BIOGRAPHICAL SKETCH

DO NOT EXCEED FIVE PAGES.

NAME: Nussinov, Ruth

OPEN RESEARCHER AND CONTRIBUTOR ID (ORCID): 0000-0002-8115-6415

POSITION TITLE: Professor, Senior Principal Scientist and Senior Principal Investigator, Head, Computational Structural Biology Group, CIL, Frederick National Laboratory for Cancer Research, NCI

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Rutgers University	PHD	05/1977	Biochemistry
Rutgers University	MS	05/1967	Biochemistry
University of Washington, Seattle	BS	05/1966	Microbiology

A. Personal Statement

I am a biologist by training. My dissertation proposed the dynamic programming algorithm for predicting the secondary structure of single stranded RNA. To date, it is still the leading method for RNA folding. In 1999 my group proposed the landmark concept that all possible protein conformations pre-exist, and that evolution has exploited them for function. At the time it was believed that a protein only has two conformations, 'open' and 'closed'. Our concept is significant since it explained that rather than the ligand 'inducing' a conformational change, the ligand can 'select' a preexisting conformation that fits it. This led us to the groundbreaking "conformational selection and population shift" idea (also published as of 1999) as an alternative to the "induced fit" text-book model to explain molecular recognition. More importantly, it offered that binding of the ligand will 'shift of the population' toward the bound conformation to maintain chemical equilibrium. Being a biologist, **I conceived of the conformational ensemble in terms of function and suggested the transformational concept that the 'population shift' is the origin of the allosteric effect, and this is how allostery impacts function**. **I further proposed that the ability to perform function is determined by how populated a protein is in its active functional state, and that the propensities of the conformational ensembles determine not only the protein–but especially also the cell– function**. Activation by oncogenic mutations mimic the mechanism of the wild-type protein. Data over three decades supported these transformative concepts. We applied them to unravel the structural mechanisms of allosteric drug action and formulate determinants of agonist/antagonist drug design. Finally, we offered that signaling strength and duration determine cell fate, not the mutations that initiated it. We defined signaling strength in terms of the population of the active state. **My pioneering pivotal concepts contributed to extraordinary advances in understanding the conformational behaviors of biological macromolecules, and their uncontrolled actions in disease. Recently I was recognized as a Pioneer in Molecular Biology for my contribution to the understanding of conformational ensembles in molecular recognition, allostery, and cell function**. I have advised/co-advised tens of students and postdocs from computer science, engineering, physics, chemistry, genetics, and biology.

B. Positions and Employment

2001- Present	Senior Principal Investigator, Leidos (Formerly SAIC), Cancer Innovation Laboratory, Frederick National Laboratory for Cancer Research, National Cancer Institute, Frederick, MD
2001-2013	Senior Principal Scientist, SAIC, Center for Cancer Research Nanobiology Program (formerly LECB), National Cancer Institute, Frederick, MD
2017- Present	Adjunct Professor, Department of Chemistry & Biochemistry, University of Maryland, College Park, College Park, MD
1990-2012	Professor of Biochemistry, Sackler School of Medicine, Tel Aviv University, Tel Aviv, Israel
1984-1990	Associate Professor, Sackler School of Medicine, Tel Aviv University, Tel Aviv, Israel
1983-1984	Visiting Associate, NIH, National Child Health and Human Development, Bethesda, Maryland
1981-1983	Senior Lecturer, Dept. of Computer Science, School of Mathematics, Tel Aviv University, Tel Aviv, Israel
1983-1983	Visiting Scientist, Los Alamos National Laboratory, Los Alamos, NM
1981-1981	Visiting Scientist, Biochemistry Department, Harvard University, Cambridge, MA
1981-1981	Visiting Scientist, Chemistry Department, Cornell University, Ithaca, NY
1980-1981	Visiting Scientist, Chemistry Department, University of California at Berkeley, CA
1977-1980	Postdoctoral Fellow, Structural Chemistry Department, Weizmann Institute, Rehovot, Israel

