Chemical Science*, the flagship journal of the Royal Society of Chemistry, among the “Most popular 2019-2020 physical and theoretical chemistry articles”. One tops the list; the second is among those selected. <https://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=sc&themeid=d4362257-448d-4dbc-8d11-fc0cce3ca91f> 2022

- **Ranked 63 in the world, and 44 in United States among the Top 1000 Female Scientists in the World according to [Research.com](https://research.com), a leading academic platform for researchers (2022)**
- **According to <https://research.com/scientists-rankings/best-scientists> Ranked within the 1000 most highly researchers in the World (851) in the world, and 548 in the US <https://research.com/scientists-rankings/best-scientists/us> (2022)**
- Developmental Core leadership Duke Center for HIV Structural Biology (2022)
- Advisory board, the RWTH Center for Computational Life Science, Germany, “Computational Chemistry”, bridging the Clinics, departments of Physics, Chemistry, and Biology, and Mechanical Engineering.
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### 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 établissements d’Enseignement Supérieur) 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; Developmental Core leadership Duke Center for HIV Structural Biology (2022)

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, 52<sup>nd</sup> Biophysical Society Meeting & 16<sup>th</sup> 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
- **A 3.5 Day symposium in honor of Ruth Nussinov ACS Fall 2020 meeting “Dynamic ensembles, cell signaling and drug discovery: A symposium in honor of Ruth Nussinov” ACS Fall 2020 meeting, San Francisco, August 2020**  
“Ruth Nussinov is a computational biologist who has made extraordinary contributions to advances in the understanding of structure and function of biomacromolecules. Early on she proposed the first algorithm for the prediction of RNA secondary structure, which is still the leading algorithm today. She was also a pioneer of DNA sequence analysis. Especially, she proposed the “Conformational Selection and Population Shift” as an alternative to the textbook “Induced-Fit” model in molecular recognition, a paradigm of vast importance in signaling and drug discovery. She further proposed that energy landscapes are dynamic with the shifts in the conformational ensembles following perturbation events the basis of allostery under normal conditions and in disease. Building on these concepts, recently she has been studying Ras signaling in cancer. The symposium will invite scientists from academia, industries, and national labs who have worked on these topics or collaborated with Ruth Nussinov in the areas of conformational ensembles, allostery in signaling and drug discovery, Ras and oncogenic signaling, etc. Speakers are by invitation only.” <https://callforpapers.acs.org/sanfrancisco2020/COMP>
- **A Festschrift Special Issue in honor of Ruth Nussinov Achievements, ACS, Journal of Physical Chemistry, 2020**
- Special Achievement Award of the Frederick National Laboratory for cancer Research with the following citation: “Dr. Ruth Nussinov received the highest score possible on a recent site visit and has received numerous international awards and honors. Dr. Nussinov’s work reaches a level of mechanistic detail that is hard for experimental or big data strategies alone to attain, leading to deeper understanding and innovative ideas. Dr. Nussinov is recognized world-wide as having made significant contributions to the area of protein dynamics and function and the intramural research program benefits greatly from her expertise and insights.”
- Annual **Achievement Award Frederick National Laboratory for Cancer Research, 2020** “... The NCI Intramural Research Program benefits greatly from her expertise and insight. ... Her ability to conceive ideas and influence the research community to adopt and follow them is a testament to her scientific leadership. Dr. Nussinov’s work reaches a

level of mechanistic detail that other strategies struggle to attain alone. Her efforts have expanded scientists' knowledge and inspired new ideas....”

- **Consulted the NCI subcommittee on ‘Intelligent drug discovery based on biochemistry, structure, and mechanisms**, including computational and artificial intelligence-driven drug discovery’ for a workshop focusing on ‘Intelligent drug discovery’. 2021
- **Steering Committee of a machine learning platform for drug discovery, developed at Mila AI research institute in Montreal, Quebec, Canada. 2021**  
<https://deepgraphlearning.github.io/torchdrug-site-dev/> TorchDrug is a machine learning platform designed for drug discovery, covering techniques from graph machine learning (graph neural networks, geometric deep learning & knowledge graphs), deep generative models to reinforcement learning. It provides a comprehensive and flexible interface to support rapid prototyping of drug discovery models in PyTorch.
- **Advisory board IIT-FZJ (Helmholtz European Partnering Project), Genoa, Italy, 2021-2022**
- **Personal invitation to join the Royal Society of Medicine, London, as a member (fellow)**
- **Ranked 63 in the world, and 44 in United States among the Top 1000 Female Scientists in the World according to [Research.com](https://research.com), a leading academic platform for researchers (2022)**
- **According to <https://research.com/scientists-rankings/best-scientists> Ranked within the 1000 most highly researchers in the World (851) in the world, and 548 in the US <https://research.com/scientists-rankings/best-scientists/us> (2022)**
- **Developmental Core leadership Duke Center for HIV Structural Biology (2022)**
- **Advisory board, the RWTH Center for Computational Life Science, Germany, “Computational Chemistry” ”, bridging the Clinics, departments of Physics, Chemistry, and Biology, and Mechanical Engineering.**
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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 14<sup>th</sup> 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, 234<sup>th</sup> 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, 2<sup>nd</sup> 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, 9<sup>th</sup> 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, 2<sup>nd</sup> 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, 240<sup>th</sup> 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, 10<sup>th</sup> 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 Superieure 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, Nové 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- $\beta$  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 to speak in 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”**, Philadelphia, 2019
323. Invited Speaker, Annual Symposium of the Center of Excellence in Immunology at the National Cancer Institute, Bethesda, 2019
324. Keynote Speaker, the IV International Conference on Cancer Research & drug Development, Baltimore, 2019

325. Invited Speaker, joint meeting between NCI/CIP and German Cancer Research Center (DKFZ), Bethesda, 2019
326. Invited Speaker, FAST Foundation (<https://fast.foundation/>) meeting, Armenia, 2019 (could not attend)
327. Invited Speaker, Biochemistry Department Colloquium, the University of Wisconsin-Madison. 2019
328. Invited Commencement MolTag (Molecular Targets) Doctoral Program Opening Event Speaker, University of Vienna, 2019
329. Invited Speaker, Pathomechanisms of Amyloid Diseases, Miami Beach, Florida, 2019
330. Keynote Speaker (following dinner following dinner), 2020 Protein Folding Dynamics Gordon Research Conference, Galveston, Texas, 2020
331. Invited Speaker, “**Systems immunology**: Repertoire and beyond”. “Beyond”: **Single cell applications to immunology** and structural studies of antibodies. University of Surrey, UK, 2020
332. Invited Distinguished University Colloquium Series, “Biophysics Can Help Resolve Biological Mysteries: Examples from Oncogenic Signaling”, Koc University, Istanbul, 2020
333. Invited Speaker, ACS meeting, Philadelphia, 2020
334. Invited Speaker, The Biophysics Program Seminars series, University of Maryland, College Park, 2020
334. Invited Speaker, Biophysical Society thematic meeting, Biophysics at the Dawn of Exascale Computers, Hamburg, Germany, 2020 (postponed 2021)
336. Invited Speaker, Trieste/Sissa, Italy, 2020 (postponed 2021)
337. Invited Distinguished Speaker, Forschungszentrum Juelich GmbH, Germany, 2020 (postponed)
338. Invited speaker, Symposium on Pathomechanisms of Amyloid Diseases, Catania, Italy, 2020 (postponed)
339. **A 3.5 Day symposium in honor of Ruth Nussinov ACS Fall 2020 meeting “Dynamic ensembles, cell signaling and drug discovery: A symposium in honor of Ruth Nussinov” ACS Fall 2020 meeting, San Francisco, August 2020** (postponed to 2021)

340. Invited speaker, Univ of Pennsylvania Physiology (<https://www.med.upenn.edu/physiol/>), 2020
341. Invited Speaker, Colloquium, Univ. of Maryland, College Park, 2020 (postponed 2021)
342. Invited Speaker, HITS Colloquium series, Heidelberg, Germany, 2020 (postponed 2021)
343. Invited Speaker, **American Physical Society Awards Symposium**, 2021
344. Frederick National Laboratory for Cancer Research, Faculty series, 2020
345. Invited talk, Department of Pharmacology at Case Western Reserve University, 2020
346. Invited Plenary talk, ISCB Symposium for STEM students, 2021
347. Invited Plenary talk, Memoriam for Prf. Akinori Sarai. Japan, 2021
348. Invited talk, CECAM workshop on "Quantifying Protein Dynamics and Allosteric regulation in the cell with emerging technologies: From Cryo-EM and NMR to Multiscale Simulations, Networks and Machine Learning", 2021, Lausanne and virtual
349. Invited talk, Biophysical Society Symposium, "Protein Data Bank (PDB) Celebrates 50 Years". Virtual, 2021
350. **Plenary Speaker, CRD, Cancer Research and Drug Development, 2021**; along with Ethan Dmitrovsky, Director, Frederick National Laboratory for Cancer Research, President, Leidos Biomedical Research, Eric B. Kmiec, Director, Gene Editing Institute, Helen F. Graham Cancer Center & Research Institute, ChristianaCare DE, and Robert A. Weinberg, MIT Director, MIT Ludwig Center for Molecular Oncology, MA, <https://cancerresearchconference.org/plenary-keynote>
351. University of Maryland, Biophysics colloquium, 2022
352. Invited colloquium talk, Case Western University, 2022
353. Invited talk, Drexel University, PA, 2022
354. Invited Speaker at the HITS (Heidelberg Institute for Theoretical Studies) Colloquium series, Molecular and Cellular Modeling Group, DKFZ-ZMBH Alliance and Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Germany 2022
354. Invited Speaker, Hamburg Thematic Meeting, Biophysics at the Dawn of Exascale Computers, Hamburg, Germany, 2022

356. Invited Keynote Speaker, Biophysical Society of Canada (BSC) Keynote Lecture (in person) at the annual meeting of the BSC, Ottawa, Canada, 2022
357. Invited Keynote Speaker. The Precision and Personalized Medicine for Life Sciences Forum. 2022
358. Invited Speaker, Kadir Has, Istanbul, Turkey (2022)
359. Invited Keynote Speaker, CECAM Flagship Workshop on “Biomolecular simulation and machine learning in the exascale era: first applications and perspectives”. The workshop is sponsored by the CECAM-DE-JUELICH node, the CECAM-IT-SIMUL node and the CECAM-IT-SISSA-SNS node. June 2023

## BIBLIOGRAPHY

### Published:

1. Nussinov, R.: Secondary structure analysis of nucleic acids. Ph.D. thesis, Rutgers University. 374, 1977.
2. Nussinov, R., Pieczenik, G., Griggs, J., and Kleitman, D.: Algorithms for loop matchings, Soc. Ind. Appl. Math. (C). J. Appl. Math. 35: 68-82, 1978.
3. Nussinov, R.: Some rules in the ordering of nucleotides in the DNA. Nucleic Acids Res. 8: 4545-4562, 1980.
4. Nussinov, R.: Strong adenine clustering in nucleotide sequences. J. Theor. Biol. 85: 285-291, 1980.
5. Nussinov, R.: Three dimensional structure and sequence homology determine splicing sites in eukaryotic precursor RNA. J. Theor. Biol. 83: 647-662, 1980.
6. Nussinov, R. and Jacobson, A. B.: Fast algorithm for predicting the secondary structure of single stranded RNA. Proc. Natl. Acad. Sci. USA 77: 6309-6313, 1980.
7. Nussinov, R., Sussman, J. L., and Trifonov, E. N.: MS2 RNA has a potential to form an unusually large number of stable hairpins. J. Theor. Biol. 85: 481-486, 1980.
8. Nussinov, R.: Nearest neighbor nucleotide patterns: Structural and biological implications. J. Biol. Chem. 256: 8458-8462, 1981.

9. Nussinov, R.: The eukaryotic dinucleotide preference rules and their implications on degenerate codon choice. J. Mol. Biol. 149: 125-131, 1981.
10. Nussinov, R.: The universal dinucleotide asymmetry rules in DNA and the amino acid codon choice. J. Mol. Evol. 17: 237-244, 1981.
11. Nussinov, R. and Tinoco, I., Jr.: Sequential folding of a messenger RNA molecule. J. Mol. Biol. 151: 519-533, 1981.
12. Wain-Hobson, S., Nussinov, R., Brown, R. J., and Sussman, J. L.: Preferential codon usage in genes. Gene 13: 355-364, 1981.
13. Nussinov, R.: Some indications for inverse DNA duplication. J. Theor. Biol. 95: 783-791, 1982.
14. Nussinov, R.: Splicing and transport of eukaryotic mRNAs: A theoretical model. J. Theor. Biol. 97: 129-140, 1982.
15. Nussinov, R.: RNA folding is unaffected by the nonrandom degenerate codon choice. Biochim. Biophys. Acta 698: 111-115, 1982.
16. Nussinov, R., Tinoco, I., Jr., and Jacobson, A. B.: Secondary structure model for the complete simian virus 40 late precursor RNA. Nucleic Acids Res. 10: 351-364, 1982.
17. Nussinov, R., Tinoco, I., Jr., and Jacobson, A. B.: Small changes in free energy assignments for unpaired bases do not affect predicted structures in single stranded RNA. Nucleic Acids Res. 10: 341-350, 1982.
18. Nussinov, R.: An efficient code searching for sequence homology and DNA duplication. J. Theor. Biol. 100: 319-238, 1983.
19. Nussinov, R.: Efficient algorithms for searching for exact repetition of nucleotide sequence. J. Mol. Evol. 19: 283-285, 1983.
20. Comay, E., Nussinov, R., and Comay, O.: An extremely accelerated algorithm for calculating the secondary structure of single stranded RNA. Nucleic Acids Res. 12: 53-66, 1984.
21. Lennon, G. G., and Nussinov, R.: Homonyms, synonyms and mutations of the sequence/structure vocabulary. J. Mol. Biol. 175: 425-430, 1984.
22. Nussinov, R.: Doublet frequencies in evolutionary distinct groups. Nucleic Acids Res. 12: 1749-1763, 1984.
23. Nussinov, R.: Effects of secondary structure in RNA on interlocking probabilities. J. Math. Biol. 19: 95-107, 1984.

24. Nussinov, R.: Promoter helical structure variation at the *E. Coli* polymerase interaction sites. J. Biol. Chem. 259: 6798-6805, 1984.
25. Nussinov, R.: Strong doublet preferences in nucleotide sequences and DNA geometry. J. Mol. Evol. 20: 111-119, 1984.
26. Nussinov, R. and Lennon, G. G.: Periodic structurally similar oligomers are found on one side of the axes of symmetry in the lac, trp and gal operators. J. Biomol. Struct. Dyn. 2: 387-396, 1984.
27. Nussinov, R. and Lennon, G. G.: Structural features are as important as sequence homologies in Drosophila heat shock gene upstream regions. J. Mol. Evol. 20: 106-110, 1984.
28. Nussinov, R. and Pieczenik, G.: Folding two large polynucleotide chains. J. Theor. Biol. 106: 261-273, 1984.
29. Nussinov, R. and Pieczenik, G.: Structural and combinatorial constraints on base pairing in large nucleotide sequences. J. Theor. Biol. 106: 245-259, 1984.
30. Nussinov, R., Shapiro, B., Lipkin, L. E., and Maizel, J. V., Jr.: DNAase I hypersensitive sites may be correlated with genomic regions of large structural variation. J. Mol. Biol. 177: 591-608, 1984.
31. Nussinov, R., Shapiro, B., Lipkin, L. E., and Maizel, J. V., Jr.: Enhancer elements share local homologous twist angle variations with a helical periodicity. Biochim. Biophys. Acta 783: 246-257, 1984.
32. Nussinov, R.: Large helical conformational deviation from ideal B-DNA and prokaryotic regulatory sites. J. Theor. Biol. 115: 179-189, 1985.
33. Greif, P. C., Nussinov, R., Kanehisa, M., and DeLisi, C.: Highly nonrandom recurrence of consecutive repeats in non-coding mammalian sequences. Journal of Mathematical Bioscience 81: 43-52, 1986.
34. Jernigan, R. L., Sarai, A., Ting, K. -L., and Nussinov, R.: Hydrophobic interactions in the major groove can influence DNA local structure. J. Biomol. Struct. Dyn. 4: 41-48, 1986.
35. Landau, G., Vishkin, U., and Nussinov, R.: An efficient string matching algorithm with k differences for nucleotide and amino acid sequences. Nucleic Acids Res. 14: 31-46, 1986.
36. Lennon, G. G. and Nussinov, R.: Eukaryotic oligomer frequencies are correlated with certain DNA helical parameters. J. Theor. Biol. 116: 427-434, 1986.

37. Nussinov, R.: Compilation of eukaryotic sequences around transcription initiation sites. J. Theor. Biol. 120: 479-487, 1986.
38. Nussinov, R.: Presence of large helical structure variation in yeast His-4 upstream region is correlated with general amino acid control on the CYC-1 gene. J. Biomol. Struct. Dyn. 3: 349-362, 1986.
39. Nussinov, R.: Sequence signals which may be required for efficient formation of mRNA 3' termini. Nucleic Acids Res. 14: 3557-3572, 1986.
40. Nussinov, R.: Some guidelines for identification of recognition sequences: Regulatory sequences frequently contain (T)GTG/CAC(A), TGA/TCA and (T)CTC/GAG(A). Biochim. Biophys. Acta 866: 93-108, 1986.
41. Nussinov, R.: Structural wrinkles and eukaryotes genomic regulatory sites. J. Mol. Evol. 22: 150-159, 1986.
42. Nussinov, R.: TGTG, G clustering and other signals near non-mammalian vertebrate mRNA 3' termini: Some implications. J. Biomol. Struct. Dyn. 3: 1145-1154, 1986.
43. Nussinov, R., Owens, J., and Maizel, J. V., Jr.: Sequence signals in eukaryotic upstream regions. Biochim. Biophys. Acta 866: 109-119, 1986.
44. Nussinov, R. and Weisberg, R. A.: Bacteriophage lambda into protein may recognize structural features of the attachment sites. J. Biomol. Struct. Dyn. 3: 1133-1144, 1986.
45. Shapiro, B., Nussinov, R., Lipkin, L., and Maizel, J. V., Jr.: A sequence analysis system encompassing rules for DNA helical distortion. Nucleic Acids Res. 14: 75-85, 1986.
46. Jernigan, R. L., Sarai, A., Shapiro, B., and Nussinov, R.: Relationship between curved DNA conformations and slow gel migration. J. Biomol. Struct. Dyn. 4: 561-567, 1987.
47. Landau, G., Vishkin, U., and Nussinov, R.: An efficient string matching algorithm with k mismatches for nucleotide and amino acid sequences. J. Theor. Biol. 126: 483-490, 1987.
48. Le, S., Currey, K. M., Nussinov, R., and Maizel, J. V., Jr.: Studies of frequently recurring substructures in human alpha-like globin mRNA precursors. Comput. Biomed. Res. 20: 563-582, 1987.
49. Nussinov, R.: (A)GGG(A), (A)CCC(A) and other potential 3' splice signals in primate pre-mRNA sequences. Biochim. Biophys. Acta 910: 261-270, 1987.

50. Nussinov, R.: Asymmetry and sharp differences in the distribution of the four nucleotides at mRNA initiation and 3' termini: Some implications. Biochim. Biophys. Acta 908: 143-149, 1987.
51. Nussinov, R.: Conserved putative signals in 3' intron junctions in rodents. J. Biomol. Struct. Dyn. 4: 1051-1064, 1987.
52. Nussinov, R.: Nucleotide quartets in the vicinity of transcription initiation sites: Some DNA and chromatin structural implications. DNA 6: 13-22, 1987.
53. Nussinov, R.: Theoretical molecular biology: Prospectives and perspectives. J. Theor. Biol. 125: 219-235, 1987.
54. Nussinov, R., Barber, A., and Maizel, J. V., Jr.: The distribution of nucleotides near bacterial transcription initiation and termination sites show distinct signals that may affect DNA geometry. J. Mol. Evol. 26: 187-197, 1987.
55. Shapiro, B., Nussinov, R., Lipkin, L., and Maizel, J. V., Jr.: An interactive dot matrix system for locating significant features in nucleic acids molecules. J. Biomol. Struct. Dyn. 4: 697-706, 1987.
56. Landau, G., Vishkin, V., and Nussinov, R.: Locating alignments with k differences for nucleotide and amino acid sequences. Comput. Appl. Biosci. 4: 19-25, 1988.
57. Le, S., Chen, K-H., Nussinov, R., and Maizel, J. V., Jr.: An improved secondary structure computation method and its application to intervening sequences in the human alpha-like globin mRNA precursors. Comput. Appl. Biosci. 4: 337-344, 1988.
58. Margalit, H., Shapiro, B. A., Nussinov, R., Owens, J., and Jernigan, R. L.: Helix stability in prokaryotic promoter regions. Biochemistry 27: 5179-5188, 1988.
59. Nussinov, R.: Conserved quartets near 5' intron junctions in primate nuclear pre-mRNAs. J. Theor. Biol. 133: 73-84, 1988.
60. Nussinov, R.: Putative viral elements in the vicinity of transcription initiation sites. Int. J. Biochem. 20: 721-730, 1988.
61. Nussinov, R., Sarai, A., Smythers, G. W., and Jernigan, R. L.: Sequence context of oligomer tracts in eukaryotic DNA: Biological and conformational implications. J. Biomol. Struct. Dyn. 6: 543-562, 1988.
62. Nussinov, R., Sarai, A., Wang, D., and Jernigan, R. L.: Sequence context of homooligomer tracts in eukaryotic genomes: Some DNA conformational implications. In Olson, W. K., Sarma, M. H., Sarma, R. H., and Sundaralingam, M. (Eds.): Proceedings of the 6th Conversation of Stereodynamics. DNA Bending and Curvature. Albany, Adenine Press, 1988, (3) pp. 129-138.



63. Owens, J., Chatterjee, D., Nussinov, R., Konopka, A. K., and Maizel, J. V., Jr.: A fixed-point alignment technique for detection of recurrent and common sequence motifs associated with biological features. Comput. Appl. Biosci. 4: 73-77, 1988.
64. Sarai, A., Mazur, J., Nussinov, R., and Jernigan, R. L.: Origin of DNA helical structure and its sequence dependence. Biochemistry 27: 8498-8502, 1988.
65. Sarai, A., Mazur, J., Nussinov, R., and Jernigan, R. L.: Sequence dependence of DNA conformations: Means and fluctuations. In Olson, W. K., Sarma, M. H., Sarma, R. H., and Sundaralingam, M. (Eds.): Proceedings of the 6th Conversation of Stereodynamics. DNA Bending and Curvature. Albany, Adenine Press, 1988, (3) pp. 213-223.
66. Le, S. -Y., Nussinov, R., and Maizel, J. V., Jr.: Tree graphs of RNA secondary structures and their comparisons. Comput. Biomed. Res. 22: 461-473, 1989.
67. Le, S. -Y., Owens, J., Nussinov, R., Chen, J-H., Shapiro, B., and Maizel, J. V., Jr.: RNA secondary structures: Comparison and determination of frequently recurring substructures. Comput. Appl. Biosci. 5: 205-210, 1989.
68. Nussinov, R.: Conserved signals around the 5' splice sites in eukaryotic nuclear precursor mRNAs: G-runs are frequent in the introns and C in the exons near both 5' and 3' splice sites. J. Biomol. Struct. Dyn. 6: 985-1000, 1989.
69. Nussinov, R.: The ordering of the nucleotides in the DNA: Computational problems in molecular biology. Computers in Biology and Medicine 19: 269-281, 1989.
70. Nussinov, R., Sarai, A., Smythers, G. W., and Jernigan, R. L.: Distinct patterns in homooligomer tract sequence context in prokaryotic and eukaryotic DNA. Biochim. Biophys. Acta 1008: 329-338, 1989.
71. Nussinov, R., Sarai, A., Smythers, G., Wang, D., and Jernigan, R. L.: Strong patterns in homooligomer tracts occurrences in non-coding and in potential regulatory sites in eukaryotic genomes. J. Biomol. Struct. Dyn. 7: 707-722, 1989.
72. Sarai, A., Mazur, J., Nussinov, R., and Jernigan, R. L.: Sequence dependence of DNA conformation flexibility. Biochemistry 28: 7842-7849, 1989.
73. Landau, G. M., Vishkin, V., and Nussinov, R.: Fast alignment of DNA and protein sequences. Methods Enzymol. 183: 487-502, 1990.
74. Le, S. -Y., Nussinov, R., and Maizel, J. V., Jr.: Studies of local stability in histone, U-snRNA and globin precursor mRNA around transcription termination sites. Computers and Mathematics with Applications 20: 49-56, 1990.

