IVET BAHAR

Current position
Louis and Beatrice Laufer Endowed Chair Director, Laufer Center for Physical & Quantitative Biology Professor, Department of Biochemistry and Cell Biology Renaissance School of Medicine, Stony Brook University, NY 11794 ivet.bahar@stonybrook.edu; bahar@laufercenter.org https://laufercenter.stonybrook.edu/Faculty/bahar/ Phone: 631 632 5422

EDUCATION

Institution	Degree(s)	Year	Area
Bogazici University, Istanbul, Turkey	BS, MS	1980, 1983	Chemical Engineering
Istanbul Technical University, Turkey	PhD	1986	Chemistry

POSITIONS

Dates	Institution	Department	Title
1/2023 - present	Stony Brook University	Laufer Center for Physical and Quantitative Biology	Louis and Beatrice Laufer Chair and Center Director (1/2023-present)
	Stony Brook U, Renaissance School of Medicine	Biochemistry and Cell Biology	Professor (1/2023 – present)
	U of Pittsburgh School of Medicine	Computational & Systems Biology	Adjunct Professor (1/2023 – present)
3/2001 – 12/2022	University of Pittsburgh, School of Medicine	Department of Computational & Systems Biology	Distinguished Professor (2013 -22)
			Founding Chair (2009 –2022) Professor (2009-2013)
		Department of Computational Biology	John K. Vries Chair (2005 - 2022)
			Founding Chair & Prof (2004-09)
		Mol Gen & Biochem Dept	Professor (2001-2004)
		Center for Computational Biology & Bioinformatics	Founding Director (2001-2004)
2010-2022	U of Pittsburgh	Drug Discovery Institute	Associate Director (2010 - 2022)
2005 - 2022	U of Pittsburgh and Carnegie Mellon U (CMU)	Joint PhD Program in Computational Biology	Co-Founder with RF Murphy, CMU Co-Director (2005-2009) Training Faculty (2005 - 2022)
1986-2001	Bogazici University, School of Engineering	Chemical Engineering Department	Professor (1993-2001) Associate Professor (1987-1993) Assistant Professor (1986-1987)
1992-2001	Bogazici University	Polymer Research Center	Co-founder & Director (1994-2001)
Short-term visits/positions			

1992-2000 (summers)	NIH National Cancer Institute	Lab of Exp & Comp Biol, Division Basic Sci	Fogarty Fellow (1992) and Visiting Professor/Scientist (1993-2000)
1989-1998 (winter breaks)	Ecole Supérieure de Phys & Chimie Paris, France	Laboratoire de Physico-chimie Structurale et Macromoléculaire	Visiting Scientist
1987-1991 (summers)	University of Akron	Institute of Polymer Science	UNESCO Fellow (1987) Visiting Professor (1988-91)

OTHER RECENT AFFILIATIONS

- Director/PI, NIGMS Biomedical Technology & Research Resource on Multiscale Modeling of Biological Systems (MMBioS) (Joint between U of Pittsburgh (Pitt) (lead), Carnegie Mellon U (CMU), Pittsburgh Supercomputing Center & the Salk Institute for Biological Studies (2012-2021)
- Co-PI (with Xiang-Qun Xie (Pitt) and Eric Xing (CMU)) NIDA Center for Computational Drug Abuse Research (CDAR) (Joint between U of Pittsburgh and Carnegie Mellon U) (2014-2020)
- Faculty, Founding Director (2005-2009) and Executive Committee Member, Carnegie Mellon University/Pitt Joint PhD Program in Computational Biology (2005-2022)
- Executive Committee Member, Integrative Systems Biology Program, Pitt (2015-2022)
- Faculty, PhD Program in Structural Biology and Molecular Biophysics (CMU-Pitt) (2005-2023)
- Faculty, Program in Integrative Molecular Biology (PIMB) (2005 - 2014)
- Faculty, Peterson Institute of Nanoscience and Nanotechnology (2005 - 2022)
- Faculty; Pittsburgh Medical Informatics Training Program (2001-2022)
- Faculty Interdisciplinary Biomedical Graduate Program, School of Medicine (2002-2022)
- Member, McGowan Institute for Regenerative Medicine (2002-2022)
- Member, Pitt Center for Simulations and Modeling (SAM) (2008 - 2022).
- Member, Mol & Cellular Cancer Biology Program, UPMC Hillman Cancer Center (2008-2022)
- Member, University of Pittsburgh Center for Protein Conformational Diseases (2016-2022)
- Scientific Committee Member, RiMed Biomedical Research Center, Palermo, Italy (2008-2022)