C. Other Experience and Professional memberships

Complete List, including committees in the NIH/NCI are in my CV at
https://ccr.cancer.gov/sites/default/files/pubs-files/Ruth_Nussinov-CV_Website-CCR_0.pdf

1. Editor-in-Chief, *Current Opinion in Structural Biology* (on-going)
2. Editor-in-Chief, *PLOS Computational Biology* (former, for 7 years)
3. Guest Editor for several JMB issues
4. Guest Editor for the Biophysical Journal
5. Developmental Core leadership Duke Center for HIV Structural Biology (2025)
6. Editorial Boards (former and on-going): JBC, Physical Biology, Proteins, Protein Engineering, Design and Selectivity; BMC Bioinformatics; Biophysical Journal; Expert Opinion in Drug Discovery
7. Member, Biophysical Society, International Society for Computational Biology (ISCB), American Chemical Society; American Society for Biochemistry and Molecular Biology (ASBMB)
   Guest Editor of Focus/Thematic Issues: Physical Biology, Seminars in Seminars in Cell and Developmental Biology, Chemical Reviews, Current Opinion in Structural Biology
8. Scientific Advisory Board (SAB) Center for HIV Structural Biology, Duke (2023-2025)
9. Advisory board or the panel of the Helmholtz European Partnering project "Innovative High-Performance Computing Approaches for Molecular Neuromedicine" (2024-2025)
10. Organizing committee of the Modeling of Protein Interactions
11. Organizing committee of the Telluride Science Research Center Coarse-Grained Modeling workshop
12. Advisory board, the RWTH Center for Computational Life Science, Germany, “Computational Chemistry”, bridging the Clinics, departments of Physics, Chemistry, and Biology, and Mechanical Engineering (2022)
13. Developmental Core leadership Duke Center for HIV Structural Biology (2022)
14. Advisory board IIT-FZJ (Helmholtz European Partnering Project), Genoa, Italy, 2021-2022
15. 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/)
16. Organizing Committee, Workshops on evolutionary medicine, Institute for Mathematics and its Applications (IMA), at the University of Minnesota, 2021
17. Chairperson of the AACR Award for Outstanding Achievement in Chemistry in Cancer Research Committee (2018-2019)
18. Site visit committee GMD Institute of Algorithms, Bonn, Germany
19. Scientific Council, Forschungszentrum Juelich GmbH, Germany, 2019

20. Los Alamos National Laboratory Site Visit to assess LANL capability to address Gene Function Discovery
21. Site Visit Committee, RWTH Aachen University and the Forschungszentrum Julich, German Research School
22. International Scientific Advisory Board, Center for Computer-Aided Drug Design, China Pharmaceutical University, Nanjing, China, 2015
23. Review Committee, Universite' de Toulouse, LAAS, CNRS, Toulouse, France, 2014
24. Advisory Board, to overview "the future of structural biology is hybrid" in the Protein Data Bank (PDB). UK, 2014
25. NSF Advisory Board, University of Chicago, 2013Site Visit Committee, Chair, the German Research School for Simulation Science, FZ-Julich and RWTH Aachen, 2011
26. Reviewing committee in CEA Saclay, Agence d'Evaluation de la Recherche et des establissement d'Enseignement Superieur, Paris, France, 2010
27. Site Visitor, Biomolecular Modeling Laboratory, Cancer Research UK London Research Institute, 2009
28. MSFD NIH Study Section, Long Term Member, 2009-2015; Ad hoc multiple times earlier and later
29. INRIA-NIH; Organized on behalf of NIH together with French Embassy, 2007

Honors/Awards
Complete List in my CV at
https://ccr.cancer.gov/sites/default/files/pubs-files/Ruth_Nussinov-CV_Website-CCR_0.pdf