75. Nussinov, R.: General nearest neighbor preferences in G/C oligomers interrupted by A/T Correlation with DNA structure. J. Biomol. Struct. Dyn. 8: 399-412, 1990.
76. Nussinov, R.: Sequence signals in eukaryotic upstream regions. Crit. Rev. Biochem. Mol. Biol. 25: 185-224, 1990.
77. Nussinov, R., Shapiro, B., Le, S. -Y., and Maizel, J. V., Jr.: Speeding up the dynamic algorithm for planar folding. Math. Biosci. 100: 33-47, 1990.
78. Le, S-Y, Shapiro, B. A., Chen, J. -H., Nussinov, R., and Maizel, J. V., Jr.: RNA pseudoknots downstream of the frameshift sites of retroviruses. Genet. Anal. Tech. Appl. 8: 191-205, 1991.
79. Nussinov, R.: Compositional variations in DNA sequence. Comput. Appl. Biosci. 7: 287-293, 1991.
80. Nussinov, R.: Distinct patterns in the dinucleotides nearest neighbors to G/C and A/T oligomers in eukaryotic sequences. J. Mol. Evol. 33: 259-266, 1991.
81. Nussinov, R.: Long-range and symmetry considerations in the DNA. DNA Seq. 2: 69-79, 1991.
82. Nussinov, R.: Signals in DNA sequences and their potential properties. Comput. Appl. Biosci. 7: 295-299, 1991.
83. Nussinov, R.: The ordering of nucleotides in the DNA: Strong pyrimidine-purine patterns near homooligomer tracts. J. Theor. Biol. 149: 21-42, 1991.
84. Nussinov, R. and Smythers, G.: Trends in the 5' vs 3' flanks of oligonucleotides in eukaryotic and prokaryotic genomes: The roles played by cytosine and guanine. J. Theor. Biol. 153: 111-135, 1991.
85. Nussinov, R. and Wolfson, H. J.: Efficient detection of motifs in biological macromolecules by computer vision techniques. Proc. Natl. Acad. Sci. USA 88: 10495-10499, 1991.
86. Fischer, D., Bachar, O., Nussinov, R., and Wolfson, H.: An efficient automated computer-vision based technique for three-dimensional structural comparison of proteins. J. Biomol. Struct. Dyn. 9: 769-789, 1992.
87. Fischer, D., Nussinov, R. and Wolfson, H.: Three dimensional substructural matching in protein molecules. Proceedings of 3rd Symposium on Combinatorial Pattern Matching. Tuscon, Arizona, 1992, pp. 133-147.
88. Nussinov, R.: DNA sequences at and between the GC and TATA boxes: Potential looping and spatial juxtapositioning of the protein factors. J. Biomol. Struct. Dyn. 9: 1213-1238, 1992.

89. Nussinov, R.: DNA spatial considerations in the arrangement of G/C and A/T blocks. Computers in Biology and Medicine 22(1/2): 97-112, 1992.
90. Nussinov, R.: Intervening, looped sequences between CCAAT and TATA in primates are rigid upstream and flexible downstream. In Sarma, R. and Sarma M. (Eds.): Proceedings of the 8th Conversation of Stereodynamics. Structure and Function. Albany, Adenine Press, 1992, (1) pp. 183-212.
91. Nussinov, R.: The Eukaryotic CCAAT and TATA boxes, DNA spacer flexibility and looping. J. Theor. Biol. 55: 243-270, 1992.
92. Bachar, O., Fischer, D., Nussinov, R., and Wolfson, H.: A computer vision based technique for 3-D sequence-independent structural comparison of proteins. Protein Eng. 6: 279-288, 1993.
93. Fischer, D., Norel, R., Wolfson, H., and Nussinov, R.: Surface motifs by a computer vision technique: Searches, detection and implications for protein-ligand recognition. Proteins Struct. Funct. Genet. 16: 278-292, 1993.
94. Fischer, D., Nussinov, R., and Wolfson, H.: Three dimensional substructural matching in protein molecules. In Apostolico, A., Crochemore, M, Galil, Z., and Manber, U. (Eds.): Lecture Notes in Computer Science, (644). New York, Springer Verlag, 1993, pp. 136-150.
95. Fischer, D., Wolfson, H., and Nussinov, R.: Spatial, sequence-order independent structural comparisons of  $\square\square\square$  proteins. J. Biomol. Struct. Dyn. 11: 367-380, 1993.
96. Norel, R., Fischer, D., Nussinov, R., and Wolfson, H-J.: 3-D docking of protein molecules. Proceedings of 4th Symposium on Combinatorial Pattern Matching and Lecture Notes in Computer Science. Padova, Italy, Springer Verlag, 1993, (684) pp. 20-34.
97. Nussinov, R.: Strong sequence patterns in eukaryotic promoter regions: Potential implications for DNA structure. Int. J. Biochem. 25: 597-607, 1993.
98. Fischer, D., Lin, S. L., Nussinov, R., and Wolfson, H.: Docking of protein molecules. Proceedings of the 12th International Conference on Pattern Recognition, Vol. II: Pattern recognition and neural networks. Los Alamitos, CA, IEEE Press, 1994, pp. 145-149.
99. Fischer, D., Wolfson, H., Lin, S. L., and Nussinov, R.: 3-D, sequence-order independent structural comparison of trypsin against the crystallographic database reveals active site similarities to serine protease: Potential implications to evolution and to protein folding. Protein Science 3: 769-778, 1994.

100. Lin, S. L., Nussinov, R., Fischer, D., and Wolfson, H.: Molecular surface representation by sparse critical points. Proteins Struct. Funct. Genet. 18(1): 94-101, 1994.
101. Norel, R., Fischer, D., Wolfson, H. and Nussinov, R.: Molecular surface recognition by a computer-vision based technique. Protein Eng. 7: 39-46, 1994.
102. Norel, R., Lin, S. L., Wolfson, H, and Nussinov, R.: Shape complementarity at protein-protein interfaces. Biopolymers 34: 933-940, 1994.
103. Sandak, B., Nussinov, R., and Wolfson, J. H.: 3-D flexible docking of molecules. In Califano A., Rigoutsos I., Wolfson H. (Eds.): Proceedings of the workshop on shape and pattern matching in computational biology. IEEE Conference on Computer Vision and Pattern Recognition. Seattle, IEEE Press, 1994, pp. 41-54.
104. Alexandrov, N., Nussinov, R., and Zimmer, R. M.: Fast protein fold recognition via sequence to structure alignment and contact capacity potentials. In Hunter, L. and Klein, T. E. (Eds.): Proceedings of the Pacific Symposium on Biocomputing. Singapore, World Scientific Publishing Co., 1995, pp. 53-72.
105. Fischer, D., Lin, S. L., Wolfson, H., and Nussinov, R.: A geometry-based suite of molecular docking processes. J. Mol. Biol. 248: 459-477, 1995.
106. Fischer, D., Tsai, C. -J., Nussinov, R., and Wolfson, H. A 3-D sequence-independent representation of the protein data bank. Protein Eng. 8: 981-997, 1995.
107. Lin, S. L. and Nussinov, R.: A disulfide-reinforced structural scaffold shared by small proteins with diverse functions. Nature Structural Biol. 2: 835-837, 1995.
108. Lin, S. L., Tsai, C. -J., and Nussinov, R.: A study of four-helix bundles: Investigating protein folding *via* similar architectural motifs in protein cores and subunit interfaces. J. Mol. Biol. 248: 151-161, 1995.
109. Norel, R., Lin, S. L., Wolfson, H., and Nussinov, R.: Molecular surface complementarity at protein-protein interfaces: The critical role played by surface normals at well placed, sparse, points in docking. J. Mol. Biol. 252(2): 263-273, 1995.
110. Sandak, B., Wolfson, H., and Nussinov, R.: An automated computer vision and robotics-based technique for 3-D flexible biomolecular docking and matching. Comput. Appl. Biosci. 11: 87-99, 1995.
111. Alesker, V., Nussinov, R., and Wolfson, H.: Detection of non-topological motifs in protein structures. Protein Eng. 9(12): 1103-1119, 1996.
112. Lin, S. L. and Nussinov, R.: Molecular recognition via the face center representation of molecular surface. Journal of Molecular Graphics 14: 78-97, 1996.

113. Naor, D., Fischer, D., Jernigan, R. L., Wolfson, H. J., and Nussinov, R.: Amino acid pair interchanges at spatially conserved locations. J. Mol. Biol. 256: 924-938, 1996.
114. Sandak, B., Nussinov, R., and Wolfson, H.: Docking of conformationally flexible molecules. Combinatorial pattern matching. Lecture Notes in Computer Science. Vol. (1) 1075: 271-287, 1996.
115. Sandak, B., Wolfson, H., and Nussinov, R.: Hinge-bending at molecular interfaces: automated docking of a dihydroxyethylene - containing inhibitor to the HIV-1 protease. In Sarma, R. H. and Sarma, M. H. (Eds.): Biological Structure and Dynamics (Proceedings of the 9th Conversation in Stereodynamics). Albany, Adenine Press, 1996, (1) pp. 233-252.
116. Tsai, C. -J., Lin, S. L., Wolfson, H. J., and Nussinov, R.: A dataset of protein-protein interfaces generated with a sequence-order-independent comparison technique. J. Mol. Biol. 260: 604-620, 1996.
117. Tsai, C. -J., Lin, S. L., Wolfson, H., and Nussinov, R.: Protein-protein interfaces: architectures and interactions in protein-protein interfaces and in protein cores. Their similarities and differences. Crit. Rev. Biochem. Mol. Biol. 31: 127-152, 1996.
118. Tsai, C. J., Lin, S. L., Wolfson, H., and Nussinov, R.: Techniques for searching structural similarities between protein cores, surfaces and between protein-protein interfaces. Techniques in Protein Chemistry VII: 419-429, 1996.
119. Azarya-Sprinzak, E., Naor, D., Wolfson, H. J., and Nussinov, R.: Interchanges of spatially neighboring residues in structurally conserved environments. Protein Eng. 10(10): 1109-1122, 1997.
120. Lin, S. L., Xu, D., Li, A., Rosen, M., Wolfson, H. J., and Nussinov, R.: Investigation of the enzymatic mechanism by docking a transition state analog to the yeast chorismate mutase. J. Mol. Biol. 271: 838-845, 1997.
121. Tsai, C. J., Lin, S. L., Wolfson, H., and Nussinov, R.: Studies of protein-protein interfaces: Statistical analysis of the hydrophobic effect. Protein Science 6: 53-64, 1997.
122. Tsai, C. -J. and Nussinov, R.: Hydrophobic folding units at protein-protein interfaces: Implications to protein folding and protein-protein association. Protein Science 6: 1426-1437, 1997.
123. Tsai, C. -J. and Nussinov, R.: Hydrophobic folding units derived from dissimilar monomer structures and their interactions. Protein Science 6: 24-42, 1997.

124. Tsai, C. -J., Xu, D. and Nussinov, R.: Structural motifs at protein-protein interfaces: Protein cores versus two-state and three-state model complexes. Protein Science 6: 1793-1805, 1997.
125. Xu, D., Lin, S. L., and Nussinov, R.: Protein binding versus protein folding: The role of hydrophilic bridges in protein associations. J. Mol. Biol. 265: 68-84, 1997.
126. Xu, D. and Nussinov, R.: Favorable domain size in proteins. Folding and Design 3: 11-17, 1997.
127. Xu, D., Tsai, C-J., and Nussinov, R.: Hydrogen bonds and salt-bridges across protein-protein interfaces. Protein Eng. 10: 999-1012, 1997.
128. Li, A-J. and Nussinov, R.: A set of van der Waals and coulombic radii of protein atoms for molecular and solvent-accessible surface calculation, packing evaluation, and docking. Proteins Struct Funct Genet 32: 111-127, 1998.
129. Lin, S. L., Xu, D., Li, A., and Nussinov, R.: Electrostatics, allostery and activity of yeast chorismate mutase. Proteins 31: 445-452, 1998.
130. Norel, R., Lin, S. L., Xu, D., Wolfson, H., and Nussinov, R.: Molecular surface variability and induced conformational changes upon protein-protein association. In Sarma, R. H. and Sarma, M. H. (Eds.): Proceedings of the 10th Conversation of Stereodynamics. Structure, Motions, Interaction and Expression of Biological Macromolecules. Albany, Adenine Press, 2: 33-52, 1998.
131. Rosen, M., Lin, S. L., Wolfson, H., and Nussinov, R.: Molecular shape comparisons in searches for active sites and functional similarity. Protein Eng. 11: 263-277, 1998.
132. Sandak, B., Nussinov, R., and Wolfson, H. J.: A method for biomolecular structural recognition and docking allowing conformational flexibility. J. Computat. Biol. 5: 631-654, 1998.
133. Sandak, B., Wolfson, H., and Nussinov R.: Flexible docking allowing induced fit in proteins: Insights from an open to closed conformational isomers. Proteins 32: 159-174, 1998.
134. Tsai, C. -J., Xu, D., and Nussinov, R.: Protein folding via binding and vice versa. Folding and Design 3: R71-R80, 1998.
135. Xu, D., Tsai, C. -J., and Nussinov, R.: Mechanism and evolution of protein dimerization. Protein Science 7: 533-544, 1998.
136. Kumar, S., Ma, B., Tsai, C. -J., Wolfson, H., and Nussinov, R.: Folding funnels and conformational transitions via hinge-bending motions. Cell Biochem. Biophys. 31: 23-46, 1999.

137. Kumar, S. and Nussinov, R.: Salt bridge stability in monomeric proteins. J. Mol. Biol. 293: 1241-1255, 1999.
138. Leibowitz, N., Fligelman, Z. Y., Nussinov, R., and Wolfson, H-J.: Multiple structural alignment and core detection by geometric hashing. In Lengauer, T., et.al. (Eds.): Proceedings of the 7th International Conference on Intelligent Systems in Molecular Biology. Menlo Park, AAAI Press, 169-177, 1999.
139. Ma, B., Kumar, S., Tsai, C. -J., and Nussinov, R.: Folding funnels and binding mechanisms. Protein Eng. 12: 713-720, 1999.
140. Ma, B. and Nussinov, R.: Explicit water and implicit water simulation of a  $\alpha$ -hairpin peptide. Proteins 37: 73-87, 1999.
141. Norel, R., Petrey, D., Wolfson, H., and Nussinov, R.: Examination of shape complementarity in docking of unbound proteins. Proteins Struct. Funct. Genet. 36: 307-317, 1999.
142. Norel, R., Wolfson, H., and Nussinov, R.: Small molecule recognition: Solid angles surface representation and shape complementarity. Combinatorial Chemistry & High Throughput Screening 2: 177-191, 1999.
143. Nussinov, R. and Wolfson, H.: Efficient computational algorithms for docking and for generating and matching a library of epitopes. I. Rigid and flexible docking algorithms. Combinatorial Chemistry and High Throughput Screening 2: 249-259, 1999.
144. Nussinov, R. and Wolfson, H.: Efficient computational algorithms for docking and for generating and matching a library of epitopes. II. Computer vision-based techniques for the generation and utilization of functional epitopes. Combinatorial Chemistry and High Throughput Screening 2: 289-297, 1999.
145. Tsai, C. -J., Kumar, S., Ma, B., and Nussinov, R.: Folding funnels, binding funnels and protein function. Protein Science 8: 1181-1190, 1999.
146. Tsai, C. -J., Ma, B., and Nussinov, R.: Folding and binding cascades: Shifts in energy landscapes. Proc. Natl. Acad. Sci. USA 96: 9970-9972, 1999.
147. Tsai, C. -J., Maizel, J. V. Jr., and Nussinov, R.: Distinguishing between sequential and non-sequentially folded proteins: Implications for folding and misfolding. Protein Science 8: 1591-1604, 1999.
148. Verbitzky, G., Nussinov, R., and Wolfson, H.: Flexible structural comparison allowing hinge bending, swivelling motions. Proteins 34: 232-254, 1999.

149. Hu, Z., Ma, B., Wolfson, H., and Nussinov, R.: Conservation of polar residues as hot spots of protein interfaces. Proteins Struct. Funct. Genet. 39: 331-342, 2000.
150. Kumar, S., Ma, B., Tsai, C. -J., and Nussinov, R.: Electrostatic strengths of salt bridges in thermophilic and mesophilic glutamate dehydrogenase monomers. Proteins: Struct. Funct. Genet. 38: 368-383, 2000.
151. Kumar, S., Ma, B., Tsai, C. -J., Sinha, N., and Nussinov, R.: Folding and binding cascades: Dynamic landscapes and population shifts. Protein Science 9: 10-19, 2000.
152. Kumar, S. and Nussinov, R.: Fluctuations between stabilizing and destabilizing electrostatic contributions of ion pairs in conformers of the c-Myc-Max leucine zipper. Proteins: Struct. Funct. Genet. 41: 485-497, 2000.
153. Kumar, S., Tsai, C. -J., Ma, B., and Nussinov, R.: Contribution of salt bridges toward protein thermostability. J. Biomol. Struct. Dyn. 1: 79-86, 2000.
154. Kumar, S., Tsai, C. -J., and Nussinov, R.: Factors enhancing protein thermostability. Protein Eng. 13(3): 179-191, 2000.
155. Ma, B., Kumar, S., Tsai, C. -J., Hu, Z., and Nussinov, R.: Transition state ensemble in enzyme catalysis: Possibility, reality, or necessity? J. Theor. Biol. 203: 383-397, 2000.
156. Ma, B. and Nussinov, R.: Molecular dynamics simulation of a beta-hairpin fragment of protein G: Balance between side chain and backbone forces. J. Mol. Biol. 296:1091-1104, 2000.
157. Ma, B., Tsai, C. -J., and Nussinov, R.: Binding and folding: In search of intra-molecular chaperone-like building block fragments. Protein Eng. 13: 617-627, 2000.
158. Ma, B., Tsai, C. -J., and Nussinov, R.: Protein folding energy landscape and vibrational entropy: A systematic study. Biophys. J. 79: 2739-2753, 2000.
159. Ma, B., Xiong, J., Lubkowski, J., and Nussinov, R.: Homology modeling and molecular dynamics simulations of lymphotactin. Protein Sci. 9: 2192-2199, 2000.
160. Shatsky, M., Fligelman, Z., Nussinov, R., and Wolfson, H.: Alignment of flexible protein structures. In Alman, et al (Eds.): Proceedings of the 8th Conference on Intelligent Systems in Molecular Biology. Menlo Park, CA, AAI Press, 329-343, 2000.
161. Tsai, C. -J., Maizel, J. V., and Nussinov, R.: Anatomy of protein structures: Visualizing how a 1-D protein chain folds into a 3-D shape. Proc. Natl. Acad. Sci. USA 97: 12038-120431, 2000.
162. Kumar, S. and Nussinov, R.: Fluctuations in ion pairs and their stabilities in proteins. Proteins Struct. Funct. Genet. 43: 433-454, 2001.



163. Kumar, S. and Nussinov, R.: How do thermophilic proteins deal with heat? Cellular and Molecular Life Sciences 58: 1216-1233, 2001.
164. Kumar, S., Sham, Y. Y., Tsai, C. -J., and Nussinov, R.: Folding and function: The N-terminal building block in adenylate kinase. Biophys. J. 80: 2439-2454, 2001.
165. Kumar, S., Tsai, C. -J., and Nussinov, R.: Thermodynamic differences among homologous thermophilic and mesophilic proteins. Biochemistry 40: 14152-14165, 2001.
166. Kumar, S., Wolfson, H., and Nussinov, R.: Protein flexibility and electrostatic interactions. IBM Journal of Research and Development, Issue On Life Sciences 45: 499-511, 2001.
167. Leibowitz, N., Fligelman, Z., Nussinov, R., and Wolfson, H.: Automated multiple structure alignment and detection of a common substructural motif. Proteins: Struct. Funct Genet. 43: 235-245, 2001.
168. Leibowitz, N., Nussinov, R., and Wolfson, H.: MUSTA: A general, efficient, automated method for multiple structure alignment and detection of a common motif: Application to proteins. J. Comp. Biol. 8: 93-121, 2001.
169. Ma, B., Wolfson, H. J., and Nussinov, R.: Protein functional epitopes: Hot spots, dynamics and combinatorial libraries. Current Opinion in Structural Biology 11: 364-369, 2001.
170. Sham, Y. Y., Ma, B., Tsai, C. -J., and Nussinov, R.: Molecular dynamics simulation of *Escherichia coli* dihydrofolate reductase and its protein fragments: Relative stabilities in experiment and simulations. Protein Sci. 10(1): 135-148, 2001.
171. Sinha, N., Kumar, S., and Nussinov, R.: Inter-domain interactions in hinge-bending transitions. Structure, 9: 1165-1181, 2001.
172. Sinha, N. and Nussinov, R.: Point mutations and sequence variability in proteins: Redistribution of populations. Proc. Natl. Acad. Sci. USA. 98(6): 3139-3144, 2001.
173. Sinha, N., Tsai, C. -J., and Nussinov, R.: A proposed structural model for amyloid fibril elongation: Domain swapping forms an inter-digitating beta-structure polymer. Protein Eng. 14(2): 93-103, 2001.
174. Tsai, C. -J., Ma, B., Kumar, S., Wolfson, H., and Nussinov, R.: Protein folding: Binding of building blocks via population selection. Crit. Rev. Biochem. Mol. Biol. 36: 399-433, 2001.

175. Tsai, C. -J., Ma, B., Kumar, S., Sham, Y., Wolfson, H., and Nussinov, R.: A hierarchical, building-blocks based computational scheme for protein structure prediction. IBM Journal of Research and Development, Issue On Life Sciences 45: 513-523, 2001.
176. Tsai, C. -J., Ma, B., Sham, Y., Kumar, S., and Nussinov, R.: Structured disorder and conformational selection. Proteins 44: 418-427, 2001.
177. Tsai, C. -J. and Nussinov, R.: The building blocks folding model and the kinetics of protein folding. Protein Eng. 14: 717-727, 2001.
178. Tsai, C. -J. and Nussinov, R.: Transient, highly populated, building blocks folding model. Cell Biochem. and Biophys. 34: 209-235, 2001.
179. Duhovny, D., Nussinov, A., and Wolfson, H.: Efficient unbound docking of rigid molecules. Proceedings of ALGO 02. Algorithms in Bioinformatics. Lecture Notes in Computer Science. Springer Verlag, 2452: 185-200, 2002.
180. Kumar, S. and Nussinov, R.: Close range electrostatic interactions in proteins. Chembiochem 3: 604-617, 2002.
181. Kumar, S. and Nussinov, R.: Relationship between ion pair geometries and electrostatic strengths in proteins. Biophysical J. 83: 1595-1612, 2002
182. Kumar, S., Tsai, C. -J., and Nussinov, R.: Maximal stabilities of reversible two state proteins. Biochemistry 41(17): 5359-5374, 2002.
183. Halperin, I., Ma, B., Wolfson, H., and Nussinov, R.: Principles of docking: An overview of search algorithms and a guide to scoring functions. Proteins Struct. Funct. Genet. 47: 409-443, 2002.
184. Ma, B. and Nussinov, R.: Molecular dynamics simulations of alanine rich  $\beta$ -sheets oligomers: Insights into amyloid formation. Protein Sci. 11: 2335-2350, 2002.
185. Ma, B. and Nussinov, R.: Stabilities and conformations of Alzheimer's  $\beta$ -amyloid peptide oligomers ( $A\beta_{1-40}$ ,  $A\beta_{16-35}$  and  $A\beta_{10-35}$ ): Sequence effects. Proc. Natl. Acad. Sci. 99: 14126-14131, 2002.
186. Ma, B., Shatsky, M., Wolfson, H., and Nussinov, R.: Multiple ligands binding at a single site: A matter of pre-existing populations. Protein Sci. 11: 184-197, 2002.
187. Sham, Y. Y., Ma, B., Tsai, C. -J., and Nussinov, R.: Thermal unfolding molecular dynamics simulation of Escherichia coli dihydrofolate reductase: Thermal stability of protein domains and unfolding pathway. Proteins Struct. Funct. Genet. 46: 308-320, 2002.