SCHOLARSHIP

HONORS

- 2024 Society Fellow, awarded by the Biophysical Society 2024
- **Elected Member of the National Academy of Sciences (NAS), USA** **2020-**
- 2022 Vehbi Koc Science Prize 2022
- Kadir Has Foundation Science Award 2019
- 2018 Prose Award for Best Textbook in Biological and Life Sciences 2018
  for "Protein Actions: Principles and Modeling" by Bahar, Jernigan & Dill, 2017
- Invited Speaker at the White House, National Strategic Computing Initiative 2016
- Distinguished Lecturer, TIGP, Academia Sinica, Taiwan 2016
- International Society for Computational Biology (ISCB), Elected Senior Member 2015-
- Chancellor's Distinguished Research Award, U of Pittsburgh 2014
- Distinguished Professor, University of Pittsburgh 2013
- John K. Vries Endowed Chair 2005
- **European Molecular Biology Organization (EMBO) Elected Member** **2000-**

- Excellence in Research Award, Bogazici University 1998
- Turkish Academy of Sciences (TUBA) Principal Member (elected) 1997- 2011
- The Science Academy (BA), Principal Member (elected)[1] 2012-
- TWAS Science Prize (awarded by the President of the Republic, Turkey)[2] 1995
- Sedat Simavi Physical Sciences Prize (joint with B. Erman) 1991
- TUBITAK Chemistry Award for Young Scientists 1990
- UNESCO Fellowship

Other

2022	Steelman Lecturer, U of North Carolina Chapel Hill, Pharmacology Department.
2019	Laureate Lecture Speaker, Pitt Senior Vice Chancellor's Laureate Lecture Series
2016	Distinguished Lecturer TIGP, Academica Sinica, Taiwan
2013	Keynote Speaker, Symposium 'Comput Biology: Then and Today" Weizmann Inst, Israel
2011	Keynote Speaker, ISCB Student Council Symposium, 19th Annu International Conference
2009	Keystone Symposium Organizer on Protein Dynamics, Allostery & Function, Keystone, CO.
2008	Keynote Speaker, ISMB Annual Satellite on Struct Bioinf & Comp Biophys, Toronto
2008	Plenary Lecturer, President's Meeting, Int Soc of Quantum Biol & Pharmacol, Switzerland
2007	First Main Talk; Swiss National Meeting of Biological Sciences
2006	Plenary Lecture; Annual Meeting of the Soc for Math Biology and SIAM Life Sciences

[1]BA is a member of ALLEA (All European Academies; European Federation of Academies of Sciences and Humanities, representing the Academies from over 40 countries in Europe; [2] TWAS: Third World Academy of Science

RESEARCH AREA

Bahar is known for pioneering novel models and methods in structural and computational biology, biochemistry, and molecular biophysics, including the widely used elastic network models (ENMs) for protein dynamics. Application of ENMs to biomolecular systems dynamics, including the interactions of protein, DNA/RNA and lipid molecules with small molecules, revealed mechanisms of substrate- and drug-binding, allosteric regulation, and supramolecular machinery, bridging structure and function. Her studies established fundamental concepts in molecular biology and biochemistry such as the role of entropy-driven fluctuations in mediating signal transmission, enzymatic and transport functions of proteins and their complexes; the evolutionary pressure for selecting structures that enable functional mechanisms; the molecular basis of adaptation to promiscuous interactions and mutations and their implications for precision medicine, personalized therapeutics and molecular design.

In the last decade, she led the development and applications of quantitative molecular and systems pharmacology models and methods, including druggability simulations, pharmacophore modeling, for computer-aided discovery of allosteric modulators, with applications to neurological disorders, cancer biology, lipid-peroxidation-associated ferroptotic or cytotoxic effects, and other diseases. ENMs applied to chromosomal dynamics recently shed light on 4D properties of the chromatin that underlie gene co-expression and regulation. More recently, she has contributed to understanding the molecular origin of multi-inflammatory (long) effects of Covid-19 as well as reduced neutralization ability of antibodies or nanobodies against SARS-CoV-2 variants. She is currently working on anticancer drug development, including in particular the development of immunotherapeutic strategies again triple negative breast cancer, as well as development of modulators of neurotransmitter's transport in the central nervous system.