2025 **Elected to the National Academy of Sciences https://ccr.cancer.gov/news/article/ruth-nussinov-elected-to-the-national-academy-of-sciences ; https://irp.nih.gov/about-us/honors/the-national-academy-of-sciences ; https://www.nasonline.org/news/2025-nas-election/**
2025 Elected Molecular Biology Pioneer by the Journal of Molecular Biology (**doi: 10.1016/j.jmb.2025.169044)**
2024 Elected an EMBO member
2024 Highly Cited Researcher awards in 2024, https://clarivate.com/highly-cited-researchers/
2024 Designated a Best Female Scientist (H-Index 134) Best Female Scientists in the World 2024 Ranking
2024 Ranked 269 in the world and 193 in United States according to https://research.com/scientists-rankings/biology-and-biochemistry
2023 Highly Cited Researcher 2023, Clarivate
2022 Ranked 63 in the world, and 44 in the US among the Top 1000 Female Scientists in the World according to Research.com, a leading academic platform for researchers, and overall 851 in the world, and 548 in the US (https://research.com/scientists-rankings/best-scientists)
2021 A Festschrift Special Issue in honor of Ruth Nussinov Achievements, ACS, *Journal of Physical Chemistry*
2021 Special Issue in honor of Professor Ruth Nussinov, *Biophysical Chemistry*
2021 Featured as the woman in science in Women's History by ISCB
2021 Elected Fellow of the AIMBE (Medical and Biological Engineering)
2020 Elected Fellow of the American Physical Society
2020 A 3.5 Day "Symposium in honor of Ruth Nussinov" ACS Fall 2020 meeting "Dynamic ensembles, cell signaling and drug discovery" (postponed due to Covid-19)
2020 Achievement Award Frederick National Laboratory for Cancer Research
2018 Ho Chi Minh City, the KeyLab Vietnam Award in Computational Translational Medicine
2018 ISCB, Accomplished by a Senior Fellow Award, Chicago
2017 AACR Award for the 2015 paper in *Molecular Cancer Research* (http://sm.aacr.org/BE1230aDESh).
2017 Xingda Award Peking University
2016 Elected Senior Fellow, International Society for Computational Biology Keynote, ISMB, Orlando
2015 Elected a Theodore von Kármán Fellow, Germany
2015 Elected The 2015 Sarkar Lecturer, the Hospital for Sick Children (SickKids), Canada
2015 Special Life Time Award. The Israeli Society for Bioinformatics and Computational Biology (ISBCB)

2015 A Mini Symposium on Computational Molecular Medicine, dedicated to Ruth Nussinov, Aachen, Germany
2015 Highly Cited Researcher; ranking among the top 1% most cited for their subject field and year of publication, earning the mark of exceptional impact." (http://highlycited.com/ Thomson Reuters, 2015, 2018)
2014 Awarded the Michael and Ada Anbar Lectureship in the Biophysical Sciences publication, earning the mark of exceptional impact." (http://highlycited.com/ Thomson Reuters, 2015, 2018)
2013 Elected Fellow of the International Society of Computational Biology for her "for significant contributions to the fields of computational biology and biochemistry"
2012 Fellow, Institute of Physics, London, UK
2012 Distinguished Ulam Scholar, The Center for Nonlinear Studies (CNLS), Los Alamos National Lab
2012 Distinguished Visitor, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany
2011 Elected Fellow of the Biophysical Society