188. Sinha, N., Tsai, C. -J. and Nussinov, R.: Building blocks, hinge-bending motions and protein topology. J. Biomol. Struct. Dyn. 19(3): 369-380, 2002.
189. Shatsky, M., Nussinov, R., and Wolfson, H.: Flexible protein alignment and hinge-bending detection. Proteins 48: 242-256, 2002.
190. Shatsky, M., Nussinov, R., and Wolfson, H.: MultiProt: A multiple protein structural alignment Proceedings of ALGO 02. Algorithms in Bioinformatics. Lecture Notes in Computer Science 2452: 235-250, 2002.
191. Tsai, C. -J., Maizel, J. V., Jr., and Nussinov, R.: The hydrophobic effect: A new insight from cold denaturation and a two-state water structure. Critical Reviews in Biochemistry and Molecular Biology 37(2): 55-69, 2002.
192. Tsai, C. -J., Polverino de Laureto, P., Fontana, A. and Nussinov, R.: Comparison of protein fragments identified by limited proteolysis and computational cutting of proteins. Protein Sci. 11: 1753-1770, 2002.
193. Benyamini, H., Gunasekaran, K., Wolfson, H., and Nussinov, R.:  $\beta_2$ -Microglobulin amyloidosis: Insights from conservation analysis and fibril modelling by protein docking techniques. J. Mol. Biol. 330: 159-174, 2003.
194. Benyamini, H., Gunasekaran, K., Wolfson, H., and Nussinov, R.: Conservation and amyloid formation: A study of the gelsolin-like family. Proteins 51: 266-282, 2003.
195. Dror, O., Benyamini, H., Nussinov, R., and Wolfson, H.: MASS: A method for multiple structural alignment by secondary structures. Proceedings ISMB, Bioinformatics. Suppl. 1: I95-I104, 2003.
196. Dror, O., Benyamini, H., Nussinov, R., and Wolfson, H.: Multiple structural alignment by secondary structures: Algorithms and applications. Protein Sci. 12(11): 2492-2507, 2003.
197. Duhovny, D., Inbar, Y., Polak, V., Shatsky, M., Halperin, I., Benyamini, H., Barzilai, A., Dror, O., Haspel, N., Nussinov, R., and Wolfson, H.: Taking geometry to its edge: Fast unbound rigid (and hinge-bent) docking. Proteins 52: 107-112, 2003.
198. Gunasekaran, K., Ma, B., and Nussinov, R.: Triggering loops and enzyme function: Identification of loops that trigger and modulate movements. J. Mol. Biol. 332: 143-159, 2003.
199. Gunasekaran, K., Ma, B., Ramakrishnan, B., Qasba, P. K., and Nussinov, R.: The interdependence of backbone flexibility, sequence conservation and function in  $\beta$ 1,4-galactosyltransferase-I. Biochemistry 42(13): 3674-3687, 2003.

200. Gunasekaran, K., Tsai, C. -J., Kumar, S., Zanuy, D. and Nussinov, R.: Extended disordered protein states and protein functions: An obligate solution to large interface, yet smaller proteins and assembly sizes. Trends Biochem. Sci. 28: 81-85, 2003.
201. Halperin, I., Wolfson, H., and Nussinov, R.: SiteLight: Binding site prediction using phage display libraries. Protein Sci. 12: 1344-1359, 2003.
202. Haspel, N., Tsai, C. -J., Wolfson, H. and Nussinov, R.: Hierarchical protein folding pathways. A computational study of protein fragments. Proteins 51(2): 203-15, 2003.
203. Haspel, N., Tsai, C. -J., Wolfson, H., and Nussinov, R.: Reducing the computational complexity of protein folding via fragment folding and assembly. Protein Sci. 12: 1177-1187, 2003.
204. Inbar, Y., Benyamini, H., Nussinov, R., and Wolfson, H.: Protein structure prediction via combinatorial assembly of sub-structural units. Proceedings ISMB, Bioinformatics. Suppl. 1: I158-I168, 2003.
205. Kumar, S., Tsai, C. -J., and Nussinov, R.: Temperature range of thermodynamic stability for the native state of reversible two-state proteins. Biochemistry 42: 4864-4873, 2003.
206. Ma, B., Elkayam, T., Wolfson, H., and Nussinov, R.: Protein-protein interactions: Structurally conserved residues distinguish between binding sites and exposed protein surfaces. Proc. Natl. Acad. Sci (USA) 100: 5772-5777, 2003.
207. Ma, B. and Nussinov, R.: Energy landscape and dynamics of the  $\beta$ -hairpin G peptide and its isomers: Topology and sequences. Protein Sci. 12: 1882-1983, 2003.
208. Ma, B. and Nussinov, R.: Molecular dynamics simulations of the unfolding of  $\beta$ -2 microglobulin and its variants. Protein Eng. 16: 561-575, 2003.
209. Oron, A., Gunasekaran, K., Wolfson, H., and Nussinov, R.: Computation of electrostatic potentials and their contribution to interactions. G. Petsko (Ed.): Current Protocols in Bioinformatics. 8.4.1-8.4.12, 2003.
210. Zanuy, D. and Nussinov, R.: The sequence dependence of fiber organization. A comparative molecular dynamics study of the islet amyloid polypeptide segments 22-27 and 22-29. J. Mol. Biol. 329: 565-584, 2003.
211. Zanuy, D., Ma, B., and Nussinov, R.: Short peptide amyloid organization: Stabilities and conformations of the islet amyloid peptide NFGAIL Biophys. J. 84: 1884-1894, 2003.
212. Barzilai, A., Kumar, S., Wolfson, H., and Nussinov, R. Potential Folding-Function Interrelationship in Proteins. Proteins 56: 635-649. 2004.

213. Dror, O., Shulman-Peleg, A., Nussinov, R., and Wolfson, H. Predicting Molecular Interactions In Silico: I. A Guide to Pharmacophore Identification and its Applications to Drug Design. Curr. Med. Chem. 11: 71-90, 2004.
214. Gunasekaran, K., Ma, B., and Nussinov, R. Is Allostery an Intrinsic Property of all Dynamic Proteins? Implications for Drug Discovery. Proteins 57: 433-443, 2004.
215. Gunasekaran, K. and Nussinov, R. Modulating Functional Loop Movements: The Role of Conserved Residues in the Correlated Loop Motions. ChemBioChem 5(2): 224-230, 2004.
216. Gunasekaran, K., Tsai, C-J., and Nussinov, R. Analysis of Ordered and Disordered Protein Complexes Reveals Structural Features Discriminating between Stable and Unstable Monomers. J. Mol. Biol. 341: 1327-1341, 2004.
217. Halperin, I., Wolfson, H., and Nussinov, R. Protein-Protein Interactions: Coupling of Structurally Conserved Residues and of Hot Spots Across Protein-Protein Interfaces. Structure 12: 1027-1038, 2004.
218. Keskin, O., Tsai, C.-J., Wolfson, H., and Nussinov, R. A New Structurally Non-Redundant Dataset of Protein-Protein Interfaces and its Implications. Protein Sci. 13: 1043-1055, 2004.
219. Kumar, S. and Nussinov, R. Different Roles of Electrostatics in Heat and in Cold: Adaptation by Citrate Synthase. Chem. Bio. Chem 5: 280-290, 2004.
220. Kumar, S. and Nussinov, R. Experiment-Guided Thermodynamic Simulations on Reversible Two-State Proteins: Implications for Protein Thermostability. Biophys. Chem. 111: 235-246, 2004.
221. Li, X., Keskin, O., Ma, B., Nussinov, R., and Liang, J. Protein-Protein Interactions: Hot Spots and Structurally Conserved Residues often Locate in Complemented Pockets that are Pre-Organized in the Unbound States. Implications for Docking. J. Mol. Biol. 344: 781-795, 2004.
222. Ma, B. and Nussinov, R. From Computational Quantum Chemistry to Computational Biology: Experiments and Computations are (Full) Partners. Physical Biol. 1: P23-P26, 2004.
223. Ma, B. and Nussinov, R. Release Factors eRF1 and RF2: A Universal Mechanism Controls the Large Conformational Changes. J. Biol. Chem. 279( ): 53875-53885, 2004.
224. Pan, Y., Ma, B., Keskin, O., and Nussinov, R. Characterization of the Conformational State and Flexibility of HIV-1 Glycoprotein gp120 Core Domain. J. Biol. Chem. 279: 30523-30530, 2004.

225. Schneidman-Duhovny, D., Nussinov, R., and Wolfson, H. J. Predicting Molecular Interactions In Silico: II. Protein-Protein and Protein-Drug Docking. Curr. Med. Chem. 11: 91-107, 2004.
226. Shatsky, M., Dror, O., Schneidman-Duhovny, D., Nussinov, R., and Wolfson, H. J. BioInfo3D: A Suite of Tools for Structural Bioinformatics. Nucleic Acids Res. 32: W503-W507, 2004.
227. Shatsky, M., Nussinov, R., and Wolfson, H. FlexProt: Alignment of Flexible Protein Structures without a Predefinition of the Hinge Regions. J. Computational Biol. 11: 83-106, 2004.
228. Shatsky, M., Nussinov, R., and Wolfson, H. A Method for Simultaneous Alignment of Multiple Protein Structures. Proteins 56: 143-156, 2004.
229. Shulman-Peleg, A., Mintz, S., Nussinov, R., and Wolfson, H. J. Protein-Protein Interfaces: Recognition of Similar Spatial and Chemical Organizations. In Jonassen and Kim, J. (Eds.): Algorithms in Bioinformatics: 4<sup>th</sup> International Workshop, WABI 2004. Lecture Notes in Computer Science. Bergen, Norway, Springer-Verlag, 2004, Vol. 3240, pp. 194-205.
230. Shulman-Peleg, A., Nussinov, R., and Wolfson, H. Recognition of Functional Sites on Protein Structures. J. Mol. Biol. 339: 607-633, 2004.
231. Tsai, H.-H., Tsai, C-J., Ma, B., and Nussinov, R. *In Silico* Protein Design by Combinatorial Assembly of Protein Building Blocks. Protein Sci. 13: 2753-2765, 2004.
232. Tsai, H-H., Zanuty, D., Haspel, N., Gunasekaran, K., Ma, B., Tsai, C-J., and Nussinov, R. The Stability and Dynamics of the Human Calcitonin Amyloid Peptide DFNKF. Biophysical J. 87: 146-158, 2004.
233. Zanuty, D., Gunasekaran, K., Ma, B., Tsai, H-H. Tsai, C-J., and Nussinov, R. Insights into Amyloid Structural Formation and Assembly through Computational Approaches. Amyloid 11: 143-161, 2004.
234. Zanuty, D., Haspel, N., Tsai, H. -H. (G.), Ma, B., Gunasekaran, K., Wolfson, H., and Nussinov, R. Side Chain Interactions Determine the Amyloid Organization: A Single Layer  $\beta$ -Sheet Molecular Structure of the Calcitonin Peptide Fragment DFNKF. Physical Biology 1: 89-99, 2004.
235. Zanuty, D., Porat, Y., Gazit, E., and Nussinov, R. Peptide Sequence and Amyloid Formation: Molecular Simulations and Experimental Study of a Human Ilet Amyloid Polypeptide Fragment and its Analogs. Structure 12: 439-455, 2004.
236. Benyamini, H., Gunasekaran, K., Wolfson, H., and Nussinov, R. Fibril Modelling by Sequence and Structure Conservation Analysis Combined with Protein Cocking

- Techniques:  $\beta_2$ -Microglobulin Amyloidosis. Biochimica et Physics Acta 1753: 121-130, 2005.
237. Dror, O., Nussinov, R., and Wolfson, H. ARTS: Alignment of RNA Tertiary Structures. Bioinformatics 21: ii47-ii53, 2005.
238. Haliloglu, T., Keskin, O., Ma, B., and Nussinov, R. How Similar are Protein Folding and Binding Nuclei? Examination of Vibrational Motions of Energy Hot Spots and Conserved Residues. Biophys. J. 88: 1552-1559, 2005.
239. Haspel, N., Zanuy, D., Ma, B., Wolfson, H. J., and Nussinov, R. A Comparative Study of Amyloid Fibril Formation by Residues 15-19 of the Human Calcitonin Hormone: A Single  $\beta$ -Sheet Model with a Small Hydrophobic Core. J. Mol. Biol. 345: 1213-1227, 2005.
240. Inbar, Y., Benyamini, H., Nussinov, R., and Wolfson, H. J. Prediction of Multi-Molecular Assemblies by Multiple Docking. J. Mol. Biol. 349: 435-447, 2005.
241. Inbar, Y., Benyamini, H., Nussinov, R., and Wolfson, H. J. Combinatorial Docking Approach for Structure Prediction of Large Proteins and Multi-Molecular Assemblies. Physical Biol. 2: S156-65, 2005.
242. Inbar, Y., Nussinov, R., and Wolfson, H. J. Multiple Docking for Protein Structure Prediction. Int. J. Robotics Res 24; 131-150, 2005.
243. Inbar, Y., Schneidman-Duhovny, D., Halperin, I., Oron, A., Nussinov, R., and Wolfson, H.J. Approaching the CAPRI Challenge with an Efficient Geometry based Docking. Proteins 60: 217-223, 2005.
244. Keskin, O., Ma, B., and Nussinov, R. Hot regions in Protein—Protein Interactions: The Organization and Contribution of Structurally Conserved Hot Spot Residues. J. Mol. Biol. 345: 1281-1294, 2005.
245. Keskin, O. and Nussinov, R. Favorable scaffolds: Proteins with Different Sequence, Structure and Function may Associate in Similar Ways. Protein Eng. Des. Sel. 18: 11-24, 2005.
246. Keskin, O., Ma, B., Rogale, K., Gunasekaran, K., and Nussinov, R. Protein-Protein Interaction: Organization, Cooperativity and Mapping in a Bottom-Up Systems Biology Approach. Phys. Biol. 2: 524-535, 2005.
247. Lasker, K., Dror, O., Benyamini, H., Nussinov, R., and Wolfson, H. J. Discovery of Protein Substructures in EM Maps. Lecture Notes in Computer Science 3692: 423-434, 2005.

248. Ma, B., Pan, Y., Gunasekaran, K., Keskin, O., Venkataraghavan, R. B., Levine, A. J., and Nussinov, R. The Contribution of the Trp/Met/Phe Residues to Physical Interactions of p53 with Cellular Proteins. Physical Biol. 2: S56-S66, 2005.
249. Ma, B., Pan, Y., Gunasekaran, K., Venkataraghavan, R. B., Levine, A. J., and Nussinov, R. Comparison of the Protein-Protein Interfaces in the p53-DNA Crystal Structures: Towards Elucidation of the Biological Interface. Proc. Natl. Acad. Sci. (USA) 102: 3988-3993, 2005.
250. Mintz, S., Shulman-Peleg, A., Wolfson, H. J., and Nussinov, R. Generation and Analysis of a Protein-Protein Interface Dataset with Similar Chemical and Spatial Patterns of Interactions. Proteins 61: 6-20, 2005.
251. Ogmen, U., Keskin, O., Aytuna, S., Nussinov, R., and GURSOY, A. PRISM: Protein Interactions by Structural Matching. Nucleic Acids Res. 33: W331-W336, 2005.
252. Pan, Y., Ma, B., and Nussinov, R. CD4 Binding Partially Locks the Bridging Sheet in gp120 but Leaves the  $\beta$  2/3 Strands Flexible. J. Mol. Biol. 350: 514-527, 2005.
253. Pan, Y., Ma, B., Venkataraghavan, R. B., Levine, A. J., and Nussinov, R. In the Quest for Stable Rescuing Mutants of p53: Computational Mutagenesis of Flexible Loop L1. Biochemistry 44: 1423-1432, 2005.
254. Schneidman-Duhovny, D., Inbar, Y., Nussinov, R., and Wolfson, H. J. Geometry Based Flexible and Symmetric Protein Docking. Proteins. 60: 224-231, 2005.
255. Schneidman-Duhovny, D., Inbar, Y., Nussinov, R., and Wolfson, H. PatchDock and SymmDock: Servers for Rigid and Symmetric Docking. Nucleic Acids Res. 33: W363-W367, 2005.
256. Shatsky, M., Shulman-Peleg, A., Nussinov, R., and Wolfson, H. J. Recognition of Binding Patterns Common to a Set of Protein Structures. Lecture Notes in Computer Science, 3500: 440-455, 2005.
257. Shulman-Peleg, A., Nussinov, R., and Wolfson, H. J. SiteEngine: Recognition and Comparison of Binding Sites and Protein-Protein Interfaces. Nucleic Acids Res. 33: W337-W341, 2005.
258. Shulman-Peleg, A., Shatsky, M., Nussinov, R., and Wolfson, H. J. MAPPIS: Multiple 3D Alignment of Protein-Protein Interfaces. Lecture Notes in Computer Science, Vol. 3695, pp. 91-103, 2005.
259. Tsai, C. -J., and Nussinov, R. Protein-Protein Interactions. Principles and Prediction. Phys. Biol. 2: 51, 2005.



260. Tsai, C. –J. and Nussinov, R. The Implications of Higher (or Lower) Success in Secondary Structure Predication of Chain Fragments. Protein Sci. 14: 1943-1944, 2005.
261. Tsai, H–H., Reches, M., Tsai, C–J., Gunasekaran, K., Gazit, E., and Nussinov, R. Energy Landscape of Amyloidogenic Peptide Oligomerization by Parallel-Tempering MD Simulation: Significant Role of Asparagine Ladder. Proc. Natl. Acad. Sci. (USA) 102: 8174-8179, 2005.
262. Wolfson, H., Shatsky, M., Duhovny, D., Shulman, A., and Nussinov, R. From Structure to Function: Methods and Applications. Curr. Protein Pept. Sci. 6: 171-183, 2005.
263. Aleman, C., Zanuy, D., Casanovas, J., Cativiela, C., and Nussinov, R. Backbone Conformational Preferences and Pseudorotational Ring Puckering of 1-Aminocyclopentane-1-Carboxylic Acid. J. Phys. Chem. B Condens. Matter Mater Surf Interfaces Biophys. 110(: 21264-21271, 2006.
264. Aleman, C., Zanuy, D., Jimenez, A. I., Cativiela, C., Haspel, N., Zheng, J., Casanovas, J., Wolfson, H., and Nussinov, R. Concepts and Schemes for the ReEngineering of Physical Protein Modules: Generating Nanodevices Via Targeted Replacements with Constrained Amino Acids. Phys. Biol. 3: S54-S62, 2006.
265. Del Sol, A., Fujihashi, H., Amoros, D., and Nussinov, R. Residue Centrality, Functionally Important Residues, and Active Site Shape: Analysis of Enzyme and Non-Enzyme Families. Protein Sci. 15: 2120-2128, 2006.
266. Del Sol, A., Fujihashi, H., Amoros, D., and Nussinov, R. Residues Crucial for Maintaining Short Paths in Network Communication Mediate Signalling in Proteins. Mol. Syst. Biol. 2: 2006.0019, 2006.
267. Dror, O., Nussinov, R., and Wolfson, H.J. The ARTS Web Server for Aligning RNA Tertiary Structures. Nucleic Acids Res. 34: W412-W415, 2006.
268. Ertekin, A., Nussinov, and Haliloglu, T. Association of Putative Concave Protein-Binding Sites with the Fluctuation Behavior of Residues. Protein Sci. 15: 2265-2277, 2006.
269. Gnanakaran, S., Nussinov, R., and Garcia, A. E. Atomic-Level Description of Amyloid Beta-Dimer Formation. J. Am. Chem. Soc. 128: 2158-2159, 2006.
270. Halperin, I., Wolfson, H., and Nussinov, R. Correlated mutations: Advances and Limitations. A Study on Fusion Proteins and on the Cohesin-Dockerin Families. Proteins 63: 832-845, 2006.
271. Haspel, N., Zanuy, D., Aleman, C., Wolfson, H., and Nussinov, R. De Novo Tubular Nanostructure Design Based on Self-Assembly of Beta-Helical Protein Motifs. Structure 14: 1137-1148, 2006.

272. Jang, H., Ma, B., Woolf, T., and Nussinov, R. Interaction of Protegrin-1 (PG-1) with Lipid Bilayers: Membrane Thinning Effect. Biophys. J. 91: 2848-2859, 2006.
273. Liu, J., Pan, Y., Ma, B., and Nussinov, R. Protein-Protein Interactions could be Carcinogenic: Simulations of p53 Core Domain Complexed with 53BP1 and BRCA1 BRCT Domains. Structure 14: 1811-1821, 2006.
274. Ma, B. and Nussinov, R. Simulations as Analytical Tools to Understand Protein Aggregation and Predict Amyloid Conformation. Curr. Opin. Chem. Biol. 10: 445-452, 2006.
275. Ma, B. and Nussinov, R. The Stability of Monomeric Intermediates Controls Amyloid Formation: A $\beta$ 25-35 and its N27Q Mutant. Biophysical J. 90: 3365-3374, 2006.
276. Nussinov, R. and Aleman, C. Nanobiology: From Physics and Engineering to Biology. Physical Biology 3: S0, 2006.
277. Pan, Y., Ma, B., Levine, A. J., and Nussinov, R. Comparison of the Human and Worm p53 Structures Suggests a Way for Enhancing p53 Stability. Biochemistry 45: 3925-3933, 2006.
278. Shatsky, M. Nussinov, R., and Wolfson, H. J. Optimization of Multiple-Sequence Alignment Based on Multiple-Structure Alignment. Proteins 62: 209-217, 2006.
279. Shatsky, M., Shulman-Peleg, A., Nussinov, R., and Wolfson, H. The Multiple Common Point Set Problem and its Application to Molecule Binding Pattern Detection. J. Comput. Biol. 13: 407-428, 2006.
280. Shaul, S., Nussinov, R., and Pupko, T. Paths of Lateral Gene Transfer of Lysyl-Aminoacyl-tRNA Synthetases with a Unique Evolutionary Transition Stage of Prokaryotes Coding for Class I and II Varieties by the Same Organisms. BMC Evol. Biol. 6: 22, 2006.
281. Tsai, H-H., Gunasekaran, K., and Nussinov, R. Sequence and Structure Analysis of Parallel  $\beta$ -helices: Implication for Constructing Amyloid Structural Models. Structure 14: 1059-1072, 2006.
282. Tsai, C-J., Zheng, J., Aleman, C., and Nussinov, R. Structure by Design: From Single Proteins and their Building Blocks to Nanostructures. Trends Biotechnol. 24: 449-454, 2006.
283. Tsai, C-J., Zheng, J., and Nussinov, R. Designing a Nanotube using Naturally Occurring Protein Building Blocks. PLoS Comput. Biol. 2: e42, 2006.

284. Wainreb, G., Haspel, N., Wolfson, H., and Nussinov, R. A Permissive Secondary Structure-Guided Superposition Tool for Clustering of Protein Fragments toward Protein Structure Prediction Via Fragment Assembly. Bioinformatics 22: 1343-1352, 2006.
285. Zanuy, D., Gunasekaran, K., Lesk, A. M., and Nussinov, R. Computational Study of the Fibril Organization of Polyglutamine Repeats Reveals a Common Motif Identified in  $\beta$ -Helices. J. Mol. Biol. 358: 330-345, 2006.
286. Zanuy, D., Nussinov, R., and Aleman, C. From Peptide-Based Material Science to Protein Fibrils: Discipline Convergence in Nanobiology. Phys. Biol. 3: S80-S90, 2006.
287. Zheng, J., Ma, B., and Nussinov, R. Consensus Repeats in Amyloid Fibrils: Sheet-Sheet Recognition Via a (Polar or Nonpolar) Zipper Structure. Phys. Biol. 3: P1-4, 2006.
288. Zheng, J., Ma, B., Tsai, C-J., and Nussinov, R. The Stability and Dynamics of an Amyloid-Forming Peptide GNNQQNY from Yeast Prion sup-35. Biophys. J. 91: 824-833, 2006.
289. Andrusier, N., Nussinov, R., and Wolfson, H. J. FireDock: Fast Interaction Refinement in Molecular Docking. Proteins 69: 139-159, 2007.
290. Casanovas, J., Zanuy, D., Nussinov, R., and Aleman, C. Intrinsic Conformational Characteristics of Alpha, Alpha-Dipenylglycine. J. Org. Chem. 72: 2174-2181, 2007.
291. Cohen-Gihon, I., Nussinov, R., and Sharan, R. Comprehensive Analysis of Co-Occurring Domain Sets in Yeast Proteins. BMC Genomics 8: 161, 2007.
292. Curco, D., Nussinov, R., and Aleman, C. Coarse-Graining the Self-Assembly of  $\beta$ -Helical Protein Building Blocks. J. Phys. Chem. B. 111: 14006-14011, 2007.
293. Curco, D., Nussinov, R., and Aleman, C. Coarse-Grained Representation of  $\beta$ -Helical Protein Building Blocks. J. Phys. Chem. B. 111: 10538-10549, 2007.
294. Del Sol, A., Arauzo-Bravo, M. J., Amoros-Moya, D., and Nussinov, R. Modular Architecture of Protein Structures and Allosteric Communications: Potential Implications for Signalling Proteins and Regulatory Linkages. Genome Biol. 8: R92, 2007.
295. Dror, O., Lasker, K., Nussinov, R., and Wolfson, H. EMatch: An Efficient Method for Aligning Atomic Resolution Subunits into Intermediate-Resolution Cryo-EM Maps of Large Macromolecular Assemblies. Acta Crystallogr. D Biol. Crystallogr. 63: 42-49, 2007.
296. Fishelovitch, D., Hazan, C., Hirao, H., Wolfson, H. J., Nussinov, R., and Shaik S. QM/MM Study of the Active Species of the Human Cytochrome P450 3A4, and the

- Influence thereof of the Multiple Substrate Binding. J. Phys. Chem. B. 111: 13822-13832, 2007.
297. Fishelovitch, D., Hazan, C., Shaik, S., Wolfson, H. J., and Nussinov, R. Structural Dynamics of the Cooperative Binding of Organic Molecules in the Human Cytochrome P450 3A4 (CP3A4). J. Amer. Chem. Soc. 129: 1602-1611, 2007.
298. Flores-Ortega, A., Casanovas, J., Zanuy, D., Nussinov, R., and Aleman, C. Conformations of Proline Analogs Having Double Bonds in the Ring. J. Phys. Chem. B. 111: 5475-5482, 2007.
299. Gunasekaran, K. and Nussinov, R. How Different are Structurally Flexible and Rigid Binding Sites? Sequence and Structural Features Discriminating Proteins that do and do not Undergo Conformational Change Upon Ligand Binding. J. Mol. Biol. 365: 257-273, 2007.
300. Haspel, N., Wainreb, G., Inbar, Y., Tsai, H. H., Tsai, C. J., Wolfson, H. J., and Nussinov, R. A Hierarchical Protein Folding Scheme Based on the Building Block Folding Model. Methods Mol. Biol. 350: 189-204, 2007.
301. Haspel, N., Zanuy, D., Zheng, J., Aleman, C., Wolfson, H., and Nussinov, R. Changing the Charge Distribution of Beta-Helical Based Nanostructures can Provide the Conditions for Charge Transfer. Biophysical J. 93: 245-253, 2007.
302. Hu, Z., Bowen, D., Southerland, W. M., Del Sol, A., Pan, Y., Nussinov, R., and Ma, B. Lingand Binding and Circular Permutation Modify Residue Interaction Network in DHFR. PLoS Comput. Biol. 3: e117, 2007.
303. Jang, H., Ma, B., and Nussinov, R. Conformational Study of the Protegrin-1 (PG-1) Dimmer Interaction with Lipid Bilayers and its Effect. BMC Struct. Biol. 7: 21, 2007.
304. Jang, H., Zheng, J., and Nussinov, R. Models of Beta-Amyloid Ion Channels in the Membrane Suggest that Channel Formation in the Bilayer is a Dynamic Process. Biophys. J. 93: 1938-1949, 2007.
305. Keskin, O., Gursoy, A., Ma, B., and Nussinov, R. Towards Drugs Targeting Multiple Proteins in a Systems Biology Approach. Curr. Top. Med. Chem. 7: 943-951, 2007.
306. Keskin, O. and Nussinov, R. Similar Binding Sites and Different Partners: Implications to Shared Proteins in Cellular Pathways. Structure 15: 341-354, 2007.
307. Lasker, K., Dror, O., Shatsky, M., Nussinov, R., and Wolfson, H. EMatch: Discovery of High Resolution Structural Homologues of Protein Domains in Intermediate Resolution Cryo-EM Maps. IEEE/ACM Trans. Comput. Biol. Bioinform. 4: 28-39, 2007.

308. Ma, B. and Nussinov, R. Trp/Met/Phe Hot Spots in Protein-Protein Interactions: Potential Targets in Drug Design. Curr. Top. Med. Chem. 7: 999-1005, 2007.
309. Ma, B., Pan, Y., Zheng, J., Levine, A. J., and Nussinov, R. Sequence Analysis of p53 Response Elements Suggests Multiple Binding Modes of the p53 Tetramer to DNA Targets. Nucleic Acids Res. 35: 2986-3001, 2007.
310. Pan, Y. and Nussinov, R. Structural Basis for Specific p53 Binding-Induced DNA Bending. J. Biol. Chem. 282: 691-699, 2007.
311. Schneidman-Duhovny, D., Nussinov, R., and Wolfson, H. J. Automatic Prediction of Protein Interactions with Large-Scale Motion. Proteins 69: 764-773, 2007.
312. Shatsky, M., Nussinov, R., and Wolfson, H. J. Algorithms for Multiple Protein Structure Alignment and Structure-Derived Multiple Sequence Alignment. Methods Mol. Biol. 413: 125-146, 2007.
313. Shulman-Peleg, A., Shatsky, M., Nussinov, R., and Wolfson, H. J. Spatial Chemical Conservation of Hot Spot Interactions in Protein-Protein Complexes. BMC Biol. 5: 43, 2007.
314. Tsai, C-J., Zheng, J., Zanuy, D., Haspel, N., Wolfson, H., Aleman, C., and Nussinov, R. Principles of Nanostructure Design with Protein Building Blocks. Proteins 68: 1-12, 2007.
315. Zanuy, D., Jimenez, A. I., Cativiela, C., Nussinov, R., and Aleman, C. Use of Constrained Synthetic Amino Acids in  $\beta$ -Helix Proteins for Conformational Control. J. Phys. Chem. 111: 3236-3242, 2007.
316. Zanuy, D., Rodriguez-Ropero, F., Haspel, N., Zheng, J., Nussinov, R., and Aleman, C. Stability of Tubular Structures Based on Beta-Helical Proteins: Self-Assembled Versus Polymerized Nanoconstructs and Wild-Type Versus Mutated Sequences. Biomacromolecules 8: 3135-3146, 2007.
317. Zanuy, D., Rodriguez-Ropero, F., Nussinov, R., and Aleman, C. Testing Beta-Helix Terminal Coils Stability by Targeted Substitutions with Non-Proteogenic Amino Acids: A Molecular Dynamics Study. J. Struct. Biol. 160: 177-189, 2007.
318. Zheng, J., Jang, H., Ma, B., Tsai, C. J., and Nussinov, R. Modeling the Alzheimer A $\beta$  17-42 Fibril Architecture: Tight Intermolecular Sheet-Sheet Association and Intramolecular Hydrated Cavities. Biophys. J. 93: 3046-3057, 2007.
319. Zheng, J., Zanuy, D., Haspel, N., Tsai, C-J., Aleman, C., and Nussinov, R. NanoStructure Design using Protein Building Blocks Enhanced by Conformationally Constrained Synthetic Residues. Biochemistry 46: 1205-1218, 2007.

320. Abraham, M., Dror, O., Nussinov, R., and Wolfson, H. J. Analysis and Classification of RNA Tertiary Structures. RNA 14: 2274-2289, 2008.
321. Ahmad, S., Keskin, O., Sarai, A., and Nussinov, R. Protein-DNA Interactions: Structural, Thermodynamic and Clustering Patterns of Conserved Residues in DNA-Binding Proteins. Nucleic Acids Res. 36: 5922-5932, 2008.
322. Andrusier, N., Mashiach, E., Nussinov, R., and Wolfson, H. J. Principles of Flexible Protein-Protein Docking. Proteins 73: 271-289, 2008.
323. Ballano, G., Zanuy, D., Jimenez, A. I., Cativiela, C., Nussinov, R., and Aleman, C. Structural Analysis of a  $\beta$ -Helical Protein Motif Stabilized by Targeted Replacements with Conformationally Constrained Amino Acids. J. Phys. Chem. B 112: 13101-13115, 2008.
324. Buch, I., Tsai, C-J., Wolfson, H. J., and Nussinov, R. Self-Assembly of Fused Homo-Oligomers to Create Nanotubes. Methods Mol. Biol. 474: 117-131, 2008.
325. Casanovas, J., Jimenez, A. I., Cativiela, C., Nussinov, R., and Aleman, C. 1-amino-2-Phenylcyclopentane-1-Carboxylic Acid: A Conformationally Restricted Phenylalanine Analogue. J. Org. Chem. 73: 644-651, 2008.
326. Casanovas, J., Nussinov, R., and Aleman, C. Intrinsic Conformational Preferences of C(alpha,alpha)-dibenzylglycine. J. Org. Chem. 73: 4205-4211, 2008.
327. Dror, O., Schneidman-Duhovny, D., Shulman-Peleg, A., Nussinov, R., Wolfson, H. J., and Sharan, R. Structural Similarity of Genetically Interacting Proteins. BMC Syst. Biol. 2: 69, 2008.
328. Emekli, U., Schneidman-Duhovny, D., Wolfson, H. J., Nussinov, R., and Haliloglu, T. HingePot: Automated Prediction of Hinges in Protein Structures. Proteins 70: 1219-1227, 2008.
329. Emekli, U., Gunasekaran, K., Nussinov, R., and Haliloglu, T. What can we Learn from Highly Connected Beta-Rich Structures for Interface Design? Methods Mol. Biol. 474: 235-253, 2008.
330. Flores-Ortega, A., Casanovas, J., Nussinov, R., and Aleman, C. Conformational Preferences of  $\beta$ - and  $\gamma$ -aminated Proline Analogues. J. Phys. Chem. B 112: 14045-14055, 2008.
331. Flores-Ortega, A., Jimenez, A. I., Cativiela, C., Nussinov, R., Aleman, C., and Casanovas, J. Conformational Preferences of Alpha-Substituted Proline Analogues. J. Org. Chem. 73: 3418-3427, 2008.

332. Gazit, E. and Nussinov, R. NanoStructure Design: Methods and Protocols. Preface. Methods Mol. Biol. 474: v-vii, 2008.
333. Gursoy, A., Keskin, O., and Nussinov, R. Topological Properties of Protein Interaction Networks from a Structural Perspective. Biochem. Soc. Trans. 36: 1398-1403, 2008.
334. Jang, H., Ma, B., Lal, R., and Nussinov, R. Models of Toxic  $\beta$ -Sheet Channels of Protegrin-1 (PG-1) Suggest a Common Subunit Organization Motif Shared with Toxic Alzheimer  $\beta$ -Amyloid Ion Channels. Biophys. J. 95: 4631-4642, 2008.
335. Jang, H., Zheng, J., Lal, R., and Nussinov, R. New Structures Help the Modelling of Toxic Amyloid $\beta$  (A $\beta$ ) Ion Channels. Trends Biochem. Sci. 33: 91-100, 2008.
336. Keskin, O., Gursoy, A., Ma, B., and Nussinov, R. Principles of Protein-Protein Interactions: What are the Preferred Ways for Proteins to Interact? Chem. Rev. 108: 1225-1244, 2008.
337. Keskin, O., Nussinov, R., and Gursoy, A. PRISM: Protein-Protein Interaction Prediction by Structural Matching. Methods Mol. Biol. 484: 505-521, 2008.
338. Kifer, I., Nussinov, R., and Wolfson, H. J. Constructing Templates for Protein Structure Prediction by Simulation of Protein Folding Pathways. Proteins 73: 380-394, 2008.
339. Liu, J. and Nussinov, R. Allosteric Effects in the Marginally Stable Von Hippel Lindau Tumor Suppressor Protein and Allostery-Based Rescue Mutant Design. Proc. Natl. Acad. Sci. U.S.A. 105: 901-906, 2008.
340. Mashiach, E., Schneidman-Duhovny, D., Andrusier, N., Nussinov, R., and Wolfson, H. J. FireDock: A Web Server for Fast Interaction Refinement in Molecular Docking. Nucleic Acids Res. 36(Web Server Issue): W229-W232, 2008.
341. Pan, Y. and Nussinov, R. p53-Induced DNA Bending: The Interplay Between p53-DNA and p53-p53 Interactions. J. Phys. Chem. B 112: 6716-6724, 2008.
342. Rodriguez-Ropero, F., Zanuy, D., Casanovas, J., Nussinov, R., and Aleman, C. Application of 1-aminocyclohexane carboxylic acid to Protein Nanostructure Computer Design. J. Chem. Info. Model. 48: 333-343, 2008.
343. Schneidman-Duhovny, D., Dror, O., Inbar, Y., Nussinov, R., and Wolfson, H. J. Deterministic Pharmacophore Detection Via Multiple Flexible Alignment of Drug-Like Molecules. J. Comput. Biol. 15: 737-754, 2008.
344. Schneidman-Duhovny, D., Dror, O., Inbar, Y., Nussinov, R., and Wolfson, H. J. PharmaGist: A Webserver for Ligand-Based Pharmacophore Detection. Nucleic Acids Res. 36(Web Server Issue): W223-228, 2008.

345. Shatsky, M., Nussinov, R., and Wolfson, H. J. Algorithms for Multiple Protein Structure Alignment and Structure-Derived Multiple Sequence Alignment. Methods Mol. Biol. 413: 125-146, 2008.
346. Shulman-Peleg, A., Shatsky, M., Nussinov, R., and Wolfson, H. J. Prediction of Interacting Single-Stranded RNA Bases by Protein Binding Patterns. J. Mol. Biol. 379: 299-316, 2008.
347. Shulman-Peleg, A., Shatsky, M., Nussinov, R., and Wolfson, H. J. MultiBind and MAPPIS: Web Servers for Multiple Alignment of Protein 3D Binding Sites and their Interactions. Nucleic Acids Res. 36(Web Server Issue): W260-W264, 2008.
348. Tozluoglu, M., Karaca, E., Haliloglu, T., and Nussinov, R. Cataloging and Organizing p73 Interactions in Cell Cycle Arrest and Apoptosis. Nucleic Acids Res. 36: 5033-5049, 2008.
349. Tsai, C-J., del Sol, A., and Nussinov, R. Allosteric: Absence of a Change in Shape does not imply that Allosteric is not at Play. J. Mol. Biol. 378: 1-11, 2008.
350. Tsai, C-J., Sauna, Z. E., Kimchi-Sarfaty, C., Ambudkar, S. V., Gottesman, M. M., and Nussinov, R. Synonymous Mutations and Ribosome Stalling can Lead to Altered Folding Pathways and Distinct Minima. J. Mol. Biol. 383: 281-291, 2008.
351. Tuncbag, N., Gursoy, A., Guney, E., Nussinov, R., and Keskin, O. Architectures and Functional Coverage of Protein-Protein Interfaces. J. Mol. Biol. 381: 785-802, 2008.
352. Yaffe, E., Fishelovitch, D., Wolfson, H. J., Halperin, D., and Nussinov, R. MolAxis: A Server for Identification of Channels in Macromolecules. Nucleic Acids Res. 36(Web Server Issue): W210-W215, 2008.
353. Yaffe, E., Fishelovitch, D., Wolfson, H. J., Halperin, D., and Nussinov, R. MolAxis: Efficient and Accurate Identification of Channels in Macromolecules. Proteins 73: 72-86, 2008.
354. Yogurtcu, O. N., Erdemli, S. B., Nussinov, R., Turkay, M., and Keskin, O. Restricted Mobility of Conserved Residues in Protein-Protein Interfaces in Molecular Simulations. Biophys. J. 94: 3475-3485, 2008.
355. Zanuy, D., Flores-Ortega, A., Casanovas, J., Curco, D., Nussinov, R., and Aleman, C. The Energy Landscape of a Selective Tumor-Homing Pentapeptide. J. Phys. Chem. B 112: 8692-8700, 2008.
356. Zheng, J., Jang, H., Ma, B., and Nussinov, R. Annular Structures as Intermediates in Fibril Formation of Alzheimer A $\beta$ <sub>17-42</sub>. J. Phys. Chem. B. 112: 6856-6865, 2008.



357. Zheng, J., Jang, H., and Nussinov, R.  $\beta_2$ -microglobulin Amyloid Fragment Organization and Morphology and its Comparison to A $\beta$  Suggests that Amyloid Aggregation Pathways are Sequence-Specific. Biochemistry 47: 2497-2509, 2008.
358. Zheng, J., Ma B., Chang, Y., and Nussinov, R. Molecular Dynamics Simulations of Alzheimer A $\beta_{40}$  Elongation and Lateral Association. Front. Biosci. 13: 3919-3930, 2008.
359. Aleman C., Jimenez, A. I., Cativiela, C., Nussinov, R., and Casanovas, J. Conformational Preferences of 1-amino-2-phenylcyclohexanecarboxylic Acid, a Phenylalanine Cyclohexane Analogue. J. Organic Chem. 74: 7834-7843, 2009.
360. Boehr, D. D., Nussinov, R., and Wright, P. E. The Role of Dynamic Conformational Ensembles in Biomolecular Recognition. Nature Chem. Biol. 5: 789-796, 2009.
361. Buch, I., Brooks, B. R., Wolfson, H. J., and Nussinov, R. Computational Validation of Protein Nanotubes. Nano Lett. 9: 1096-1102, 2009.
362. Carbonell, P., Nussinov, R., and del Sol, A. Energetic Determinants of Protein Binding Specificity: Insights into Protein Interaction Networks. Proteomics 9: 1744-1753, 2009.
363. del Sol, A., Tsai, C-J., Ma, B., and Nussinov, R. The Origin of Allosteric Functional Modulation: Multiple Pre-Existing Pathways. Structure 17: 1042-1050, 2009.
364. Dror, O., Schneidman-Duhovny, D., Inbar, Y., Nussinov, R., and Wolfson, H. J. Novel Approach for Efficient Pharmacophore-Based Virtual Xcreening: Method and Applications. J. Chem. Inf. Model. 49: 2333-2343, 2009.
365. Fishelovitch, D., Shaik, S., Wolfson, H. J., and Nussinov, R. Theoretical Characterization of Substrate Access/Exit Channels in the Human Cytochrome P450 3A4 Enzyme: Involvement of Phenylalanine Residues in the Gating Mechanism. J. Phys. Chem. B. 113: 13018-13025, 2009.
366. Jang, H., Arce, F. T., Capone, R., Ramachandran, S., Lal, R., and Nussinov, R. Misfolded Amyloid Ion Channels Present Mobile  $\beta$ -Sheet Subunits in Contrast to Conventional Ion Channels. Biophys. J. 97: 3029-3037, 2009.
367. Liu, J. and Nussinov, R. The Mechanism of Ubiquitination in the Cullin-RING E3 Ligase Machinery: Conformational Control of Substrate Orientation. PLoS Comput. Biol. 5: e1000527, 2009.
368. Ma, B. and Nussinov, R. Amplification of Signalling Via Cellular Allosteric Relay and Protein Disorder. Proc. Natl. Acad. Sci. U.S.A. 106: 6887-6888, 2009.
369. Ma, B. and Nussinov, R. Regulating Highly Dynamic Unstructured Proteins and their Coding mRNAs. Genome Biol. 10: 204, 2009.

370. Miller, Y., Ma, B., and Nussinov, R. Polymorphism of Alzheimer's A $\beta$ <sub>17-42</sub> (p3) Oligomers: The Importance of the Turn Location and its Conformation. Biophys. J. 97: 1168-1177, 2009.
371. Mustata, M., Capone, R., Jang, H., Arce, F. T., Ramachandran, S., Lal, R., and Nussinov, R. The K3 Fragment of Amyloidogenic  $\beta$ <sub>2</sub>-microglobulin Forms Ion Channels: Implication for Dialysis Related Amyloidosis. J. Amer. Chem. Soc. 131: 14938-14945, 2009.
372. Pan, P. and Nussinov, R. Cooperativity Dominates the Genomic Organization of p53-Response Elements: A Mechanistic View. PLoS Computational Biol. 5: e1000448, 2009.
373. Pan, Y., Tsai, C-J., Ma, B., and Nussinov, R. How do Transcription Factors Select Specific Binding Sites Among Many Similar Ones in the Genome? Nature Struct. Mol. Biol. 16: 1118-1120, 2009.
374. Pappu, R. V. and Nussinov, R. Protein Folding: Lessons Learned and New Frontiers. Phys. Biol. 6: 10301, 2009.
375. Revilla-Lopez, G., Torras, J., Jimenez, A. I., Cativiela, C., Nussinov, R., and Aleman, C. Side-Chain to Backbone Interactions Dictate the Conformational Preferences of a Cyclopentane Arginine Analogue. J. Org. Chem. 74: 2403-2412, 2009.
376. Shulman-Peleg, A., Nussinov, R., and Wolfson, H. J. RsiteDB: A Database of Protein Binding Pockets that Interact with RNA Nucleotide Bases. Nucleic Acids Res. 37(Database Issue): D369-D373, 2009.
377. Tsai, C-J., del Sol, A., and Nussinov, R. Protein Allostery, Signal Transmission and Dynamics: A Classification Scheme of Allosteric Mechanisms. Mol. Biosyst. 5: 207-216, 2009.
378. Tsai, C-J., Ma, B., and Nussinov, R. Intra-Molecular Chaperone: The Role of the N-Terminal in Conformational Selection and Kinetic Control. Phys. Biol. 6: 13001, 2009.
379. Tsai, C-J., Ma, B. and Nussinov, R. Protein-Protein Interaction Networks: How can a Hub Protein Bind so Many Different Partners? Trends Biochem. Sci. 34: 594-600, 2009.
380. Tuncbag, N., Kar, G., Gursoy, A., Keskin, O., and Nussinov, R. Towards Inferring Time Dimensionality in Protein-Protein Interaction Networks by Integrating Structures: The p53 Example. Mol. BioSyst. 5: 1770-1778, 2009.
381. Tuncbag, N., Kar, G., Keskin, O., Gursoy, A., and Nussinov, R. A Survey of Available Tools and Web Servers for Analysis of Protein-Protein Interactions and Interfaces. Brief. Bioinform. 10: 217-232, 2009.

382. Yu, X., Wang, Q., Yang, J-C., Buch, I., Tsai, C-J., Ma, B., Cheng, S. Z. D., Nussinov, R., and Zheng, J. Mutational Analysis and Allosteric Effects in the HIV-1 Capsid Protein Carboxyl-Terminal Dimerization Domain. Biomacromolecules 10: 390-399, 2009.
383. Zanuy, D., Ballano, G., Jimenez, A. I., Casanovas, J., Haspel, N., Cativiela, C., Curco, D., Nussinov, R., and Aleman, C. Protein Segments with Conformationally Restricted Amino Acids can Control Supramolecular Organization at the Nanoscale. J. Chem. Inf. Model. 49: 1623-1629, 2009.
384. Zanuy, D., Curco, D., Nussinov, R., and Aleman, C. Influence of the Dye Presence on the Conformational Preferences of CREKA, a Tumor Homing Linear Pentapeptide. Biopolymers 92: 83-93, 2009.
385. Zanuy, D., Flores-Ortega, A., Jimenez, A. I., Calaza, M. I., Cativiela, C., Nussinov, R., Ruoslahti, E., and Aleman, C. *In silico* Molecular Engineering for a Targeted Replacement in a Tumor-Homing Peptide. J. Phys. Chem. B 113: 7879-7889, 2009.
386. Agemy, L., Sugahara, K. N., Kotamraju, V. R., Gujraty, K., Girard, O. M., Kono, Y., Mattrey, R. F., Park, J-H., Sailor, M. J., Jimenez, A. I., Cativiela, C., Zanuy, D., Sayago, F. J., Aleman, C., Nussinov, R., and Ruoslahti, E. Nanoparticle-Induced Vascular Blockade in Human Prostate Cancer. Blood 116: 2847-2856, 2010.
387. Ahmad, S., Keskin, O., Mizuguchi, K., Sarai, A., and Nussinov, R. CCRXP: Exploring Clusters of Conserved Residues in Protein Structures. Nucleic Acids Res. 38: W398-W401, 2010.
388. Buch, I., Fishelovitch, D., London, N., Raveh, B., Wolfson, H. J., and Nussinov, R. Allosteric Regulation of Glycogen Synthase Kinase-3 $\beta$ : A Theoretical Study. Biochemistry 49: 10890-10901, 2010.
389. Capone, R., Mustata, M., Jang, H., Arce, F. T., Nussinov, R., and Lal, R. Antimicrobial Protegrin-1 Forms Ion Channels: Molecular Dynamic Simulation, Atomic Force Microscopy, and Electrical Conductance Studies. Biophys. J. 98: 2644-2652, 2010.
390. Csermely, P., Palotai, R., and Nussinov, R. Induced Fit, Conformational Selection and Independent Dynamic Segments: An Extended View of Binding Events. Trends Biochem. Sci. 35: 539-546, 2010.
391. Fishelovitch, D., Shaik, S., Wolfson, H. H., and Nussinov, R. How Does the Reductase Help to Regulate the Catalytic Cycle of Cytochrome P450 3A4 Using the Conserved Water Channel? J. Phys. Chem. B 114: 5964-5970, 2010.
392. Jang, H., Arce, F. T., Ramachandran, S., Capone, R., Azimova, R., Kagan, B. L., Nussinov, R., and Lal, R. Truncated  $\beta$ -Amyloid Peptide Channels Provide an Alternative

- Mechanism for Alzheimer's Disease and Down's Syndrome. Proc. Natl. Acad. Sci. U.S.A. 107: 6538-6543, 2010.
393. Jang, H., Arce, F. T., Ramachandran, S., Capone, R., Lal, R., and Nussinov, R. Structural Convergence Among Diverse, Toxic  $\beta$ -Sheet Ion Channels. J. Phys. Chem. B 114: 9445-9451, 2010.
394. Jang, H., Arce, F. T., Ramachandran, S., Capone, R., Lal, R., and Nussinov, R.  $\beta$ -Barrel Topology of Alzheimer's  $\beta$ -Amyloid Ion Channels. J. Mol. Biol. 404: 917-934, 2010.
395. Kar, G., Keskin, O., GURSOY, A., and Nussinov, R. Allostery and Population Shift in Drug discovery. Curr Opin Pharmacol. 10: 715-722, 2010.
396. Liu, J. and Nussinov, R. Molecular Dynamics Reveal the Essential Role of Linker Motions in the Function of Cullin-RING E3 Ligases. J. Mol. Biol. 396: 1508-1523, 2010.
397. Liu, J. and Nussinov, R. Rbx1 Flexible Linker Facilitates Cullin-RING Ligase Function Before Neddylation and After Deneddylation. Biophys. J. 99: 736-744, 2010.
398. Ma, B. and Nussinov, R. Enzyme Dynamics Point to Stepwise Conformational Selection in Catalysis. Curr. Opin. Chem. Biol. 14: 652-659, 2010.
399. Ma, B. and Nussinov, R. Polymorphic C-Terminal  $\beta$ -Sheet Interactions Determine the Formation of Fibril or Amyloid  $\beta$ -Derived Diffusible Ligand-Like Globulomer for the Alzheimer A $\beta$ 42 Dodecamer. J. Biol. Chem. 285: 37102-37110, 2010.
400. Ma, B, Tsai, C-J., Pan, Y., and Nussinov, R. Why does Binding of Proteins to DNA or Proteins to Proteins does not Necessarily Spell Function? ACS Chem. Biol. 5: 265-272, 2010.
401. Mashiach, E., Nussinov, R., and Wolfson, H. J. FiberDock: A Web Server for Flexible Induced-Fit Backbone Refinement in Molecular Docking. Nucleic Acids Res. 38(Web Server issue): W457-W461, 2010.
402. Mashiach, E., Nussinov, R., and Wolfson, H. J. FiberDock: Flexible Induced-Fit Backbone Refinement in Molecular Docking. Proteins 78: 1503-1519, 2010.
403. Mashiach, E., Schneidman-Duhovny, D., Peri, A., Shavit, Y., Nussinov, R., and Wolfson, H. J. An Integrated Suite of Fast Docking Algorithms. Proteins 78: 3197-3204, 2010.
404. Miller, Y., Ma, B., and Nussinov, R. Polymorphism in Alzheimer A $\beta$  Amyloid Organization Reflects Conformational Selection in a Rugged Energy Landscape. Chem. Rev. 110: 4820-4838, 2010.