D. Contributions to Science

1. My 1978 paper, Nussinov, R., Pieczenik, G., Griggs, J., and Kleitman, D.: Algorithms for loop matchings, *SIAM J Appl Math*, 35(1): 68-82, 1978 proposed the dynamic programming algorithm for RNA secondary structure prediction. I developed it in my dissertation. In my post doc, I followed with its application, Nussinov, R. and Jacobson, A. B.: Fast algorithm for predicting the secondary structure of single stranded RNA. *Proc Natl Acad Sci U S A* 77: 6309-13, 1980. To date, this algorithm is still the leading method for predicting RNA structure, and is taught in bioinformatics classes in universities across Europe and in the U.S. This is significant since it provided a way to model the structure of RNA, which is essential to understand its function. Its impact can be seen in Course Lecture/Reference Materials: Wikipedia: Nucleic Acid Structure; Wikiomics: RNA Secondary Structure Prediction; RNA Structure Determination (Center for Integrative Bioinformatics, Vrije Universiteit Amsterdam); and books, e.g., Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids, Durbin R, Eddy SR, Krogh A, Mitchison G, eds., Cambridge University Press, 1998); Sequence Analysis in Molecular Biology: Treasure Trove or Trivial Pursuit. (Gunnar Von Heijne, https://www.amazon.com/Sequence-Analysis-Molecular-Biology-Treasure/dp/0124337066, Acad. Press, 2012).
2. My group proposed the model of 'conformational selection and population shift' as an alternative to 'induced fit' to explain molecular recognition. Biochemistry textbooks have championed the 'induced fit' mechanism for more than 50 years. The concept of conformational selection and population shift that we introduced emphasized that all conformational states preexist, and that evolution has exploited them for function. This paradigm impacted the community's views. Population shift is now broadly recognized as the origin of allostery, and thus signaling. It explains the effects of allosteric, disease-related mutations. The new concepts that we have contributed "have changed the way biophysicists and structural biologists think about protein folding, protein-protein interactions, and ligand binding" and is now included in a semester chemistry/biochemistry course in U.S. college so the students are "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 them". A paper in Science noted, "Although biochemistry textbooks have championed the induced fit mechanism for more than 50 years, there is now growing support for the additional [conformational selection and population shift] binding mechanism" (quoted from Boehr DD and Wright PE. How do proteins interact? *Science* 320: 1429-30, 2008). Early papers include: Tsai CJ, Kumar S, Ma B, Nussinov R. Folding funnels, binding funnels, and protein function. *Protein Sci*. 8: 1181-90, 1999; Ma B, Kumar S, Tsai CJ, Nussinov R. Folding funnels and binding mechanisms. *Protein Eng.* 12: 713-20, 1999; Tsai CJ, Ma B, Nussinov R. Folding and binding cascades: shifts in energy landscapes. *Proc Natl Acad Sci U S A*. 96: 9970-72, 1999.
3. My group suggested that all proteins are allosteric (Is allostery an intrinsic property of all dynamic proteins? Gunasekaran K, Ma B, Nussinov R. *Proteins* 57: 433-43, 2004) and, more recently, we provided the unified mechanistic underpinnings of allostery (A unified view of "how allostery works".

Tsai CJ, Nussinov R. *PLoS Comput Biol*. 10: e1003394, 2014), the underappreciated role of allostery in the cell (The underappreciated role of allostery in the cellular network. Nussinov R, Tsai CJ, Ma B. *Annu Rev Biophys*. 42: 169-89, 2013), the principles of allosteric interactions in cell signaling (Principles of allosteric interactions in cell signaling. Nussinov R, Tsai CJ, Liu J. *J Am Chem Soc*. 136(51): 17692-701, 2014), its role in disease (Allostery in disease and in drug discovery. Nussinov R, Tsai CJ. *Cell* 153: 293-305, 2013), and, over the years, the design principles of allosteric drugs (e.g., Unraveling structural mechanisms of allosteric drug action. Nussinov R, Tsai CJ. *Trends Pharmacol Sci*. 35: 256-64, 2014; The design of covalent allosteric drugs. Nussinov R, Tsai CJ. *Annu Rev Pharmacol Toxicol*. 55: 249-67 2014).