405. Miller, Y., Ma, B., and Nussinov, R. Zinc Ions Promote Alzheimer A $\beta$  Aggregation Via Population Shift of Polymorphic States. PNAS 107: 9490-9495, 2010.
406. Miller, Y., Ma, B., Tsai, C-J., and Nussinov, R. Hollow Core of Alzheimer's A $\beta$ <sub>42</sub> Amyloid Observed by cryoEM is Relevant at Physiological pH. Proc. Natl. Acad. Sci. 107: 14128-14133, 2010.
407. Ozbabacan, S. E. A., Gursoy, A., Keskin, O., and Nussinov, R. Conformational Ensembles, Signal Transduction and Residue Hot Spots: Application to Drug Discovery. Curr. Opin. Drug Discov. Devel. 13: 527-537, 2010.
408. Pan, Y. and Nussinov, R. Lysine120 Interactions with p53 Response Elements can Allosterically Direct p53 Organization. PLoS Comput. Biol. 6: e1000878, 2010.
409. Pan, Y. and Nussinov, R. Preferred Drifting Along the DNA Major Groove and Cooperative Anchoring of the p53 Core Domain: Mechanisms and Scenarios. J. Mol. Recognit. 23: 232-240, 2010.
410. Pan, Y., Tsai, C-J., Ma, B. and Nussinov, R. Mechanisms of Transcription Factor Selectivity. Trends Genet. 26: 75-83, 2010.
411. Revilla-Lopez, G., Jimenez, A. I., Cativiela, C., Nussinov, R., Aleman, C., and Zanuy, D. Conformational Profile of a Proline-Arginine Hybrid. J Chem Inf Model. 50: 1781-1789, 2010.
412. Revilla-Lopez, G., Torras, J., Curco, D., Casanovas, J., Calaza, M. I., Zanuy, D., Jimenez, A. I., Cativiela, C., Nussinov, R., Grodzinski, P., and Aleman, C. NCAD, a Database Integrating the Intrinsic Conformational Preferences of Non-Coded Amino Acids. J. Phys. Chem. B 114: 7413-7422, 2010.
413. Tozluoglu, M., Karaca, E., Nussinov, R., and Haliloglu, T. A Mechanistic View of the Role of E3 in Sumoylation. PLoS Comput. Biol. 6. pii: e1000913, 2010.
414. Yu, X., Wang, J., Yang, J-C., Wang, Q., Cheng, S. Z. D., Nussinov, R., and Zheng, J. Atomic Scale Simulations Confirm that *soluble*  $\beta$ -Sheet-Rich Peptide Self-Assemblies Provide Amyloid Mimics Presenting Similar Conformational Properties. Biophysical J. 98: 27-36, 2010.
415. Zen, A., Micheletti, C., Keskin, O., and Nussinov, R. Comparing Interfacial Dynamic in Protein-Protein Complexes: An Elastic Network Approach. BMC Struct. Biol. 10: 26, 2010.
416. Arce, F. T., Jang, H., Ramachandran, S., Landon, P. B., Nussinov, R., and Lal, R. Polymorphism of Amyloid  $\beta$  Peptide in Different Environments: Implications for Membrane Insertion and Pore Formation. Soft Matter 7: 5267-52733, 2011.

417. Buch, I., Tsai, C.-J., Wolfson, H. J., Nussinov, R. Symmetry-Based Self-Assembled Nanotubes Constructed Using Native Protein Structures: The Key Role of Flexible Linkers. Protein Pept Lett. 18: 362-372, 2011.
418. Cohen-Gihon, I., Fong, J. H., Sharan, R., Nussinov, R., Przytycka, T. M., and Panchenko, A. R. Evolution of Domain Promiscuity in Eukaryotic Genomes – A Perspective from the Inferred Ancestral Domain Architectures. Mol. Biosyst. 7: 784-792, 2011.
419. Cohen-Gihon, I., Sharan, R., and Nussinov, R. Processes of Fungal Proteome Evolution and Gain of Function: Gene Duplication and Domain Rearrangement. Phys. Biol. 8: 035009, 2011.
420. Curco, D., Zanuy, D., Nussinov, R., and Aleman, C. A Simulation Strategy for the Atomistic Modeling of Flexible Molecules Covalently Tethered to Rigid Surfaces: Application to Peptides. J. Comput. Chem. 32: 607-619, 2011.
421. Dickin, R., Marden, C., Collings, A. M., Nussinov, R., and Bourne, P. E. A Review of 2010 for PLoS Computational Biology. PLoS Comput. Biol. 7: e1002003, 2011.
422. Haspel, N., Zanuy, D., Nussinov, R., Teesalu, T., Ruoslahti, E., and Aleman, C. Binding of a C-End Rule Peptide to Neuropilin-1 Receptor: A Molecular Modeling Approach. Biochemistry 50: 1755-1762, 2011.
423. Jang, H., Arce, F. T., Mustata, M., Ramachandran, S., Capone, R., Nussinov, R., and Lal, R. Antimicrobial Protegrin-1 (PG-1) Forms Amyloid-like Fibrils with Rapid Kinetics Suggesting a Functional Link. Biophysical J. 100: 1775-1783, 2011.
424. Karaca, E., Tozluoğlu, M., Nussinov, R., and Haliloğlu, T. Alternative Allosteric Mechanisms can Regulate the Substrate and E2 in SUMO Conjugation. J. Mol. Biol. 406: 620-630, 2011.
425. Kifer, I., Nussinov, R., and Wolfson, H. J. GOSSIP: A Method for Fast and Accurate Global Alignment of Protein Structures. Bioinformatics 27: 925-932, 2011.
426. Kifer, I., Nussinov, R., and Wolfson, H. J. Protein Structure Prediction using a Docking-Based Hierarchical Folding Scheme. Proteins 79: 1759-1773, 2011.
427. Kuzu, G., Keskin, O., Gursoy, A., and Nussinov, R. Expanding the Conformational Selection Paradigm in Protein-Ligand Docking. Meth. Mol. Biol. 19: 59-74, 2011.
428. Liu, J. and Nussinov, R. Flexible Cullins in Cullin-Ring E3 Ligases Allosterically Regulate Ubiquitination. J. Biol. Chem. 286: 40934-40942, 2011.
429. Luna, A., Karac, E. I., Sunshine, M., Chang, L., Nussinov, R., Aladjem, M. I., and Kohn, K. W. A Formal MIM Specification and Tools for the Common Exchange of MIM

- Diagrams: An XML-Based Format, and API, and a Validation Method. BMC Bioinformatics 12: 167, 2011.
430. Ma, B. and Nussinov, R. Polymorphic Triple  $\beta$ -Sheet Structures Contribute to Amide H/D Exchange Protection in Alzheimer's Amyloid  $\beta$ 42. J. Biol. Chem. 286: 34244-34253, 2011.
  431. Ma, B., Tsai, C-J., HaliloAlu, T., and Nussinov, R. Dynamic Allostery: Linkers are not Merely Flexible. Structure 19: 907-917, 2011.
  432. Mashiach-Farkash, E., Nussinov, R., and Wolfson, H. J. SymmRef: A Flexible Refinement Method for Symmetric Multimers. Proteins 79: 2607-2623, 2011.
  433. Miller, Y., Ma, B., and Nussinov, R. The Unique Alzheimer's  $\beta$ -Amyloid Triangular Fibril has a Cavity Along the Fibril Axis Under Physiological Conditions. J. Am. Chem. Soc. 133: 2742-2748, 2011.
  434. Miller, Y., Ma, B., and Nussinov, R. Synergistic Interactions Between Repeats in tau Protein and A $\beta$  Amyloids may be Responsible for Accelerated Aggregation Via Polymorphic States. Biochemistry 50: 5172-5181, 2011.
  435. Nussinov, R., Panchenko, A. R., and Przytycka, T. Physics Approaches to Protein Interactions and Gene Regulation. Phys. Biol. 8: 030301, 2011.
  436. Nussinov, R., Tsai, C-J., and Csermely, P. Allo-Network Drugs: Harnessing Allostery in Cellular Networks. Trends Pharmacol. Sci. 32: 686-693, 2011.
  437. Pan, Y. and Nussinov, R. The Role of Response Elements Organization in Transcription Factor Selectivity: The IFN- $\beta$  Enhanceosome Example. PLoS Comput. Biol. 7: e1002077, 2011.
  438. Parthasarathy, S., Long, F., Miller, Y., Xiao, Y., McElheny, D., Thurber, K., Ma, B., Nussinov, R., and Ishii, Y. Molecular-Level Examination of Cu<sup>2+</sup> Binding Structure for Amyloid Fibrils of 40-Residue Alzheimer's  $\beta$  by Solid-State NMR Spectroscopy. J. Am. Chem. Soc. 133: 3390-3400, 2011.
  439. Puri, A., Jang, H., Yavlovich, A., Masgood, A., Veenstra, T., Luna, C., Aranda-Espinoza, H., Nussinov, R., and Blumenthal, R. Material Properties of Matrix Lipids Determine Conformation and Intermolecular Reactivity of a Diacetylenic Phosphatidylcholine in the Lipid Layer. Langmuir 27: 15120-15128, 2011.
  440. Revilla-Lopez, G., Rodriguez-Ropero, F., Curco, D., Torras, J. Calaza, M. I., Zanuy, D., Jimenez, A. I., Cativiela, C., Nussinov, R., and Aleman, C. Integrating the Intrinsic Conformational Preferences of Noncoded  $\alpha$ -Amino Acids Modified at the Peptide Bond into the Noncoded Amino Acids Database. Proteins 79: 1841-1852, 2011.

441. Revilla-Lopez, G., Torras, J., Nussinov, R., Aleman, C., and Zanuy, D. Exploring the Energy Landscape of a Molecular Engineered Analog of a Tumor-Homing Peptide. Phys. Chem. Chem. Phys. 13: 9986-1894, 2011.
442. Tsai, C-J. and Nussinov, R. Gene-Specific Transcription Activation Via LongRange Allosteric Shape-Shifting. Biochem. J. 439: 15-25, 2011.
443. Tsai, C-J. and Nussinov, R. A Unified Convention for Biological Assemblies with Helical Symmetry. Acta Crystallogr. D. Biol Crystallogr. 67: 716-728, 2011.
444. Tuncbag, N., Gursoy, A., Nussinov, R., and Keskin, O. Predicting Protein-Protein Interactions on a Proteome Scale by Matching Evolutionary and Structural Similarities at Interfaces using PRISM. Nat. Proc. 6: 1341-1354, 2011.
445. Yuan, P., Liang, K., Ma, B., Zhang, N., Nussinov, R., and Huang, J. Multiple-Targeting and Conformational Selection in the Estrogen Receptor: Computation and Experiment. Chem. Biol. Drug Des. 78: 1137-1149, 2011.
446. Acuner Ozbabacan, S. E., Keskin, O., Nussinov, R., and Gursoy, A. Enriching the Human Apoptosis Pathway by Predicting the Structures of Protein-Protein Complexes. J. Struct. Biol. 179: 338-346, 2012.
447. Capone, R., Jang, H., Kotler, S. A., Connelly, L., Teran, Arce C., Ramachandran, S., Kagan, B. L., Nussinov, R., and Lal, R. All-d-enantiomer of  $\beta$ -Amyloid Peptide Forms Ion Channels in Lipid Bilayers. J. Chem. Theory Comput. 8: 1143-1152, 2012.
448. Capone, R., Jang, H., Kotler, S.A., Kagan, B.L., Nussinov, R., and Lal, R. Probing Structural Features of Alzheimer's Amyloid- $\beta$  Pores in Bilayers using Site-Specific Amino Acid Substitutions. Biochemistry 51: 776-785, 2012.
449. Connelly, L., Jang, H., Ramachandran, S., Kagan, B., Nussinov, R., and Lal, R. Effects of Point Substitutions on the Structure of Toxic Alzheimer's  $\beta$ -Amyloid Channels: Atomic Force Microscopy and Molecular Dynamics Simulations. Biochemistry 51: 3031-3038, 2012.
450. Connelly, L.S., Teran Arce, F., Jang, H., Capone, R., Kotler, S.A., Ramachandran, S., Kagan, B.L., Nussinov, R., and Lal, R. Atomic Force Microscopy and MD Simulations Reveal Pore-Like Structures of All-d-Enantiomer of Alzheimer's  $\beta$ -Amyloid Peptide: Relevance to the Ion Channel Mechanism of AD Pathology. J. Phys. Chem. B. 116: 1728-1735, 2012.
451. Csermely, P., Sandhu, K. S., Hazai, E., Hoksza, Z., Kiss, H. J. M., Miozzo, F., Veres, D. V., Piazza, F., and Nussinov, R. Disordered Proteins and Network Disorder in Network Descriptions of Protein Structure, Dynamics and Function. Hypotheses and a Comprehensive Review. Curr. Protein Pept. Sci. 13: 19-33, 2012.



452. Dickin, R., Hall, C.J., Taylor, L.K., Collings, A.M., Nussinov, R., and Bourne, P.E. A Review of 2011 for PLoS Computational Biology. PLoS Comput Biol. 8: e1002387, 2012.
453. Engin, H. B., Keskin, O., Nussinov, R., and Gursoy, A. A Strategy Based on Protein-Protein Interface Motifs may Help in Identifying Drug Off-Targets. J. Chemical Information and Modeling. 52: 2273-2286, 2012.
454. Kagan, B. L., Jang, H., Capone, R., Teran Arce, F., Ramachandran, S., Lal, R., and Nussinov, R. Antimicrobial Properties of Amyloid Peptides. Mol. Pharm. 9: 708-717, 2012.
455. Kar, G., Keskin, O., Nussinov, R., and Gursoy, A. Human Proteome-Scale Structural Modelling of E2-E3 Interactions Exploiting Interface Motifs. J. Proteome Res. 11: 1196-1207, 2012.
456. Korkmaz, E. N., Nussinov, R., and Haliloglu, T. Conformational Control of the Binding of the Transactivation Domain of the MLL Protein and c-Myb to the KIX Domain of CREB. PLoS Comput. Biol. 8: e1002420, 2012.
457. Kuzu, G., Keskin, O., Gursoy, A., and Nussinov, R. Constructing Structural Networks of Signaling Pathways on the Proteome Scale. Curr. Opin. Struct. Biol. 22: 367-377, 2012.
458. Kuzu, G., Keskin, O., Gursoy, A., and Nussinov, R. Expanding the Conformational Selection Paradigm in Protein-Ligand Docking. Methods Mol. Biol. 819: 59-74, 2012.
459. Ma, B. and Nussinov, R. Selective Molecular Recognition in Amyloid Growth and Transmission and Cross-Species Barriers. J. Mol. Biol. 421: 172-184, 2012.
460. Miller, Y., Ma, B., and Nussinov, R. Metal Binding Sites in Amyloid Oligomers: Complexes and Mechanisms. Coord. Chem. Rev. 19-20: 2245-2252, 2012.
461. Nussinov, R. Allosteric Modulators can Cestore Function in an Amino Acid Neurotransmitter Receptor by Slightly Altering Intra-Molecular Communication Pathways. Br. J. Pharmacol. 165: 2110-2112, 2012.
462. Nussinov, R. A Future Vision for PLoS Computational Biology. PLoS Comput Biol 8: e1002727, 2012.
463. Nussinov, R. How do Cellular Signals Travel Long Distances? Mol. Biosyst. 8(1): 22-26, 2012.
464. Nussinov, R. and Ma, B. Protein Dynamics and Conformational Selection in Bidirectional Signal Transduction. BMC Biol. 10: 2, 2012.
465. Nussinov, R., and Tsai, C. J. The Different Ways Through which Specificity Works in

- Orthosteric and Allosteric Drugs. Curr. Pharm. Des. 18: 1311-1316, 2012.
466. Nussinov, R., Tsai, C-J., Xin, F., and Radivojac, P. Allosteric Post-Translational Modification Codes. Trends Biochem. Sci. 37: 447-455, 2012.
467. Papp, D., Lenti, K., Modos, D., Fazekas, D., Dul, Z., Turei, D., Foldvari-Nagy, L., Nussinov, R., Csermely, P., and Korcsmaros, T. The NRF2-Related Interactome and Regulome Contain Multifunctional Proteins and Fine-Tuned Autoregulatory Loops. FEBS Lett. 586: 1795-802, 2012.
468. Siddiqua, A., Luo, Y., Meyer, V., Swanson, M.A., Yu, X., Wei, G., Zheng, J., Eaton, G.R., Ma, B., Nussinov, R., Eaton, S.S., and Margittai, M. Conformational Basis for Asymmetric Seeing Barrier in Filaments of Three- and Four-Repeat Tau. J. Am. Chem. Soc. 134: 10271-10278, 2012.
469. Tuncbag, N., Keskin, O., Nussinov, R., and Gursoy, A. Fast and Accurate Modelling of Protein-Protein Interactions by Combining Template-Interface-Based Docking with Flexible Refinement. Proteins 80: 1239-1249, 2012.
470. Xu, Y., Ma, B., Nussinov, R. Structural and Functional Consequences of Phosphate-Arsenate Substitutions in Selected Nucleotides: DNA, RNA and ATP. J. Phys. Chem. B. 116: 4801-4811, 2012.
471. Yu, X., Luo, Y., Dinkel, P., Zheng, J., Wei, G., Margittai, M., Nussinov, R., and Ma, B. Cross-Seeding and Conformational Selection Between Three- and Four-Repeat Human tau Proteins. J. Biol. Chem. 287: 14950-14959, 2012.
472. Zhao, J., Luo, Y., Jang, H., Yu, X., Wei, G., Nussinov, R., and Zheng, J. Probing Ion Channel Activity of Human Islet Amyloid Polypeptide (Amylin). Biochim Biophys Acta (Membranes) 1818: 3121-3130, 2012.
473. Csermely, P., Korcsmaros, T., Kiss, H. J. M., London, G., and Nussinov, R. Structure and Dynamics of Molecular Networks: A Novel Paradigm of Drug Discovery. Pharmacology and Therapeutics. 138: 333-408, 2013.
474. Csermely, P., Nussinov, R., and Szilagyi, A. From Allosteric Drugs to Allo-Network Drugs: State of the Art and Trends of Design, Synthesis, and Computational Methods. Curr. Top. Med. Chem. 13: 2-4, 2013.
475. Gupta, K., Jang, H., Harlen, K., Puri, A., Nussinov, R., Schneider, J., Blumenthal, R., Mechanism of Membrane Permeation Induced by Synthetic  $\beta$ -Hairpin Peptides. J. Biophysical Chemistry, 105: 2093-2103, 2013.
476. Guven Maiorov, E., Keskin, O., Gursoy, A., and Nussinov, R. The Structural Network of Inflammation and Cancer: Merits and Challenges. Semin. Cancer Biol. 23: 243-251, 2013.

477. Haspel, N., Laurent, A. D., Zanuy, D., Nussinov, R., Aleman, C., Puiggali, J., and Revilla-Lopez, G. Conformational Exploration of Two Peptides and Their Hybrid Polymer Conjugates: Potentialities as Self-Aggregating Materials. J. Phys. Chem. B. 116: 13941-13952, 2013.
478. Huang, Q., Yu, L., Levine, A. J., Nussinov, R., and Ma, B. Dipeptide Analysis of p53 Mutations and Evolution of p53 Family Proteins. Biochim. Biophys. Acta. 844: 198-206, 2013.
479. Jang, H., Connelly, L., Arce, F. T., Ramachandran, S., Kagan, B. L., Lal, R., and Nussinov, R. Mechanisms for the Insertion of Toxic, Fibril-like  $\beta$ -Amyloid Oligomers into the Membrane. J. Chemical Theory Comput. 9: 822-833, 2013.
480. Jang, H., Connelly, L., Teran Arce, F., Ramachandran, S., Lal, R., Kagan, B. L., and Nussinov, R. Alzheimer's Disease: Which Type of Amyloid-Preventing Drug Agents to Employ? Physical Chemistry Chemical Physics. 15: 8868-8877, 2013.
481. Jang, H., Teran Arce, F., Ramachandran, S., Kagan, B. L., Lal, R., and Nussinov, R. Familial Alzheimer's Disease Osaka Mutant ( $\Delta E22$ )  $\beta$ -Barrels Suggest an Explanation for the Different A $\beta$ 1-40/42 Preferred Conformational States Observed by Experiment. J. Physical Chemistry. 117:11518-11529, 2013.
482. Kuzu, G., GURSOY, A., Nussinov, R., and Keskin, O. Exploiting Conformational Ensembles in Modelling Protein-Protein Interactions on the Proteome Scale. J. Proteome Research 12: 2641-4653, 2013.
483. Lengauer, T. and Nussinov, R. New Methods Section in PLoS Computational Biology. PLoS Comput Biol 9: e1002972, 2013.
484. Liu, J. and Nussinov, R. The Role of Allostery in the Ubiquitin-Proteasome System. Crit. Rev. Biochem. Mol. Biol. 48: 89-97, 2013.
485. Luo, Y., Dinkel, P., Yu, X., Margittai, M., Zheng, J., Nussinov, R., Wei, G., and Ma, B. Molecular Insights into the Reversible Formation of Tau Protein Fibrils. Chemical Communications 49: 3582-3584, 2013.
486. Ma, B. and Nussinov, R. Structured Crowding and its Effects on Enzyme Catalysis. Topics in Current Chemistry. 337: 123-137, 2013.
487. Nussinov, R. The Spatial Structure of Cell Signaling Systems. Physical Biology 10: 045004, 2013.
488. Nussinov R. How Can PLoS Computational Biology Help the Biological Sciences? PLOS Computational Biology 9: e1003262, 2013.

489. Nussinov, R., Ma, B., and Tsai, C.-J. A Broad View of Scaffolding Suggests that Scaffolding Proteins can Actively Control Regulation and Signalling of Multienzyme Complexes through Allostery. BBA-Proteomics 1834: 820-829, 2013.
490. Nussinov, R., Ma, B., Tsai, C.J., and Csermely, P. Allosteric Conformational Barcodes Direct Signaling in the Cell. Structure 21: 1509-1521, 2013.
491. Nussinov, R. and Tsai, C.-J. Allostery in Disease and in Drug Discovery. Cell 153: 293-305, 2013.
492. Nussinov, R., Tsai, C.-J., and Ma, B. The Underappreciated Role of Allostery in the Cellular Network. Annual Reviews in Biophysics 42: 169-189, 2013.
493. Nussinov, R, Tsai, CJ, Mattos, C. Pathway Drug Cocktail': Targeting Ras Signaling Based on Structural Pathways. Trends Mol Med. 19: 695-704, 2013.
494. Szilagy, A., Nussinov, R., and Csermely, P. Allo-Network Drugs: Extension of the Allosteric Drug Concept to Protein-Protein Interaction and Signaling Networks. Curr. Top. Med. Chem. 13: 64-77, 2013.
495. Tsai, C. J. and Nussinov, R. The Molecular Basis of Targeting Protein Kinases in Cancer Therapeutics. Semin. Cancer Biol. 23: 235-242, 2013.
496. Xu, Y., Wang, H., Nussinov, R., and Ma, B. Protein Charge and Mass Contribute to the Spatio-Temporal Dynamics of Protein-Protein Interactions in a Minimal Proteome. Proteomics 13: 1339-1351, 2013.
497. Zanut, D. Kotla, R., Nussinov, R., Teesalu, T., Sugahara, K. N., Aleman, C., and Haspel, N. Sequence Dependence of C-End Rule Peptides in Binding and Activation of Neuropilin-1 Receptor. J. Struct. Biol. 182: 78-86, 2013.
498. Zanut, D., Sayago, F. J., Revilla-Lopez, G., Ballano, G., Agemy, L., Kotamraju, V. R., Jimenez, A. I., Cativiela, C., Nussinov, R., Sawvel, A. M., Stucky, G., Ruoslahti, E., and Alman, C. Engineering Strategy to Improve Peptide Analogs: From Structure-Based Computational Design to Tumor Homing. J. Computer Aided Mol. Design 27: 31-43, 2013.
499. Acuner-Ozbabacan, E.S., Engin, H.B., Guven-Maiorov, E., Kuzu, G., Muratcioglu, S., Baspinar, A., Chen, Z., Van Waes, C., Gursoy, A., Keskin, O., and Nussinov, R. The Structural Network of Interleukin-10 and its Implications in Inflammation and Cancer. BMC Genomics. 15: S2, 2014.
500. Acuner Ozbabacan, S.E., Gursoy, A., Nussinov, R., and Keskin, O. The Structural Pathway of Interleukin 1 (IL-1) Initiated Signaling Reveals Mechanisms of Oncogenic Mutations and SNPs in Inflammation and Cancer. PLoS Comput Biol. 10: e1003470, 2014.

501. Baspinar, A., Cukuroglu, E., Nussinov, R., Keskin, O. and Gursoy, A. PRISM: A Web Server and Repository for Prediction of Protein-Protein Interactions and Modelling their 3D Complexes. Nucleic Acids Research 42 (Web Server issue): W285-289, 2014.
502. Cronin, M., Coolbaugh, M.J., Nellis, D., Zhu, J., Wood, D.W., Nussinov, R., and Ma, B. Dynamics Differentiate Between Active and Inactive Inteins. Eur. J. Med. Chem. 32(6):236-46, 2014.
503. Cui, Q. and Nussinov R. Making Biomolecular Simulations Accessible in the Post-Nobel Prize Era. PLoS Comput. Biol. 10: e1003786, 2014.
504. Cukuroglu, E., Gursoy, A., Nussinov, R. and Keskin, O. Non-Redundant Unique Interface Structures as Templates for Modelling Protein Interactions. PLoS ONE 9: e86738, 2014
505. Dai, D., Huang, Q., Nussinov, R., and Ma, B. Promiscuous and Specific Recognition Among Ephrins and Eph Receptors. Biochim. Biophys. Acta. 1844: 1729-1740, 2014.
506. Engin, H. B., Gursoy, A., Nussinov, R., and Keskin, O. Network-Based Strategies can help Mono- and Poly-Pharmacology Drug Discovery: A Systems Biology View. Current Pharmaceutical Design 20: 1201-1207, 2014.
507. Gillman, A.L., Jang, H., Lee, J., Ramachandran, S., Kagan, B.L., Nussinov, R., Teran Arce, F. Activity and Architecture of Pyroglutamate-Modified Amyloid- $\beta$  (A $\beta$ E3-42) Pores. J Phys Chem B. 118(26):7335-44. 2014.
508. Guven-Maiorov, E., Acuner-Ozbabacan, S. E., Keskin, O., Gursoy, A. and Nussinov, R. Structural Pathways of Cytokins May Illuminate their Roles in Regulation of Cancer Development and Immunotherapy. Cancers (Basel) 6: 663-683, 2014.
509. Jang, H., Teran Arce, F., Ramachandran, S., Kagan, B.L., Lal, R., and Nussinov, R. Disordered Amyloidogenic Peptides May Insert into the Membrane and Assemble into Common Cyclic Structural Motifs. Chem. Soc. Rev. 43(19):6750-64, 2014.
510. Ji, X., Huang, Q., Yu, L., Nussinov, R., and Ma, B. Bioinformatics Study of Cancer-Related Mutations Within p53 Phosphorylation Site Motifs. Int. J. Mol. Sci. 15: 13275-13298, 2014.
511. Kuzu, G., Keskin, O., Nussinov, R., and Gursoy, A. Modeling Protein Assemblies in the Proteome. Mol. Cell Proteomics 13:887-96, 2014.
512. Lee, J., Gillman, A.L., Jang, H., Ramachandran, S., Kagan, B.L., Nussinov, R., and Teran Arce, F. Role of the Fast Kinetics of Pyroglutamate-Modified Amyloid- $\beta$  Oligomers in Membrane Binding and Membrane Permeability. Biochemistry 53: 4704-4714, 2014.

513. Lu, S., Huang, W., Wang, Q., Shen, Q., Li, S., Nussinov, R., and Zhang, J. The structural basis of ATP as an allosteric modulator. PLoS Comput Biol. 10(9):e1003831, 2014.
514. Luo, Y., Ma B, Nussinov, R., and Wei, G. Structural Insight into Tau Protein's Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. J Phys Chem Lett. 5(17):3026-3031, 2014.
515. Ma, B., Kolb, S., Diprima, M., Karna, M., Tosato, G., Yang, Q., Huang, Q. and Nussinov, R. Investigation of the interactions between the EphB2 receptor and SNEW peptide variants. Growth Factors 32(6):236-46, 2014.
516. Ma, B., and Nussinov, R. Druggable Orthosteric and Allosteric Hot Spots to Target Protein-Protein Interactions. Current Pharmaceutical Design 20: 1293-1301, 2014.
517. Meyer, V., Dinkel, P. D., Luo, Y., Yu, X., Wei, G., Zheng, J., Eaton, G. R., Ma, B., Nussinov, R., Eaton, S. S., and Margittai, M. Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. Angewandte Chemie 53: 1590-1593, 2014.
518. Murase, S.K., Haspel, N., del Valle, L., Perpete, E.A., Michaux, C., Nussinov, R., Puiggali, J. and Aleman, C. Molecular characterization of L-phenylalanine terminated poly(L-lactide) conjugates RSC Advances 4(44):23231-23241, 2014.
519. Nussinov, R. The Significance of the 2013 Nobel Prize in Chemistry and the Challenges Ahead. PLoS Comput Biol. 10: e1003423, 2014.
520. Nussinov R, Jang H. Dynamic Multiprotein Assemblies Shape the Spatial Structure of Cell Signaling. Prog. Biophys. Mol. Biol., 116(2-3):158-64, 2014.
521. Nussinov, R. Jang, H. and Tsai, C.-J. The Structural Basis for Cancer Treatment Decisions. Oncotarget, 15(17): 7285-7302, 2014.
522. Nussinov, R., Ma, B., and Tsai, C.-J. Multiple Conformational Selection and Induced Fit Events Take Place in Allosteric Propagation. Biophys. Chem. 86: 22-30, 2014.
523. Nussinov, R. and Tsai, C.-J. Unraveling Structural Mechanisms of Allosteric Drug Action. Trends Pharmacol. Sci. 35(5): 256-264, 2014.
524. Nussinov, R. and Tsai, C.-J. Free Energy Diagrams for Protein Function. Chemistry and Biology 21: 311-318, 2014.
525. Nussinov, R., Tsai, C.-J. and Liu, J. Principles of allosteric interactions in cell signaling. J Am Chem Soc. 136(51):17692-701, 2014
526. Nussinov, R. and Wolynes, P.G. A Second Molecular Biology Revolution? The Energy Landscapes of Biomolecular Function. Phys. Chem. Chem. Phys. 16: 6321-6322, 2014.

527. Qi, R., Luo, Y., Ma, B., Nussinov, R. and Wei, G. Conformational Distribution and  $\alpha$ -Helix to  $\beta$ -Sheet Transition of Human Amylin Fragment Dimer. Biomacromolecules 15: 122-131, 2014.
528. Ozbabacan, S. E. A., Gursoy, A., Nussinov, R., and Keskin, O. The Structural Pathway of Interleukin 1 (IL-1) Initiated Signalling Reveals Mechanisms of Oncogenic Mutations and SNPs in Inflammation and Cancer. PLoS Computational Biology 10: e1003470, 2014.
529. Sudha, G., Nussinov, R., and Srinivasan, N. An Overview of Recent Advances in Structural Bioinformatics of Protein-Protein Interactions and a Guide to their Principles. Prog. Biophys. Mol. Biol. 116(2-3):141-50, 2014.
530. Szalay, K.Z., Nussinov, R., and Csermely, P. Attractor Structures of Signaling Networks: Consequences of Different Conformational Barcode Dynamics and their Relations to Network-Based Drug Design. Molecular Informatics 33(6-7): 463-468, 2014.
531. Tsai, C.-J. and Nussinov, R. A Unified View of 'How Allostery Works'. PLoS Computational Biology 10: e1003394, 2014.
532. Tsai, C.-J. and Nussinov, R. The Free Energy Landscape in Translational Science: How can Somatic Mutations Result in Constitutive Oncogenic Activation? Physical Chemistry Chemical Physics 16: 6332-6341, 2014.
533. Chavan, T.S., Jang, H., Khavrutskii, L., Abraham, S. J., Banerjee, A., Freed B. J., Johannessen, L., Tarasov, S. G., Gaponenko, V., Nussinov, R. and Tarasova, NI. High Affinity Interaction of the K-Ras4B Hypervariable Region with the Ras Active Site. Biophysical J. 109(12):2602-13, 2015.
534. Clausen, R., Ma, B., Nussinov, R. and Shehu, A. Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Comput Biol. 11(9):e1004470, 2015
535. Datta, S.A., Clark, P.K., Fan, L., Ma, B., Harvin, D.P., Sowder, R.C. 2nd, Nussinov, R., Wang, Y.X. and Rein, A. J. Virol. 90(4):1773-87, 2015.
536. Fetics, S. K., Guterres, H., Kearney, B. M., Buhrman, G., Ma, B., Nussinov, R. and Mattos, C. Allosteric Effects of the Oncogenic RasQ61L Mutant on Raf-RBD. Structure 23(3): 505-516, 2015.
537. Guven-Maiorov, E., Keskin, O., Gursoy, A. and Nussinov, R. A Structural View of Negative Regulation of the Toll-like Receptor-Mediated Inflammatory Pathway. Biophys J. 109(6), 1214-26, 2015

538. Guven-Maiorov, E., Keskin, O., Gursoy, A., VanWaes, C., Chen, Z., Tsai, C.J. and Nussinov, R. The Architecture of the TIR Domain Signalosome in the Toll-like Receptor-4 Signaling Pathway. Sci Rep. 5:13128, 2015.
539. Jang, H., Abraham, S. J., Chavan, T. S., Hitchinson, B., Khavrutskii, L., Tarasova, N. I., Nussinov, R. and Gaponenko, V. Mechanisms of Membrane Binding of Small GTPase K-Ras4B Farnesylated Hypervariable Region. J Biol Chem, 290(15):9465-77, 2015.
540. Lengauer, T. and Nussinov, R. How to write a presubmission inquiry. PLoS Comput Biol. 11(2):e1004098, 2015.
541. Lu, S., Deng, R., Jiang, H., Song, H., Li, S., Shen, Q., Huang, W., Nussinov, R., Yu, J. and Zhang J. The Mechanism of ATP-Dependent Allosteric Protection of Akt Kinase Phosphorylation. Structure 23(9):1725-34, 2015.
542. Lu, S., Banerjee, A., Jang, H., Zhang, J., Gaponenko, V. and Nussinov, R. GTP Binding and Oncogenic Mutations May Attenuate Hypervariable Region (HVR)-Catalytic Domain Interactions in Small GTPase KRAS4B, Exposing the Effector Binding Site. J. Biol Chem. 290(48):28887-900, 2015.
543. Miller, Y., Ma, B., and Nussinov R. Polymorphism in Self-Assembly of Peptide-Based  $\beta$ -Hairpin Contributes to Network Morphology and Hydrogel Mechanical Rigidity. J Phys Chem B. 119(2):482-90, 2015.
544. Muratcioglu, S., Chavan, T.S, Freed, B.C., Jang, H., Khavrutskii, L., Freed, R.N., Dyba, M.A., Stefanisko, K., Tarasov, S.G., Gursoy, A., Keskin, O., Tarasova, N.I., Gaponenko, V. and Nussinov, R. GTP-Dependent K-Ras Dimerization. Structure 23(7):1325-35, 2015.
545. Muratcioglu, S., Presman, D.M., Pooley, J.R., Grøntved, L., Hager, G.L., Nussinov, R., Keskin, O. and Gursoy, A. Structural Modeling of GR Interactions with the SWI/SNF Chromatin Remodeling Complex and C/EBP. Biophys J. 109(6), 1227-39, 2015.
546. Nussinov, R. Advancements and challenges in computational biology. PLoS Comput Biol. 8;11(1):e1004053, 2015.
547. Nussinov, R., Bonhoeffer, S., Papin, J.A., and Sporns O. From "What Is?" to "What Isn't?" Computational Biology. PLoS Comput Biol. 11(7):e1004318, 2015.
548. Nussinov, R., Jang, H. and Tsai, C.-J. Oligomerization and Nanocluster Organization Render Specificity. Biological Reviews Camb. Philos. Soc., 90(2):587-98, 2015.
549. Nussinov, R., Muratcioglu, S., Tsai, C.J., Jang, H., Gursoy, A. and Keskin, O. The Key Role of Calmodulin in KRAS-Driven Adenocarcinomas. Mol Cancer Res. 13(9):1265-73, 2015.



550. Nussinov, R. and Tsai, C.-J. The Design of Covalent Allosteric Drugs. *Ann. Review of Pharmacology and Toxicology*, 55:249-67, 2015.
551. Nussinov, R. and Tsai, C.J. The Role of Allostery in the Termination of Second Messenger Signaling. *Biophys J.* 109(6), 1080-1, 2015
552. Nussinov, R. and Tsai, C. -J. Allostery without a conformational change? Revisiting the paradigm. *Curr Opin Struct Biol.* 30:17-24, 2015.
553. Nussinov, R. and Tsai, C. -J. 'Latent drivers' expand the cancer mutational landscape. *Curr Opin Struct Biol.* 13(9):1265-73, 2015.
554. Nussinov, R. and Tsai, C. -J. Tandem Domains with Tuned Interactions Are a Powerful Biological Design Principle. *PLoS Biol.* 13(11):e1002306. 2015.
555. Nussinov, R., Tsai, C.J., Muratcioglu, S., Jang, H., Gursoy, A. and Keskin, O. Principles of K-Ras effector organization and the role of oncogenic K-Ras in cancer initiation through G1 cell cycle deregulation. *Expert Rev Proteomics.* 12(6):669-82, 2015.
556. Sali, A., Berman, H.M., Schwede, T., Trewheella, J., Kleywegt, G., Burley, S.K., Markley, J., Nakamura, H., Adams, P., Bonvin, A.M., Chiu, W., Peraro, M.D., Di Maio, F., Ferrin, T.E., Grünewald, K., Gutmanas, A., Henderson, R., Hummer, G., Iwasaki, K., Johnson, G., Lawson, C.L., Meiler, J., Marti-Renom, M.A., Montelione, G.T., Nilges, M., Nussinov, R., Patwardhan, A., Rappsilber, J., Read, R.J., Saibil, H., Schröder, G.F., Schwieters, C.D., Seidel, C.A., Svergun, D., Topf, M., Ulrich, E.L., Velankar, S. and Westbrook, J.D. Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure* 23(7):1156-67, 2015.
557. Shehu, A. and Nussinov, R. Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics. *PLoS Comput Biol.* 11(10):e1004585, 2015.
558. Xiao, Y., Ma, B., McElheny, D., Parthasarathy, S., Long, F., Hoshi, M., Nussinov, R. and Ishii, Y. A $\beta$ (1-42) fibril structure illuminates self-recognition and replication of amyloid in Alzheimer's disease. *Nat Struct Mol Biol.* 22(6):499-505, 2015.
559. Xu, L., Shan, S., Chen, Y., Wang, X., Nussinov, R. and Ma, B. Coupling of Zinc-Binding and Secondary Structure in Nonfibrillar A $\beta$ 40 Peptide Oligomerization. *J Chem Inf Model.* 55(6):1218-1230, 2015.
560. Zhou, P., Zhang, N., Nussinov, R. and Ma, B. Defining the Domain Arrangement of the Mammalian Target of Rapamycin Complex Component Rictor Protein. *J Comput Biol.* 22(9):876-86, 2015.
561. Zhu, Y., Yang, S., Qi, R., Zou, Y., Ma, B., Nussinov, R. and Zhang, Q. Effects of the C-Terminal Tail on the Conformational Dynamics of Human Neuronal Calcium Sensor-1 Protein. *J Phys Chem B.* 119(44):14236-44, 2015.

562. Baram, M., Atsmon-Raz, Y., Ma, B., Nussinov, R. and Miller, Y. Amylin-A $\beta$  oligomers at atomic resolution using molecular dynamics simulations: a link between Type 2 diabetes and Alzheimer's disease. Phys Chem Chem Phys. 18(4):2330-8, 2016.
563. Banerjee, A., Jang, H., Nussinov, R. and Gaponenko, V. The disordered hypervariable region and the folded catalytic domain of oncogenic K-Ras4B partner in phospholipid binding. Curr Opin Struct Biol. 36:10-17, 2016.
564. Csermely P, Korcsmáros T, Nussinov R. Intracellular and intercellular signaling networks in cancer initiation, development and precision anti-cancer therapy: RAS acts as contextual signaling hub. Semin Cell Dev Biol. 58:55-9, 2016.
565. Chakrabarti, M., Jang, H. and Nussinov, R. Comparison of the Conformations of KRAS Isoforms, K-Ras4A and K-Ras4B, Points to Similarities and Significant Differences. J Phys Chem B. 120(4):667-79, 2016.
566. Chavan, T.S., Muratcioglu, S., Marszalek, R., Jang, H., Keskin, O., Gursoy, A., Nussinov, R. and Gaponenko, V. Plasma membrane regulates Ras signaling networks. Cell Logist. 5(4):e1136374, 2016.
567. Guven-Maiorov, E., Keskin, O., Gursoy, A., VanWaes, C., Chen, Z., Tsai, C.J. and Nussinov, R. TRAF3 Signaling: Competitive Binding and Evolvability of Adaptive Viral Molecular Mimicry. Biochim Biophys Acta. 1860(11 Pt B):2646-55, 2016.
568. Guven-Maiorov, E., Tsai, C.J. and Nussinov, R. Pathogen mimicry of host protein-protein interfaces modulates immunity. Semin Cell Dev Biol. 58:136-45, 2016.
569. Hewitt, W.M., Lountos, G.T., Zlotkowski, K., Dahlhauser, S.D., Saunders, L.B., Needle, D., Tropea, E., Zhan, C., Wei, G., Ma, B., Nussinov, R., Waugh, D.S. and Schneekloth, J.S. Jr. Insights into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angew Chem Int Ed Engl. 55(19):5703-7, 2016
570. Jang, H., Arce, F.T., Lee, J., Gillman, A.L., Ramachandran, S., Kagan, B.L., Lal, R., and Nussinov R. Computational Methods for Structural and Functional Studies of Alzheimer's Amyloid Ion Channels. Methods Mol Biol. 1345:251-68, 2016.
571. Jang, H., Muratcioglu, S., Gursoy, A., Keskin, O. and Nussinov, R. Membrane-associated Ras dimers are isoform-specific: K-Ras dimers differ from H-Ras dimers. Biochem J. 473(12):1719-32, 2016.
572. Jang, H., Banerjee, A., Chavan, T.S., Lu, S., Zhang, J., Gaponenko, V., and Nussinov, R. The higher level of complexity of K-Ras4B activation at the membrane. FASEB J. 30(4):1643-55, 2016.

573. Karchin R, Nussinov R. Genome Landscapes of Disease: Strategies to Predict the Phenotypic Consequences of Human Germline and Somatic Variation. PLoS Comput Biol. 12(8):e1005043, 2016.
574. Kuzu G, Keskin O, Nussinov R, Gursoy A. PRISM-EM: template interface-based modelling of multi-protein complexes guided by cryo-electron microscopy density maps. Acta Crystallogr D Struct Biol. 72(Pt 10):1137-1148, 2016.
575. Lambrughi M, De Gioia L, Gervasio FL, Lindorff-Larsen K, Nussinov R, Urani C, Bruschi M, and Papaleo E. DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. Nucleic Acids Res. 44(19):9096-9109, 2016.
576. Lei, J., Qi, R., Wei, G., Nussinov, R. and Ma, B. Self-aggregation and coaggregation of the p53 core fragment with its aggregation gatekeeper variant. Phys Chem Chem Phys. 18(11):8098-107, 2016.
577. Liao TJ, Tsai CJ, Jang H, Fushman D, Nussinov R. RASSF5: An MST activator and tumor suppressor in vivo but opposite in vitro. Curr Opin Struct Biol. 41:217-224, 2016
578. Liu, J. and Nussinov, R. Allosterity: An Overview of Its History, Concepts, Methods, and Applications. PLoS Comput Biol. 12(6):e1004966. 2016.
579. Lu, S., Jang, H., Nussinov, R. and Zhang, J. The Structural Basis of Oncogenic Mutations G12, G13 and Q61 in Small GTPase K-Ras4B. Sci Rep. 6:21949, 2016.
580. Lu S, Jang H, Gu S, Zhang J, Nussinov R. Drugging Ras GTPase: a comprehensive mechanistic and signaling structural view. Chem Soc Rev. 45(18):4929-52. 2016.
581. Lu, S., Jang, H., Zhang, J. and Nussinov, R. Inhibitors of Ras-SOS Interactions. ChemMedChem. 18(11):8098-107, 2016.
582. Lu, S., Jang, H., Muratcioglu, S., Gursoy, A., Keskin. O., Nussinov, R. and Zhang, J. Ras Conformational Ensembles, Allosterity, and Signaling. Chem Rev. 116(11):6607-65, 2016.
583. Ma B, Nussinov R. Protein dynamics: Conformational footprints. Nat Chem Biol. 12(11):890-891, 2016.
584. Ma, B., Zhao, J. and Nussinov, R. Conformational selection in amyloid-based immunotherapy: Survey of crystal structures of antibody-amyloid complexes. Biochim Biophys Acta. 1860(11 Pt B):2672-81, 2016.
585. Maximova, T., Moffatt, R., Ma, B., Nussinov, R. and Shehu, A. Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Comput Biol. 12(4):e1004619, 2016.

586. Nussinov, R. Introduction to Protein Ensembles and Allostery. Chem Rev. 116(11):6263-6, 2016.
587. Nussinov, R., Muratcioglu, S., Tsai, C.J., Jang H., Gursoy, A. and Keskin, O. Ras4B/calmodulin/PI3K $\alpha$ : A promising new adenocarcinoma-specific drug target? Expert Opin Ther Targets. 12:1-12, 2016.
588. Nussinov R, Papin JA. Computing Biology. PLoS Comput Biol. 2016 2(7):e1005050.
589. Nussinov, R., Tsai, C.-J., Chakrabarti, M., Jang, H. A New View of Ras Isoforms in Cancers. Cancer Research. 76(1):18-23, 2016.
590. Nussinov R, Tsai CJ, Jang H. Independent and core pathways in oncogenic KRAS signaling. Expert Rev Proteomics. 13(8):711-6, 2016.
591. Nussinov, R., Tsai, C.J., Jang, H., Korcsmáros, T. and Csermely, P. Oncogenic KRAS signaling and YAP1/ $\beta$ -catenin: Similar cell cycle control in tumor initiation. Semin Cell Dev Biol. 58:79-85, 2016.
592. Nussinov, R. and Udgaonkar, J. B. Folding and binding: Dynamic conformational heterogeneity is pivotal to cell life. Curr Opin Struct Biol. 36:iv-vi, 2016.
593. Papaleo, E., Saladino, G., Lambrugh, M., Lindorff-Larsen, K., Gervasio, F. L. and Nussinov, R. The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chem Rev. 116(11):6391-423, 2016.
594. Tuncbag, N., Gursoy, A., Keskin, O. and Nussinov, R. The potential impact of recent developments in three-dimensional quantitative interaction proteomics on structural biology. Expert Rev Proteomics 13(5):447-9, 2016.
595. Wei, G., Xi, W., Nussinov, R. and Ma, B. Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. Chem Rev. 116(11):6516-51, 2016.
596. Xu, L., Nussinov, R. and Ma, B. Allosteric stabilization of the amyloid- $\beta$  peptide hairpin by the fluctuating N-terminal. Chem Commun (Camb). 52(8):1733-6, 2016.
597. Xu L, Nussinov R, Ma B. Coupling of the non-amyloid-component (NAC) domain and the KTK(E/Q)GV repeats stabilize the  $\alpha$ -synuclein fibrils. Eur J Med Chem. 121:841-50, 2016.
598. Xu, L., Zheng, J., Margittai, M., Nussinov, R. and Ma, B. How Does Hyperphosphorylation Promote Tau Aggregation and Modulate Filament Structure and Stability? ACS Chem Neurosci. 7(5):565-75, 2016.