4. My group uncovered the structural basis for cancer signaling by key protein nodes in the MAPK and PI3K/mTOR pathways, and their mechanistic principles; elucidated calmodulin's role in KRAS-driven adenocarcinomas; and proposed a new view of Ras isoforms. This new view argues for multiple signaling states of palmitoylated Ras isoforms, such as K-Ras4A. This view questions the completeness and accuracy of small GTPase Ras isoform statistics in different cancer types and calls for reevaluation of concepts and protocols. Importantly, the multiple signaling states also call for reconsideration of oncogenic Ras therapeutics. These works were all published. Examples include A New View of Ras Isoforms in Cancers. Nussinov R, Tsai CJ, Chakrabarti M, Jang H. *Cancer Res*. 76(1):18-23. 2016; Oncogenic Ras Isoforms Signaling Specificity at the Membrane. Nussinov R, Tsai CJ, Jang H. *Cancer Res*. 78(3):593-602. 2018; The mechanism of full activation of tumor suppressor PTEN at the phosphoinositide-enriched membrane. Jang H, Smith IN, Eng C, Nussinov R. *iScience*.;24(5):102438. 2021 The mechanism of PI3Kα activation at the atomic level. Zhang M, Jang H, Nussinov R. *Chem Sci*. 2019 Feb 20;10(12):3671-3680; A New View of Activating Mutations in Cancer. Nussinov R, Tsai CJ, Jang H. *Cancer Res*. 2022 Nov 15;82(22):4114-4123.
5. My group has pioneered the concept, conceived and developed the algorithm and applied it for prediction of protein-protein interaction by interface structural mimicry. Our innovative concept of prediction of protein-protein interactions through interface mimicry has been made possible by our amino acid sequence-order independent computer vision-based algorithm for comparisons of protein structures, including their surfaces, Efficient detection of three-dimensional structural motifs in biological macromolecules by computer vision techniques. Nussinov R, Wolfson HJ. *Proc Natl Acad Sci U S A*. 88(23):10495-9. 1991; A geometry-based suite of molecular docking processes. Fischer D, Lin SL, Wolfson HL, Nussinov R. *J Mol Biol*. 248(2):459-77 1995. Recently, we applied it to predict host-microbe interactions. Interface-Based Structural Prediction of Novel Host-Pathogen Interactions. Guven-Maiorov E, Tsai CJ, Ma B, Nussinov R. *Methods Mol Biol*.;1851:317-335, 2019. HMI-PRED 2.0: a biologist-oriented web application for prediction of host-microbe protein-protein interaction by interface mimicry. Lim H, Tsai CJ, Keskin O, Nussinov R, Gursoy A. *Bioinformatics*. 2022 Oct 31;38(21):4962-4965. Its concept is that the architectures of protein-protein interfaces have been conserved by evolution, much in the same way as motifs in protein structures. To evade host defense, pathogens hijack host proteins at different levels: sequence, structure, motif, and binding surface, i.e., interface. Interface similarity allows pathogen proteins to compete with host counterparts to bind to a target protein, rewire physiological signaling, and result in persistent infections, as well as cancer. The concept of interface mimicry promises to identify more host-microbe protein-protein interactions than complete sequence or structural similarity.
6. My group has pioneered studies on the molecular level resolving the puzzling question of How can same-gene mutations promote both cancer and developmental disorders? Nussinov R, Tsai CJ, Jang H. *Sci Adv*. 2022 Jan 14;8(2):eabm2059. Our innovative concept proposed that cell type–specific expression of the mutant protein, and of other proteins in the respective pathway, timing of activation (during embryonic development or sporadic emergence), and the absolute number of molecules that the mutations activate, alone or in combination, are pivotal in determining the pathological phenotypes—cancer and (or) developmental disorders. We further proposed that Neurodevelopmental disorders, immunity, and cancer are connected. Nussinov R, Tsai CJ, Jang H. *iScience*. 2022 May 30;25(6):104492.
7. Our innovative broad outlook harnesses cell biology and protein conformational ensembles, helping us to define signaling strength, clarify cell cycle decisions, and thus cell fate. Nussinov R, Zhang W, Liu Y,

Jang H. Sci Adv. 2024 Jul 5;10(27):eadm9211. doi: 10.1126/sciadv.adm9211. Mitogen signaling strength and duration can control cell cycle decisions.

E. Research Support

Complete List of Published Works in My Bibliography

Total of 782 papers (in PubMed) 83131 citations, **H-index**: 143 (based on Google Scholar)
See the complete list of publications: View Dr. Nussinov's Complete Bibliography at NCBI
http://www.ncbi.nlm.nih.gov/pubmed/?term=Nussinov%20R or in Google Scholar
https://scholar.google.com/citations?hl=en&user=L3n3n8UAAAAJ

Invited Talks (Last 10 Years)

1. Invited Keynote, Gordon Research Conference (GRC) on Enzymes, Coenzymes, and Metabolic Pathways, Waterville Valley, NH, USA. July 2025
2. Invited talk, Weizmann Institute, Israel, April 2025
3. Invited talk, seminar series, City College of New York seminar series on Biochemistry, Biophysics, NYC, March 2025
4. Invited talks, Computational Biomedicine, Institute of Bioscience and Medicine, Julich, Germany, February 2025 https://www.fz-juelich.de/en/inm/inm-9/conferences/racb/program
5. Faculty talk, NCI-Frederick, January 2025
6. Invited Departmental Seminar, Karolinska Institute, Sweden, September 2024
7. Invited Speaker, conference of the Helmholtz European Partnering project "Innovative HPC Approaches for
8. Molecular Neuromedicine", organized by Paolo Carloni and Michele Parrinello, Julich, Germany, November 2024
9. Invited Speaker, Biowulf, NIH-Bethesda, September 2024
10. Invited Speaker, European Calcium Society (ECS) meeting, Cambridge, UK, September 2024
11. Invited Speaker, BioTech Connector. Leidos, NCI- Frederick, August 2024
12. Invited Speaker, CECAM (Centre Européen de Calcul Atomique and Moleculaire) Flagship Workshop on Towards quantitative cell biology through AI-driven software engineering for molecular simulations, Pisa, Italy, May 2024
13. Invited Speaker, Science for the Non-Scientist. Frederick National laboratory for Cancer Research, March 2024
14. Invited Speaker, CECAM (Centre Européen de Calcul Atomique and Moleculaire) Flagship Workshop on "Making the invisible protein life visible using integrative biophysical approaches: Structural and dynamic characterization of hidden protein states and allosteric regulatory landscapes", Lugano, October 2023
15. Invited Keynote Lecture at the First NHR-Conference at the Freie Universität in Berlin-Dahlem. High-performance computing in the life science. Berlin, September 2023
16. Invited Speaker, to the international symposium entitled "Targeting RAS, new avenues and challenges", Salamanca, Spain, September 2023
17. Invited Keynote Speaker, CECAM Flagship Workshop on "Biomolecular simulation and machine learning in the exascale era: first applications and perspectives". Workshop sponsored by the CECAM-DE-JUELICH node, the CECAM-IT-SIMUL node and the CECAM-IT-SISSA-SNS node. Pisa, Italy, June 2023
18. Invited Speaker, Modeling of Protein Interactions – MPI Lawrence, KS, May 2023
19. Invited Speak, Science and Technology Group, Leidos, Frederick National Laboratory for cancer Research, January 2023
20. Invited Speaker, Kadir Has, Istanbul, Turkey (2022).
21. Invited Keynote Speaker, Biophysical Society of Canada (BSC) Keynote Lecture (in person) at the annual meeting of the BSC, Ottawa, Canada, 2022.
22. Invited Speaker, Hamburg Thematic Meeting, Biophysics at the Dawn of Exascale Computers, Hamburg, Germany, 2022. (due to Covid I did not attend)
23. 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.
24. Invited talk, Drexel University, PA, 2022.
25. Invited colloquium talk, Case Western University, 2022.
26. University of Maryland, Biophysics colloquium, 2022.
27. Plenary Speaker, CRD, Cancer Research and Drug Development, 2021.
28. Invited talk, Biophysical Society Symposium, "Protein Data Bank (PDB) Celebrates 50 Years". Virtual, 2021.
29. 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*.