599. Zhan C, Qi R, Wei G, Guven-Maiorov E, Nussinov R, Ma B. Conformational dynamics of cancer-associated MyD88-TIR domain mutant L252P (L265P) allosterically tilts the landscape toward homo-dimerization. Protein Eng Des Sel. 29(9):347-54, 2016.
600. Zhang M, Zheng J, Nussinov R, Ma B. Oncogenic Mutations Differentially Affect Bax Monomer, Dimer, and Oligomeric Pore Formation in the Membrane. Sci Rep. 6:33340, 2016.
601. Zhu, Y., Ma, B., Qi, R., Nussinov, R., and Zhang, Q. Temperature-Dependent Conformational Properties of Human Neuronal Calcium Sensor-1 Protein Revealed by All-Atom Simulations. J Phys Chem B. 120(14):3551-9, 2016.
602. Zou, Y., Sun, Y., Zhu, Y., Ma, B., Nussinov, R., and Zhang, Q. Critical Nucleus Structure and Aggregation Mechanism of the C-terminal Fragment of SOD1 Protein. ACS Chem Neurosci. 7(3):286-96, 2016.
603. Andrabi M, Hutchins AP, Miranda-Saavedra D, Kono H, Nussinov R, Mizuguchi K, Ahmad S. Predicting conformational ensembles and genome-wide transcription factor binding sites from DNA sequences. Sci Rep. 7(1):4071, 2017.
604. Dong X, Sun Y, Wei G, Nussinov R, Ma B. Binding of protofibrillar A $\beta$  trimers to lipid bilayer surface enhances A $\beta$  structural stability and causes membrane thinning. Phys Chem Chem Phys. Oct 18;19(40):27556-27569, 2017.
605. Gan W, Schneidman D, Zhang N, Ma B, Nussinov R. Probing Oligomerized Conformations of Defensin in the Membrane. Methods Mol Biol. 1529:353-362, 2017.
606. Gong Y, Zhu Y, Zou Y, Ma B, Nussinov R, Zhang Q. Human Neuronal Calcium Sensor-1 Protein Avoids Histidine Residues to Decrease pH Sensitivity. J Phys Chem B. 121(3):508-517, 2017.
607. Guven-Maiorov E, Tsai CJ, Ma B, Nussinov R. Prediction of Host-Pathogen Interactions for Helicobacter pylori by Interface Mimicry and Implications to Gastric Cancer. J Mol Biol. Dec 8;429(24):3925-3941, 2017.
608. Guven-Maiorov E, Tsai CJ, Nussinov R. Structural host-microbiota interaction networks. PLoS Comput Biol. Oct 12;13(10):e1005579, 2017.
609. Haspel N, Zheng J, Aleman C, Zanuy D, Nussinov R. A Protocol for the Design of Protein and Peptide Nanostructure Self-Assemblies Exploiting Synthetic Amino Acids. Methods Mol Biol. 1529:323-352, 2017.
610. Huang W, Nussinov R, Zhang J. Computational Tools for Allosteric Drug Discovery: Site Identification and Focus Library Design. Methods Mol Biol. 1529:439-446, 2017.
611. Ideker T, Nussinov R. Network approaches and applications in biology. PLoS Comput Biol. Oct 12;13(10):e1005771, 2017.

612. Jang H, Banerjee A, Chavan T, Gaponenko V, Nussinov R. Flexible-body motions of calmodulin and the farnesylated hypervariable region yield a high-affinity interaction enabling K-Ras4B membrane extraction. J Biol Chem. 292(30):12544-12559, 2017.
613. Lee J, Kim YH, T Arce F, Gillman AL, Jang H, Kagan BL, Nussinov R, Yang J, Lal R. Amyloid  $\beta$  Ion Channels in a Membrane Comprising Brain Total Lipid Extracts. ACS Chem Neurosci. 8(6):1348-1357, 2017.
614. Li N, Jang H, Yuan M, Li W, Yun X, Lee J, Du Q, Nussinov R, Hou J, Lal R, Zhang F. Graphite-Templated Amyloid Nanostructures Formed by a Potential Pentapeptide Inhibitor for Alzheimer's Disease: A Combined Study of Real-Time Atomic Force Microscopy and Molecular Dynamics Simulations. Langmuir 33(27):6647-6656, 2017.
615. Libardo MDJ, Bahar AA, Ma B, Fu R, McCormick LE, Zhao J, McCallum SA, Nussinov R, Ren D, Angeles-Boza AM, Cotten ML. Nuclease Activity Gives an Edge to Host-Defense Peptide Piscidin 3 over Piscidin 1, Rendering it more Effective against Persisters and Biofilms. FEBS J. 284(21):3662-3683, 2017.
616. Liao TJ, Jang H, Tsai CJ, Fushman D, Nussinov R. The dynamic mechanism of RASSF5 and MST kinase activation by Ras. Phys Chem Chem Phys. 19(9):6470-6480, 2017.
617. Liu J, Nussinov R. Energetic redistribution in allostery to execute protein function. Proc Natl Acad Sci U S A. 114(29):7480-7482, 2017.
618. Muratcioglu S, Jang H, Gursoy A, Keskin O, Nussinov R. PDE $\delta$  Binding to Ras Isoforms Provides a Route to Proper Membrane Localization. J Phys Chem B. 121(24):5917-5927, 2017.
619. Nussinov R, Jang H, Tsai CJ, Liao TJ, Li S, Fushman D, Zhang J. Intrinsic protein disorder in oncogenic KRAS signaling. Cell Mol Life Sci. 74(17):3245-3261, 2017.
620. Nussinov R, Papin JA. How can computation advance microbiome research? PLoS Comput Biol. Sep 21;13(9):e1005547, 2017.
621. Nussinov R, Papin JA, Vakser I. Computing the Dynamic Supramolecular Structural Proteome. PLoS Comput Biol. 13(1):e1005290, 2017.
622. Nussinov R, Tsai CJ, Jang H. A New View of Pathway-Driven Drug Resistance in Tumor Proliferation. Trends Pharmacol Sci. 38(5):427-437, 2017.
623. Nussinov R, Wang G, Tsai CJ, Jang H, Lu S, Banerjee A, Zhang J, Gaponenko V. Calmodulin and PI3K Signaling in KRAS Cancers. Trends in Cancer. 3(3):214-224, 2017.
624. Onel M, Sumbul F, Liu J, Nussinov R, Haliloglu T. Cullin Neddylation May Allosterically Tune Polyubiquitin Chain Length and Topology. Biochem J. 474(5):781-795, 2017.

625. Tsai CJ, Nussinov R. Allostery modulates the beat rate of a cardiac pacemaker. J Biol Chem. 292(15):6429-6430, 2017.
626. Tuncbag N, Keskin O, Nussinov R, Gursoy A. Prediction of Protein Interactions by Structural Matching: Prediction of PPI Networks and the Effects of Mutations on PPIs that Combines Sequence and Structural Information. Methods Mol Biol. 1558:255-270, 2017.
627. Xu L, Ma B, Nussinov R, Thompson D. Familial Mutations May Switch Conformational Preferences in  $\alpha$ -Synuclein Fibrils. ACS Chem Neurosci. 8(4):837-849, 2017.
628. Zhang M, Zheng J, Nussinov R, Ma B. Release of Cytochrome C from Bax Pores at the Mitochondrial Membrane. Sci Rep. 7(1):2635, 2017.
629. Zhang M, Jang H, Gaponenko V, Nussinov R. Phosphorylated Calmodulin Promotes PI3K Activation by Binding to the SH2 Domains. Biophys J. Nov 7;113(9):1956-1967, 2017.
630. Zhao J, Nussinov R, Ma B. Allosteric control of antibody-prion recognition through oxidation of a disulfide bond between the CH and CL chains. Protein Eng Des Sel. 30(1):67-76, 2017.
631. Zhao J, Nussinov R, Ma B. Mechanisms of recognition of amyloid- $\beta$  (A $\beta$ ) monomer, oligomer, and fibril by homologous antibodies J Biol Chem. Nov 3;292(44):18325-18343, 2017.
632. Cheng F, Nussinov R. KRAS Activating Signaling Triggers Arteriovenous Malformations. Trends Biochem Sci. 43(7):481-483, 2018 doi: 10.1016/j.tibs.2018.04.007
633. Kuzu G, Keskin O, Nussinov R, Gursoy A PRISM-EM: template interface-based modelling of multi-protein complexes guided by cryo-electron microscopy density maps. Corrigendum. Acta Crystallogr D Struct Biol. 74(Pt 1):65-66, 2018
634. Li X, Dong X, Wei G, Margittai M, Nussinov R, Ma B. The distinct structural preferences of tau protein repeat domains. Chem Commun (Camb). 54(45):5700-5703, 2018
635. Li S, Jang H, Zhang J, Nussinov R. Raf-1 Cysteine-Rich Domain Increases the Affinity of K-Ras/Raf at the Membrane, Promoting MAPK Signaling. Structure. 26(3):513-525.e2, 2018
636. Liao TJ, Jang H, Fushman D, Nussinov R. Allosteric KRas4B Can Modulate SOS1 Fast and Slow Ras Activation Cycles. Biophys J.;115(4):629-641. doi: 10.1016/j.bpj.2018.07.016. 2018

637. Nussinov R, Tsai CJ, Jang H. Oncogenic Ras Isoforms Signaling Specificity at the Membrane. Cancer Res. 78(3):593-602, 2018
638. Nussinov R, Tsai CJ, Jang H. Is Nanoclustering essential for all oncogenic KRas pathways? Can it explain why wild-type KRas can inhibit its oncogenic variant? Semin Cancer Biol. 2018 Jan 5. pii: S1044-579X(17)30269-9. doi: 10.1016/j.semcancer.2018.01.002.
639. Nussinov R, Tsai CJ, Jang H. Oncogenic KRas mobility in the membrane and signaling response. Semin Cancer Biol. 2018 Feb 27. pii: S1044-579X(17)30287-0. doi: 10.1016/j.semcancer.2018.02.009.
640. Nussinov R, Zhang M, Tsai CJ, Jang H. Calmodulin and IQGAP1 activation of PI3K $\alpha$  and Akt in KRAS, HRAS and NRAS-driven cancers. Biochim Biophys Acta. 1864(6 Pt B):2304-2314, 2018. doi: 10.1016/j.bbadis.2017.10.032.
641. Nussinov R, Zhang M, Tsai CJ, Liao TJ, Fushman D, Jang H. Autoinhibition in Ras effectors Raf, PI3K $\alpha$ , and RASSF5: a comprehensive review underscoring the challenges in pharmacological intervention. Biophys Rev. ;10(5):1263-1282. doi: 10.1007/s12551-018-0461-0. 2018
642. Ozdemir ES, Jang H, Gursoy A, Keskin O, Li Z, Sacks DB, Nussinov R. Unraveling the molecular mechanism of interactions of the Rho GTPases Cdc42 and Rac1 with the scaffolding protein IQGAP2. J Biol Chem. 293(10):3685-3699, 2018
643. Ozdemir ES, Jang H, Gursoy A, Keskin O, Nussinov R. Arl2-Mediated Allosteric Release of Farnesylated KRas4B from Shuttling Factor PDE $\delta$ . J Phys Chem B. 122(30):7503-7513, 2018 doi: 10.1021/acs.jpcc.8b04347.
644. Ozdemir ES, Nussinov R, Gursoy A, Keskin O. Developments in integrative modeling with dynamical interfaces. Curr Opin Struct Biol. 56:11-17. doi: 10.1016/j.sbi.2018.10.007, 2018
645. Qi R, Wei G, Ma B, Nussinov R. Replica Exchange Molecular Dynamics: A Practical Application Protocol with Solutions to Common Problems and a Peptide Aggregation and Self-Assembly Example. Methods Mol Biol. 1777:101-119. 2018
646. Qian Z, Zou Y, Zhang Q, Chen P, Ma B, Wei G, Nussinov R. Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. Biochim Biophys Acta. 2018 Feb 8. pii: S0005-2736(18)30046-4. doi: 10.1016/j.bbamem.2018.02.005.
647. Rangarajan S, He Y, Chen Y, Kerzic MC, Ma B, Gowthaman R, Pierce BG, Nussinov R, Mariuzza RA, Orban J. Peptide-MHC (pMHC) binding to a human antiviral T cell receptor induces long-range allosteric communication between pMHC- and CD3-binding sites. J Biol Chem. 293(41):15991-16005. 2018. doi: 10.1074/jbc.RA118.003832.



648. Ren B, Hu R, Zhang M, Liu Y, Xu L, Jiang B, Ma J, Ma B, Nussinov R, Zheng J. Experimental and Computational Protocols for Studies of Cross-Seeding Amyloid Assemblies. Methods Mol Biol. 1777:429-447, 2018
649. Song NY, Zhu F, Wang Z, Willette-Brown J, Xi S, Sun Z, Su L, Wu X, Ma B, Nussinov R, Xia X, Schrump DS, Johnson PF, Karin M, Hu Y. IKK $\alpha$  inactivation promotes Kras-initiated lung adenocarcinoma development through disrupting major redox regulatory pathways. Proc Natl Acad Sci U S A.; 115(4):E812-E821. 2018
650. Steklov M, Pandolfi S, Baietti MF, Batiuk A, Carai P, Najm P, Zhang M, Jang H, Renzi F, Cai Y, Abbasi Asbagh L, Pastor T, De Troyer M, Simicek M, Radaelli E, Brems H, Legius E, Tavernier J, Gevaert K, Impens F, Messiaen L, Nussinov R, Heymans S, Eyckerman S, Sablina AA. Mutations in LZTR1 drive human disease by dysregulating RAS ubiquitination. Science. 362(6419):1177-1182, doi: 10.1126/science.aap7607. 2018
651. Tsai CJ, Nussinov R. Allosteric activation of RAF in the MAPK signaling pathway. Curr Opin Struct Biol. 53:100-106. doi: 10.1016/j.sbi.2018.07.0072018
652. Wang M, Zhu D, Zhu J, Nussinov R, Ma B. Local and global anatomy of antibody-protein antigen recognition. J Mol Recognit. 31(5):e2693, 2018
653. Wang G, Zhang M, Jang H, Lu S, Lin S, Chen G, Nussinov R, Zhang J, Gaponenko V. Interaction of Calmodulin with the cSH2 Domain of the p85 Regulatory Subunit. Biochemistry 57(12):1917-1928, 2018
654. Weismiller HA, Murphy R, Wei G, Ma B, Nussinov R, Margittai M. Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. J Biol Chem. 293(45):17336-17348. doi: 10.1074/jbc.RA118.005316. PMID: 30242125, 2018
655. Wu D, Wang W, Chen W, Lian F, Lang L, Huang Y, Xu Y, Zhang N, Chen Y, Liu M, Nussinov R, Cheng F, Lu W, Huang J. Pharmacologic inhibition of dihydroorotate dehydrogenase induces apoptosis and differentiation in acute myeloid leukemia cells. Haematologica. 103(9):1472-1483, 2018 pii: haematol.2018.188185. doi: 10.3324/haematol.2018.188185.
656. Yang YA, Lee S, Zhao J, Thompson AJ, McBride R, Tsogtbaatar B, Paulson JC, Nussinov R, Deng L, Song J. In vivo tropism of Salmonella Typhi toxin to cells expressing a multiantennal glycan receptor. Nat Microbiol. 3(2):155-163, 2018 doi: 10.1038/s41564-017-0076-4.
657. Zhang M, Li Z, Wang G, Jang H, Sacks DB, Zhang J, Gaponenko V, Nussinov R. Calmodulin (CaM) Activates PI3K $\alpha$  by Targeting the "Soft" CaM-Binding Motifs in Both the nSH2 and cSH2 Domains of p85 $\alpha$ . J Phys Chem B. 122(49):11137-11146. doi: 10.1021/acs.jpcc.8b05982. 2018

658. Zhao J, Nussinov R, Ma B. Antigen binding allosterically promotes Fc receptor recognition. MAbs. 13:1-17. 2018. doi: 10.1080/19420862.2018.1522178. PMID: 30212263
659. Zhao J, Zhang B, Zhu J, Nussinov R, Ma B. Structure and energetic basis of overrepresented  $\lambda$  light chain in systemic light chain amyloidosis patients. Biochim Biophys Acta. 1864(6 Pt B):2294-2303. doi:10.1016/j.bbadis.12.009. 2018
660. Cheng F, Liang H, Butte AJ, Eng C, Nussinov R. Personal Mutanomes Meet Modern Oncology Drug Discovery and Precision Health. Pharmacol Rev. 71(1):1-19. doi: 10.1124/pr.118.016253, 2019
661. Guven-Maiorov E, Tsai CJ, Ma B, Nussinov R. Interface-Based Structural Prediction of Novel Host-Pathogen Interactions. Methods Mol Biol. 1851:317-335. doi: 10.1007/978-1-4939-8736-8, 2019
662. Guven-Maiorov E, Tsai CJ, Nussinov R. Oncoviruses Can Drive Cancer by Rewiring Signaling Pathways Through Interface Mimicry. Front Oncol. 2019 Nov 15;9:1236. doi: 10.3389/fonc.2019.01236.
663. Huang Y, Fang J, Lu W, Wang Z, Wang Q, Hou Y, Jiang X, Reizes O, Lathia J, Nussinov R, Eng C, Cheng F. A Systems Pharmacology Approach Uncovers Wogonoside as an Angiogenesis Inhibitor of Triple-Negative Breast Cancer by Targeting Hedgehog Signaling. Cell Chem Biol. 26(8):1143-1158.e6. doi: 10.1016/j.chembiol.2019.05.004. 2019.
664. Jang H, Banerjee A, Marcus K, Makowski L, Mattos C, Gaponenko V, Nussinov R. The Structural Basis of the Farnesylated and Methylated KRas4B Interaction with Calmodulin. Structure, 27(11):1647-1659.e4. doi: 10.1016/j.str.2019.08.009. 2019
665. Lei J, Qi R, Tang Y, Wang W, Wei G, Nussinov R, Ma B. Conformational stability and dynamics of the cancer-associated isoform  $\Delta 133p53\beta$  are modulated by p53 peptides and p53-specific DNA. FASEB J. 33(3):4225-4235. doi: 10.1096/fj.201801973R. 2019.
666. Nussinov R, Jang H, Tsai CJ, Cheng F. Precision medicine review: rare driver mutations and their biophysical classification. Biophys Rev. 11(1):5-19. doi: 10.1007/s12551-018-0496-2, 2019
667. Nussinov R, Jang H, Tsai CJ, Cheng F. Review: Precision medicine and driver mutations: Computational methods, functional assays and conformational principles for interpreting cancer drivers. PLoS Comput Biol. 15(3):e1006658. doi: 10.1371/journal.pcbi.1006658. eCollection 2019

668. Nussinov R, Tsai CJ, Jang H. Protein ensembles link genotype to phenotype. PLoS Comput Biol. 2019 Jun 20;15(6):e1006648. doi: 10.1371/journal.pcbi.1006648. eCollection 2019.
669. Nussinov R, Tsai CJ, Jang H. Why Are Some Driver Mutations Rare? Trends Pharmacol Sci. ;40(12):919-929. doi: 10.1016/j.tips.2019.10.003. 2019.
670. Nussinov R, Tsai CJ, Jang H. Dynamic Protein Allosteric Regulation and Disease. Adv Exp Med Biol. 1163:25-43. doi: 10.1007/978-981-13-8719-7\_2. 2019
671. Nussinov R, Tsai CJ, Jang H. Does Ras Activate Raf and PI3K Allosterically? Front Oncol. 2019 Nov 15;9:1231. doi: 10.3389/fonc.2019.01231.
672. Nussinov R, Tsai CJ, Shehu A, Jang H. Computational Structural Biology: Successes, Future Directions, and Challenges. Molecules. 24(3). doi: 0.3390/molecules24030637. 2019
673. Ozdemir ES, Halakou F, Nussinov R, Gursoy A, Keskin O. Methods for Discovering and Targeting Druggable Protein-Protein Interfaces and Their Application to Repurposing. Methods Mol Biol. 1903:1-21. doi: 10.1007/978-1-4939-8955-3\_1, 2019
674. Peng H, Zeng X, Zhou Y, Zhang D, Nussinov R, Cheng F. A component overlapping attribute clustering (COAC) algorithm for single-cell RNA sequencing data analysis and potential pathobiological implications. PLoS Comput Biol. 19;15(2):e1006772. doi: 10.1371/journal.pcbi.1006772. eCollection 2019
675. Ruff WE, Dehner C, Kim WJ, Pagovich O, Aguiar CL, Yu AT, Roth AS, Vieira SM, Kriegel C, Adeniyi O, Mulla MJ, Abrahams VM, Kwok WW, Nussinov R, Erkan D, Goodman AL, Kriegel MA. Pathogenic Autoreactive T and B Cells Cross-React with Mimotopes Expressed by a Common Human Gut Commensal to Trigger Autoimmunity. Cell Host Microbe. 26(1):100-113.e8, doi: 10.1016/j.chom.2019.05.003. 2019.
676. Tsai CJ, Nussinov R. Emerging Allosteric Mechanism of EGFR Activation in Physiological and Pathological Contexts. Biophys J. 117(1):5-13. doi: 10.1016/j.bpj.2019.05.021. 2019.
677. Wodak SJ, Paci E, Dokholyan NV, Berezovsky IN, Horovitz A, Li J, Hilser VJ, Bahar I, Karanicolas J, Stock G, Hamm P, Stote RH, Eberhardt J, Chebaro Y, Dejaegere A, Cecchini M, Changeux JP, Bolhuis PG, Vreede J, Faccioli P, Orioli S, Ravasio R, Yan L, Brito C, Wyart M, Gkeka P, Rivalta I, Palermo G, McCammon JA, Panecka-Hofman J, Wade RC, Di Pizio A, Niv MY, Nussinov R, Tsai CJ, Jang H, Padhorny D, Kozakov D, McLeish T. Allostery in Its Many Disguises: From Theory to Applications. Structure. 27(4):566-578. doi: 10.1016/j.str.2019.01.003. 2019
678. Yang X, Cheng H, Chen J, Wang R, Saleh A, Si H, Lee S, Guven-Maiorov E, Keskin O, Gursoy A, Nussinov R, Fang J, Van Waes C, Chen Z. Head and Neck Cancers Promote

- an Inflammatory Transcriptome through Coactivation of Classic and Alternative NF- $\kappa$ B Pathways. Cancer Immunol Res. 7(11):1760-1774, doi: 10.1158/2326-6066.CIR-18-0832. 2019.
679. Zeng X, Zhu S, Liu X, Zhou Y, Nussinov R, Cheng F. deepDR: A network-based deep learning approach to in silico drug repositioning. Bioinformatics. 35(24):5191-5198. doi: 10.1093/bioinformatics/btz418. 2019.
680. Zhang M, Jang H, Nussinov R. The structural basis for Ras activation of PI3K $\alpha$  lipid kinase. Phys Chem Chem Phys. 21(22):12021-12028. doi: 10.1039/c9cp00101h. 2019.
681. Zhang M, Jang H, Nussinov R. The mechanism of PI3K $\alpha$  activation at the atomic level. Chem Sci. 10(12):3671-3680. doi: 10.1039/c8sc04498h. eCollection 2019.
682. Zhang M, Li Z, Jang H, Hedman AC, Sacks DB, Nussinov R. Ca<sup>2+</sup>-Dependent Switch of Calmodulin Interaction Mode with Tandem IQ Motifs in the Scaffolding Protein. IQGAP1. Biochemistry. 58(49):4903-4911. doi: 10.1021/acs.biochem.9b00854. 2019.
683. Chen Y, Wei G, Zhao J, Nussinov R, Ma B. Computational Investigation of Gantenerumab and Crenezumab Recognition of A $\beta$  Fibrils in Alzheimer's Disease Brain Tissue. ACS Chem Neurosci. 11(20):3233-3244. doi: 10.1021/acschemneuro.0c00364. 2020.
684. Dudas B, Merzel F, Jang H, Nussinov R, Perahia D, Balog E. Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. Front Mol Biosci. 2020 Jul 10;7:145. doi: 10.3389/fmolb.2020.00145. eCollection 2020.
685. Fang J, Pieper AA, Nussinov R, Lee G, Bekris L, Leverenz JB, Cummings J, Cheng F. Harnessing endophenotypes and network medicine for Alzheimer's drug repurposing. Med Res Rev. doi: 10.1002/med.21709. 2020.
686. Guven-Maiorov E, Hakouz A, Valjevac S, Keskin O, Tsai CJ, Gursoy A, Nussinov R. HMI-PRED: A Web Server for Structural Prediction of Host-Microbe Interactions Based on Interface Mimicry. J Mol Biol. 432(11):3395-3403. doi: 10.1016/j.jmb.2020.01.025. 2020.
687. He Y, Agnihotri P, Rangarajan S, Chen Y, Kerzic MC, Ma B, Nussinov R, Mariuzza RA, Orban J. Peptide-MHC Binding Reveals Conserved Allosteric Sites in MHC Class I- and Class II-Restricted T Cell Receptors (TCRs). J Mol Biol. Dec 4;432(24):166697. doi: 10.1016/j.jmb.2020.10.031. 2020.
688. Jang H, Zhang M, Nussinov R. The quaternary assembly of KRas4B with Raf-1 at the membrane. Comput Struct Biotechnol J. 8:737-748. doi: 10.1016/j.csbj.2020.03.018. eCollection 2020.

689. Liao TJ, Jang H, Nussinov R, Fushman D. High-Affinity Interactions of the nSH3/cSH3 Domains of Grb2 with the C-Terminal Proline-Rich Domain of SOS1. J Am Chem Soc. 142(7):3401-3411. doi: 10.1021/jacs.9b10710. 2020.
690. Liao TJ, Jang H, Fushman D, Nussinov R. SOS1 interacts with Grb2 through regions that induce closed nSH3 conformations. J Chem Phys.; 153(4):045106. doi: 10.1063/5.0013926. 2020.
691. Liu C, Zhao J, Lu W, Dai Y, Hockings J, Zhou Y, Nussinov R, Eng C, Cheng F. Individualized genetic network analysis reveals new therapeutic vulnerabilities in 6,700 cancer genomes. PLoS Comput Biol. 6(2):e1007701. doi: 10.1371/journal.pcbi.1007701. 2020.
692. Muratcioglu S, Aydin C, Odabasi E, Ozdemir ES, Firat-Karalar EN, Jang H, Tsai CJ, Nussinov R, Kavakli IH, Gursoy A, Keskin O. Oncogenic K-Ras4B dimerization enhances downstream MAPK signaling. J Mol Biol. 432(4):1199-1215. doi: 10.1016/j.jmb.2020.01.002. 2020.
693. Nussinov R, Jang H, Zhang M, Tsai CJ, Sablina AA. The Mystery of Rap1 Suppression of Oncogenic Ras. Trends Cancer. 6(5):369-379. doi: 10.1016/j.trecan.2020.02.002, 2020.
694. Nussinov R, Tsai CJ, Jang H. Autoinhibition can identify rare driver mutations and advise pharmacology. FASEB J. 34(1):16-29. doi: 10.1096/fj.201901341R. 2020.
695. Nussinov R, Tsai CJ, Jang H. Ras assemblies and signaling at the membrane. Curr Opin Struct Biol. 62:140-148. doi: 10.1016/j.sbi.2020.01.009. 2020.
696. Nussinov R, Tsai CJ, Jang H. Are Parallel Proliferation Pathways Redundant? Trends Biochem Sci. 45(7):554-563. doi: 10.1016/j.tibs.2020.03.013.
697. Younger S, Jang H, Davies HA, Niemiec MJ, Garcia JGN, Nussinov R, Migrino RQ, Madine J, Arce FT. Medin Oligomer Membrane Pore Formation: A Potential Mechanism of Vascular Dysfunction. Biophys J. 2020 Jun 2;118(11):2769-2782. doi: 10.1016/j.bpj.2020.04.026.
698. Zeng X, Zhu S, Hou Y, Zhang P, Li L, Li J, Huang LF, Lewis SJ, Nussinov R, Cheng F. Network-based Prediction of Drug-Target Interactions using an Arbitrary-Order Proximity Embedded Deep Forest. Bioinformatics. 36(9):2805-2812. doi: 10.1093/bioinformatics/btaa010. 2020.
699. Zhang M, Jang H, Nussinov R. PI3K inhibitors: review and new strategies. Chemical Science 11(23): 5855-5865. <https://doi.org/10.1039/D0SC01676D> 2020.

700. Zhang M, Jang H, Nussinov R. Structural Features that Distinguish Inactive and Active PI3K Lipid Kinases. *J Mol Biol.* 432(22):5849-5859. doi: 10.1016/j.jmb.2020.09.002. 2020.
701. Zhou Y, Wang F, Tang J, Nussinov R, Cheng F. Artificial intelligence in COVID-19 drug repurposing. *Lancet Digit Health.* Dec;2(12):e667-e676. 2020 Sep 18. doi: 10.1016/S2589-7500(20)30192-8. 2020
702. Abdelkarim H, Leschinsky N, Jang H, Banerjee A, Nussinov R, Gaponenko V. The dynamic nature of the K-Ras/calmodulin complex can be altered by oncogenic mutations. *Curr Opin Struct Biol.* Jul 23;71:164-170. doi: 10.1016/j.sbi.2021.06.008. 2021
703. Brown KM, Xu M, Sargen M, Jang H, Zhang M, Zhang T, Zhu B, Jones K, Kim J, Mendoza L, Hayward NK, Tucker MA, Goldstein AM, Yang XR, Stewart DR, Hicks B, Consonni D, Pesatori AC, Fagnoli MC, Peris K, Stratigos A, Menin C, Ghiorzo P, Puig S, Nagore E; MelaNostrum Consortium, Andresson T, Nussinov R, Calista D, Landi MT. Novel MAPK/AKT-impairing germline NRAS variant identified in a melanoma-prone family. *Fam Cancer.* Jul 3. doi: 10.1007/s10689-021-00267-9. 2021
704. Cai T, Lim H, Abbu KA, Qiu Y, Nussinov R, Xie L. MSA-Regularized Protein Sequence Transformer toward Predicting Genome-Wide Chemical-Protein Interactions: Application to GPCRome Deorphanization. *J Chem Inf Model.* Apr 26;61(4):1570-1582. doi: 10.1021/acs.jcim.0c01285. 2021
705. Eren M, Tuncbag N, Jang H, Nussinov R, Gursoy A, Keskin O. Normal Mode Analysis of KRas4B Reveals Partner Specific Dynamics. *J Phys Chem B.* May 27;125(20):5210-5221. doi: 10.1021/acs.jpcc.1c00891. 2021
706. Haspel N, Jang H, Nussinov R. Active and Inactive Cdc42 Differ in Their Insert Region Conformational Dynamics. *Biophys J.* Jan 19;120(2):306-318. doi: 10.1016/j.bpj.2020.12.007. 2021
707. Jang H, Smith IN, Eng C, Nussinov R. The mechanism of full activation of tumor suppressor PTEN at the phosphoinositide-enriched membrane. *iScience.* Apr 17;24(5):102438. doi: 10.1016/j.isci.2021.102438. 2021
708. Liu C, Han Z, Zhang ZK, Nussinov R, Cheng F A network-based deep learning methodology for stratification of tumor mutations. *Bioinformatics.* 8;37(1):82-8. doi: 10.1093/bioinformatics/btaa1099. 2021
709. Lu W, Yu W, He J, Liu W, Yang J, Lin X, Zhang Y, Wang X, Jiang W, Luo J, Zhang Q, Yang H, Peng S, Yi Z, Ren S, Chen J, Siwko S, Nussinov R, Cheng F, Zhang H, Liu M. Reprogramming immunosuppressive myeloid cells facilitates immunotherapy for colorectal cancer. *EMBO Mol Med.*;13(1):e12798. doi: 10.15252/emmm.202012798. 2021

710. Lucchesi CA, Zhang J, Ma B, Nussinov R, Chen X. Survivin Expression is Differentially Regulated by a Selective Crosstalk between Rbm38 and miRNAs let-7b or miR-203a. Cancer Res. 81(7):1827-1839. doi: 10.1158/0008-5472.CAN-20-3157. 2021
711. Ma B, Bai G, Nussinov R, Ding J, Wang YX. Conformational Ensemble of TteAdoCbl Riboswitch Provides Stable Structural Elements for Conformation Selection and Population Shift in Cobalamin Recognition. J Phys Chem B. Mar 18;125(10):2589-2596. doi: 10.1021/acs.jpcc.1c00038. 2021
712. Maloney RC, Zhang M, Jang H, Nussinov R. The mechanism of activation of monomeric B-Raf V600E. Comput Struct Biotechnol J. Jun 4;19:3349-3363. doi: 10.1016/j.csbj.2021.06.007. 2021
713. Martin W, Sheynkman G, Lightstone FC, Nussinov R, Cheng F. Interpretable artificial intelligence and exascale molecular dynamics simulations to reveal kinetics: Applications to Alzheimer's disease. Curr Opin Struct Biol. Oct 7;72:103-113. doi: 10.1016/j.sbi.2021.09.001.2021
714. Nguyen PH, Ramamoorthy A, Sahoo BR, Zheng J, Faller P, Straub JE, Dominguez L, Shea JE, Dokholyan NV, De Simone A, Ma B, Nussinov R, Najafi S, Ngo ST, Loquet A, Chiricotto M, Ganguly P, McCarty J, Li MS, Hall C, Wang Y, Miller Y, Melchionna S, Habenstein B, Timr S, Chen J, Hnath B, Strodel B, Kayed R, Lesné S, Wei G, Sterpone F, Doig AJ, Derreumaux P. Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chem Rev. Feb 24;121(4):2545-2647. doi: 10.1021/acs.chemrev.0c01122. 2021.
715. Nussinov R. Autobiography of Ruth Nussinov. J Phys Chem B. Jul 1;125(25):6735-6739. doi: 10.1021/acs.jpcc.1c04719. 2021
716. Nussinov R, Jang H, Gursoy A, Keskin O, Gaponenko V. Inhibition of nonfunctional Ras. Cell Chem Biol. 28(2):121-133. doi: 10.1016/j.chembiol.2020.12.012. 2021
717. Nussinov R, Jang H, Nir G, Tsai CJ, Cheng F. A new precision medicine initiative at the dawn of exascale computing. Signal Transduct Target Ther. Jan 6;6(1):3. doi: 10.1038/s41392-020-00420-3. 2021
718. Nussinov R, Shirouzu M. Editorial overview: Catalysis and regulation: The beating heart of biology. Curr Opin Struct Biol. Dec;71:iii-v. doi: 10.1016/j.sbi.2021.09.002. 2021
719. Nussinov R, Tsai CJ, Jang H. Signaling in the crowded cell. Curr Opin Struct Biol. Jul 1;71:43-50. doi: 10.1016/j.sbi.2021.05.009. 2021
720. Nussinov R, Tsai CJ, Jang H. Anticancer drug resistance: An update and perspective. Drug Resist Updat. 2021 Dec 59:100796. doi: 10.1016/j.drug.2021.100796.

721. Nussinov R, Zhang M, Maloney R, Jang H. Drugging multiple same-allele driver mutations in cancer. Expert Opin Drug Discov. Aug;16(8):823-828. doi: 10.1080/17460441.2021.1905628. 2021
722. Nussinov R, Zhang M, Maloney R, Jang H. Ras isoform-specific expression, chromatin accessibility, and signaling. Biophys Rev. Jul 31;13(4):489-505. doi: 10.1007/s12551-021-00817-6. 2021
723. Nussinov R, Zhang M, Maloney R, Tsai CJ, Yavuz BR, Tuncbag N, Jang H. Mechanism of activation and the rewired network: New drug design concepts. Med Res Rev. Oct 25. doi: 10.1002/med.21863. 2021
724. Nussinov R, Zhang M, Tsai CJ, Jang H. Phosphorylation and Driver Mutations in PI3K $\alpha$  and PTEN Autoinhibition. Mol Cancer Res. 19(4):543-548. doi: 10.1158/1541-7786.MCR-20-0818. 2021
725. Ovek D, Taweel A, Abali Z, Tezsezen E, Koroglu YE, Tsai CJ, Nussinov R, Keskin O, Gursoy A. Web interface for 3D visualization and analysis of SARS-CoV-2-human mimicry and interactions. Bioinformatics. Dec 2;btab799. doi: 10.1093/bioinformatics/btab799. 2021
726. Senyuz S, Jang H, Nussinov R, Keskin O, Gursoy A. Mechanistic Differences of Activation of Rac1P29S and Rac1A159V. J Phys Chem B. Apr 22;125(15):3790-3802. doi: 10.1021/acs.jpcc.1c00883. 2021
727. Weako J, Jang H, Keskin O, Nussinov R, Gursoy A. The structural basis of Akt PH domain interaction with calmodulin. Biophys J. May 18;120(10):1994-2008. doi: 10.1016/j.bpj.2021.03.018. 2021
728. Zhang M, Jang H, Li Z, Sacks DB, Nussinov R. B-Raf autoinhibition in the presence and absence of 14-3-3. Structure. 29(7):768-777.e2. doi: 10.1016/j.str.2021.02.005. doi: 10.1016/j.str.2021.02.005. 2021
729. Zhang M, Jang H, Nussinov R. PI3K Driver Mutations: A Biophysical Membrane-Centric Perspective. Cancer Res. Jan 15;81(2):237-247. doi: 10.1158/0008-5472.CAN-20-0911. 2021.
730. Zhang M, Maloney R, Jang H, Nussinov R. The mechanism of Raf activation through dimerization. Chem Sci. Nov 18;12(47):15609-15619. doi: 10.1039/d1sc03444h. 2021
731. Zhao J, Mohan N, Nussinov R, Ma B, Wu WJ. Trastuzumab Blocks the Receiver Function of HER2 Leading to the Population Shifts of HER2-Containing Homodimers and Heterodimers. Antibodies (Basel). Feb 4;10(1):7. doi: 10.3390/antib10010007. 2021.
732. Zhao J, Nussinov R, Ma B. The Allosteric Effect in Antibody-Antigen Recognition. Methods Mol Biol. 2253:175-183. doi: 10.1007/978-1-0716-1154-8\_11. 2021.



733. Zhou Y, Zhao J, Fang J, Martin W, Li L, Nussinov R, Chan TA, Eng C, Cheng F. My personal mutanome: a computational genomic medicine platform for searching network perturbing alleles linking genotype to phenotype. Genome Biol. Jan 29;22(1):53. doi: 10.1186/s13059-021-02269-3. 2021.
734. Berezovsky IN, Nussinov R. Multiscale Allostery: Basic Mechanisms and Versatility in Diagnostics and Drug Design. J Mol Biol. 434(17):167751. doi: 10.1016/j.jmb.2022.167751. 2022
735. Grudzien P, Jang H, Leschinsky N, Nussinov R, Gaponenko V. Conformational Dynamics Allows Sampling of an "Active-like" State by Oncogenic K-Ras-GDP. J Mol Biol. Jun 23:167695. doi: 10.1016/j.jmb.2022.167695. Online ahead of print. 2022
636. Jain A, Mittal S, Tripathi LP, Nussinov R, Ahmad S. Host-pathogen protein-nucleic acid interactions: A comprehensive review. Comput Struct Biotechnol J. 20:4415-4436. doi: 10.1016/j.csbj.2022.08.001. 2022
637. Kabir KL, Ma B, Nussinov R, Shehu A. Fewer Dimensions, More Structures for Improved Discrete Models of Dynamics of Free versus Antigen-Bound Antibody. Biomolecules. 12(7):1011. doi: 10.3390/biom12071011. 2022
738. Lim H, Cankara F, Tsai CJ, Keskin O, Nussinov R, Gursoy A. Artificial intelligence approaches to human-microbiome protein-protein interactions. Curr Opin Struct Biol. 2022 Feb 10;73:102328. doi: 10.1016/j.sbi.2022.102328.
739. Lim H, Tsai CJ, Keskin O, Nussinov R, Gursoy A. HMI-PRED 2.0: a biologist-oriented web application for prediction of host-microbe protein-protein interaction by interface mimicry. Bioinformatics. 38(21):4962-4965. doi: 10.1093/bioinformatics/btac633. 2022
740. Liu Y, Jang H, Zhang M, Tsai CJ, Maloney R, Nussinov R. The structural basis of BCR-ABL recruitment of GRB2 in chronic myelogenous leukemia. Biophys J. 121(12):2251-2265 doi: 10.1016/j.bpj.2022.05.030. 2022
741. Liu Y, Zhang M, Tsai CJ, Jang H, Nussinov R. Allosteric regulation of autoinhibition and activation of c-Abl. Comput Struct Biotechnol J. 20:4257-4270. doi: 10.1016/j.csbj.2022.08.014. 2022
742. Maloney RC, Zhang M, Liu Y, Jang H, Nussinov R. The mechanism of activation of MEK1 by B-Raf and KSR1. Cell Mol Life Sci. May 4;79(5):281. doi: 10.1007/s00018-022-04296-0. 2022.
743. Nussinov R, Jang H, Nir G, Tsai CJ, Cheng F. Open Structural Data in Precision Medicine. Annu Rev Biomed Data Sci. Apr 28. doi: 10.1146/annurev-biodatasci-122220-012951. 2022. Online ahead of print.

744. Nussinov R, Tsai CJ, Jang H. How can same-gene mutations promote both cancer and developmental disorders? Sci Adv. Jan 14;8(2):eabm2059. doi: 10.1126/sciadv.abm2059. 2022.
745. Nussinov R, Tsai CJ, Jang H. Allosteric, and how to define and measure signal transduction. Biophys Chem. Jan 29;283:106766. doi: 10.1016/j.bpc.2022.106766. 2022.
746. Nussinov R, Tsai CJ, Jang H Neurodevelopmental disorders, immunity, and cancer are connected. iScience. May 30;25(6):104492. doi: 10.1016/j.isci.2022.104492. 2022
747. Nussinov R, Tsai CJ, Jang H. A new view of activating mutations in cancer. Cancer Res. CAN-22-2125. doi: 10.1158/0008-5472.CAN-22-2125. 2022
748. Nussinov R, Zhang M, Liu Y, Jang H. AlphaFold, Artificial Intelligence (AI), and Allosteric. J Phys Chem B. 126(34):6372-6383. doi: 10.1021/acs.jpcc.2c04346. 2022.
749. Nussinov R, Zhang M, Maloney R, Liu Y, Tsai CJ, Jang H. Allosteric: Allosteric Cancer Drivers and Innovative Allosteric Drugs. J Mol Biol. Apr 1:167569. doi: 10.1016/j.jmb.2022.167569. 2022. Online ahead of print.
750. Ozdemir ES, Ranganathan SV, Nussinov R. How has artificial intelligence impacted COVID-19 drug repurposing and what lessons have we learned? Expert Opin Drug Discov. 17(10):1061-1065. doi: 10.1080/17460441.2022.2128333. 2022
751. Song NY, Li X, Ma B, Willette-Brown J, Zhu F, Jiang C, Su L, Shetty J, Zhao Y, Shi G, Banerjee S, Wu X, Tran B, Nussinov R, Karin M, Hu Y. IKK $\alpha$ -deficient lung adenocarcinomas generate an immunosuppressive microenvironment by overproducing Treg-inducing cytokines. Proc Natl Acad Sci U S A. 2022 Feb 8;119(6):e2120956119. doi: 10.1073/pnas.2120956119.
752. Tsuji K, Hymel D, Ma B, Tamamura H, Nussinov R, Burke TR Jr. Development of ultra-high affinity bivalent ligands targeting the polo-like kinase 1. RSC Chem Biol. 3(9):1111-1120. doi: 10.1039/d2cb00153e. 2022
753. Zhang H, Ni D, Fan J, Li M, Zhang J, Hua C, Nussinov R, Lu S. Markov State Models and Molecular Dynamics Simulations Reveal the Conformational Transition of the Intrinsically Disordered Hypervariable Region of K-Ras4B to the Ordered Conformation. J Chem Inf Model. 62(17):4222-4231. doi: 10.1021/acs.jcim.2c00591. 2022
754. Zeng X, Xiang H, Yu L, Wang J, Li K, Nussinov R, Cheng F. Accurate prediction of molecular targets using a self-supervised image representation learning framework. Res Sq. 2022 Apr 7:rs.3.rs-1477870. doi: 10.21203/rs.3.rs-1477870/v1.
755. Zeng X, Wang F, Luo Y, Kang SG, Tang J, Lightstone FC, Fang EF, Cornell W, Nussinov R, Cheng F. Deep generative molecular design reshapes drug discovery. Cell Rep Med. 100794. doi: 10.1016/j.xcrm.2022.100794. 2022

In Press:

Books/Book Chapters (Last 10 years):

11. Benyamini, H., Gunasekaran, K., Wolfson, H., and Nussinov, R. Gelsolin Amyloidosis. In: Amyloid Proteins: The Beta Pleated Sheet Conformation and Disease, Sipe, J. (Ed.), Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2005, pp. 625-634.
12. Haspel, N., Zanuy, D., Tsai, H-H., Ma, B., Wolfson, H., and Nussinov, R. Computational Approaches and Tools for Establishing Structural Models for Short Amyloid-Forming Peptides. In: Amyloid Proteins: The Beta Pleated Sheet Conformation and Disease, Sipe, J. (Ed.), Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2005, pp. 301-318.
13. Dror, O., Shulman-Peleg, A., Nussinov, R., and Wolfson, H.J. Predicting Molecular Interactions In: Silico: I. A Updated Guide to Pharmacophore Identification and its Applications to Drug Design. Frontiers in Medicinal Chemistry, 2006, pp. 551-584.
14. Bai, Y. and Nussinov, R. Protocols for Protein Folding. Methods in Molecular Biology, Humana Press, Totowa, NJ, 2007, pp. 69-81.
15. Haspel, N., Wainreb, G., Inbar, Y., Tsai, H-H., Tsai, C-J., Wolfson, H. J., and Nussinov, R. A Hierarchical Protein Folding Scheme Based on the Building Block Model. In: Methods in Molecular Biology, Nussinov R. and Bai, Y. (Eds.), Humana Press, U.S.A., Totowa, NJ, 2007, Vol. 350, pp. 189-204.
16. Inbar, Y., Schneidman-Duhovny, D., Dror, O., Nussinov, R., and Wolfson, H.J. Deterministic Pharmacophore Detection Via Multiple Flexible Alignment of Drug-Like Molecules. In: Research in Computational Molecular Biology, Speed, T. (Ed.), Springer, San Francisco, CA, Volume LNBI 4453, 2007, Vol. 412, pp. 412-429.
17. Kumar, S., Arya, S., and Nussinov, R. Temperature-Dependent Molecular Adaptation Features in Proteins. In: Physiology and Biochemistry of Extremophiles, Glansdorff, N. and Gerday, C. (Eds.) American Society for Microbiology, 2007, pp. 75-85.
18. Gazit, E. and Nussinov, R. Nanostructure Design: Methods and Protocols. Methods in Molecular Biology. Humana Press, U.S.A, 2008, Vol. 474, pp. v-vii.
19. Shatsky, M., Nussinov, R., and Wolfson, H. Algorithms for Multiple Protein Structure Alignment and Structure-Derived Multiple Sequence Alignment. In: Methods in

Molecular Biology, Zaki, M.J. and Bystroff, C. (Eds.), Humana Press, U.S.A., 2008, Vol. 413, pp. 125-146.

Invited NCI Publications:

1. Ma, B., Elkayam, T., Wolfson, H., and Nussinov, R. Protein-Protein Interactions: What are the Preferred Ways in Which Proteins Interact? Center for Cancer Research Frontiers in Science, Structural Biology, Vol. 4, November 2005.
2. Keskin, O., Ma, B., Rogale, K., Gunasekaran, K., and Nussinov, R. Protein-Protein Interactions in a Bottom-Up Systems Biology Approach. Center for Cancer Research Frontiers in Science, Molecular Biology, Vol. 5, November 2006.
3. Zheng, J., Ma, B., Tsai, C J., and Nussinov, R. A Catalogue of Structural Motifs in Amyloid Fibril Organization. Center for Cancer Research Frontiers in Science, Molecular Biology, Vol. 8, April 2007.