30. Invited Plenary talk, Memoriam for Prf. Akinori Sarai. Japan, 2021.
31. Invited Plenary talk, ISCB Symposium for STEM students, 2021.
32. Invited talk, Department of Pharmacology at Case Western Reserve University, 2020.
33. Frederick National Laboratory for Cancer Research, Faculty series, 2020.
34. Invited Speaker, American Physical Society Awards Symposium, 2021.
35. Invited Speaker, HITS Colloquium series, Heidelberg, Germany, 2020 (postponed 2021).
36. Invited Speaker, Colloquim, Univ. of Maryland, College Park, 2020 (postponed 2021).
37. Invited speaker, Univ of Pennsylvania Physiology, 2020.
38. 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).
39. Invited speaker, Symposium on Pathomechanisms of Amyloid Diseases, Catania, Italy, 2020 (postponed).
40. Invited Distinguished Speaker, Forschungszentrum Juelich GmbH, Germany, 2020.
41. Invited Speaker, Trieste/Sissa, Italy, 2020 (postponed 2021).
42. Invited Speaker, Biophysical Society thematic meeting, Biophysics at the Dawn of Exascale Computers, Hamburg, Germany, 2020 (postponed 2021).
43. Invited Speaker, The Biophysics Program Seminars series, University of Maryland, College Park, 2020.
44. Invited Speaker, ACS meeting, Philadelphia, 2020.
45. Invited Distinguished University Colloquium Series, "Biophysics Can Help Resolve Biological Mysteries: Examples from Oncogenic Signaling", Koc University, Istanbul, 2020.
46. Invited Speaker, "Systems immunology: Repertoire and beyond". "Beyond": Single cell applications to immunology and structural studies of antibodies. University of Surrey, UK, 2020.
47. Keynote Speaker (following dinner following dinner), 2020 Protein Folding Dynamics Gordon Research Conference, Galveston, Texas, 2020.
48. Invited Speaker, Pathomechanisms of Amyloid Diseases, Miami Beach, Florida, 2019.
49. Invited Commencement MolTag (Molecular Targets) Doctoral Program Opening Event Speaker, University of Vienna, 2019.
50. Invited Speaker, Biochemistry Department Colloquium, the University of Wisconsin-Madison. 2019.
51. Invited Speaker, FAST Foundation (https://fast.foundation/) meeting, Armenia, 2019 (could not attend).
52. Invited Speaker, NCI/CIP and German Cancer Research Center (DKFZ), Bethesda, 2019.
53. Keynote Speaker, IV International Conference on Cancer Research & drug Development, Baltimore, 2019.
54. Invited Speaker, Symposium of the Center of Excellence in Immunology at the NCI, Bethesda, 2019.
55. Invited to speak in the AACR Innovation Summit panel Philadelphia, 2019.
56. Invited Speaker, Cleveland Clinic, Lerner College of Medicine, Case Western Reserve University, 2019.
57. Invited Speaker, ACS meeting, San Diego, 2019.
58. Invited talk Jiangsu University of Technology, Changzhou, China, 2019.
59. Invited Speaker, MIT Math & Computer Science and Artificial Intelligence Laboratory Seminar, 2019.
60. Invited Speaker, BME faculty seminar series featuring prominent nationwide and international scientists, Oregon Health & Science University (OHSU) Biomedical Engineering, Portland, Oregon, 2019.
61. Invited Speaker, ACS meeting, Orlando, Florida, 2019.
62. Invited Speaker, Biophysics Seminar series, The College of Computer, Mathematical, and Natural Sciences, University of Maryland, College Park, 2019.
63. Invited Speaker, Koc University, Istanbul, 2019.
64. Invited Speaker, Pathomechanisms of Amyloid Diseases, Miami, FL, 2018.
65. Invited Speaker, Modeling Protein Interactions, Lawrence, Kansas, 2018.
66. Invited speaker, Univ of Maryland-NCI Partnership Symposium, Univ. of Maryland, College Park, 2018.
67. Invited Speaker, Multiscale simulations of allosteric regulatory mechanisms in cancer-associated proteins and signaling protein networks, Lugano, Switzerland, 2018.
68. Invited Speaker, Cold Spring Harbor Asia Conference entitled "Frontiers in Computational Biology and Bioinformatics 2018." Dushu Lake Hotel and Conference Center, Suzhou, China.

69. Invited Keynote Speaker, Neurological Disorders, Dead Sea, Israel, 2018.
70. The ISCB 2018 Accomplishment Award by a Senior Scientist Award Keynote talk, Chicago, Il, 2018.
71. Invited Keynote KeyLab Award Lecture, workshop on "Recent computational and experimental advances in molecular medicine". Ho Chi Minh City, Vietnam, 2018.
72. Invited Speaker, Towards a Unified Approach to the Analysis and Design of Allostery, Lausanne, 2018.
73. Invited talk, ACS Meeting, Insights into Structure, Function, Dynamics and Evolution of Enzymatic Mechanisms from Computational Simulation. New Orleans, Louisiana, 2018.
74. Invited Speaker, Biophysical Society Meeting, San Francisco, CA, 2018.
75. Invited Speaker, Heidelberg International Chronic Inflammation Workshop, Heidelberg, Germany, 2017.
76. Invited Speaker, "Computational approaches to investigating allostery, Lausanne, Switzerland, 2017.
77. Invited Speaker, Laboratory of Metabolism seminar series, NIH, Bethesda MD 2017.
78. Keynote talk, Brazilian Bioinformatics and Computational Biology Association, San Paulo, Brazil, 2017.
79. Invited Distinguished Speaker, Computer Science Department, Virginia Tech, Blacksburg, Virginia 2017.
80. Invited Speaker, Xingda Lecture Series, the College of Chemistry and Molecular Engineering, Peking University, Beijing, China, 2017.
81. Invited talk, Chemistry Department, Peking University, Beijing, China, 2017.
82. Invited Speaker, ACS Symposium "Molecular recognition: Revealing the effects associated with receptor-ligand binding", Washington DC, 2017.
83. Invited Speaker, International Symposium on Protein Misfolding Diseases, University of Catania, Catania, Sicily, Italy, 2017.
84. Invited Plenary Speaker, Interdisciplinary Signalling Workshop, Visegrad, Hungary, 2017.
85. Invited Speaker, International Conference on Biological Physics (ICBP2017), Symposium on Protein Folding, Misfolding and Structural Prediction Rio de Janeiro, Brazil.
86. Invited Speaker, Computational Aspects of Biomolecular NMR. Gordon Research Conference. Maine, 2017.
87. Invited Speaker, 9th IUPAP International Conference on Biological Physics, Rio de Janeiro, Brazil, 2017.
88. Invited Speaker, ACS meeting, session on Allostery, San Francisco, CA, 2017.
89. Invited seminar speaker, Laboratory of Cell Biology, NIH. Bethesda, MD, 2017.
90. Invited Speaker, NCI-Frederick faculty seminar series, 2017.
91. Invited Keynote Address at the ISCB-Latin America in Buenos Aires. Buenos Aires, Argentina, 2016.
92. Invited Speaker, Copenhagen Bioscience Conference 2017, Novo Nordisk Foundation Denmark, 2017.
93. 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.
94. Invited Plenary talk in a Symposium titled: Advances in Enzymology: Implications in Health, Disease, and Therapeutics. Mumbai, India, 2017.
95. Keynote Speaker, the 2nd Latin American Student Council Symposium (LA-SCS), Buenos Aires, 2016.
96. Invited Keynote Address at the ISCB-Latin America in Buenos Aires. Buenos Aires, Argentina, 2016**.**