MAJOR CONTRIBUTIONS TO SCIENCE

The references below refer to publications on pages 25-51 or
https://laufercenter.stonybrook.edu/Faculty/bahar/publications.html#2023

1. Demonstrating the significance of structure-encoded dynamics as a determinant of biomolecular machinery, allostery, and response to small-molecule binding. Our basic premise is: sequence encodes structure, structure encodes dynamics; and dynamics defines mechanisms of function, which in turn feeds back to sequence (evolution) and so on. Thus, 'dynamics' bridges structure and function. Based on this hypothesis, we focused on structural dynamics and developed elastic network modes (ENMs) to elucidate the collective motions of proteins and their complexes/assemblies. ENMs opened the way to efficient characterization of biomolecular systems dynamics, including the cooperative motions of supramolecular systems of 10,000s of residues. We can determine *the* spectrum of motions specific to any architecture as a *unique analytical solution*. Applications to protein-protein[148] and protein-inhibitor[181,203,211] interactions, enzymes[104,145,205] and supramolecular machines,[141,170,180,182] have consistently shown that structural changes involved in biological functions conform to global motions uniquely defined by the fold and predicted by ENMs (for reviews see [168, 188; 191, 242]).

148. Tobi D, Bahar I (2005) "Structural Changes Involved in Protein Binding Correlate with intrinsic Motions of Proteins in the Unbound State" *Proc Natl Acad Sci (USA)* **102**: 18908-1891
181. Bakan A, Bahar I (2009) The intrinsic dynamics of enzymes plays a dominant role in determining the structural changes induced upon inhibitor binding. *Proc Natl Acad Sci USA* **106**: 14349-14354.
188. Bahar I, Lezon TR, Yang LW, Eyal E (2010) Global Dynamics of Proteins: Bridging Between Structure and Function *Annu Rev Biophys* **39**: 23-42
145. Yang L-W, Bahar I (2005) Coupling between Catalytic Site and Collective Dynamics: A requirement for Mechanochemical Activity of Enzymes *Structure* **13**: 893-904
191. Bahar I (2010) On the functional significance of soft modes predicted by coarse-grained models for membrane proteins *J Gen Physiol* **135**: 563-73

2. Elucidating the mechanisms of function of neurotransmitter transporters, their alteration by small molecule modulators and their targeting for therapeutic purposes. We focus on two major families of neurotransmitter transporters, the excitatory amino acid transporters (EAATs) or glutamate transporters, and neurotransmitter: sodium symporters (NSS) that comprise monoamine transporters such as the dopamine transporter (DAT). We demonstrated for the first time the ability of trimeric EAATs to assume a mixed structure with outward- and inward-facing subunits,[204] confirmed later by X-ray. We elucidated mutually exclusive pathways of substrate/Na^+ transport and chloride channeling in EAATs,[260] simulated the complete cycle of dopamine transport by dopamine transporter (DAT),[248] provided insights into the modulation of DAT by PIP_2[316], by amphetamine and cocaine,[240] identified a new Na^+ binding site and its coupling to neurotransmission,[236] performed spatiotemporally realistic simulations of dopamine reuptake at the synapses.[272] Significant efforts are ongoing for discovering allosteric modulators of DAT and EAATs[333], and therapeutic implications of mutations associated with neurodegenerative diseases[332] in collaboration with experimentalists.[376]

204. Jiang J, Shrivastava IH, Watts SD, Bahar I, Amara SG (2011) Large collective motions regulate the functional properties of glutamate transporter trimers *Proc Natl Acad Sci USA* **108**: 15141-6
260. Cheng MH, Torres-Salazar D, Gonzalez-Suarez AD, Amara SG, Bahar I. (2017) Substrate transport and anion permeation proceed through distinct pathways in glutamate transporters. *Elife* **DOI**: 10.7554/eLife.25850
248. MH Cheng, I Bahar (2015) Molecular mechanism of dopamine transport by human dopamine transporter *Structure* **23**: 2171-2181.
240.Cheng MH, Block E, Hu F, Cobanoglu MC, Sorkin A, Bahar I (2015) Insights into the modulation of

dopamine transporter function by amphetamine, orphenadrine, and cocaine binding *Front Neurol* **6**: 134
236. Zomot E, Gur M, Bahar I (2015) Microseconds Simulations Reveal a New Sodium-Binding Site and the Mechanism of Sodium-Coupled Substrate Uptake by LeuT *J Biol Chem* **290**: 544-55
272. Kaya C, ...,, Sejnowski TJ, Sorkin A, Faeder JR & Bahar I. (2018) Heterogeneities in Axonal Structure and Transporter Distribution Lower Dopamine Reuptake Efficiency *eNeuro* **5**(1) ENEURO. 0298-17.2017
316. Belovich AN, Aguilar JI, Mabry SJ, Cheng MH, Zanella D, Hamilton PJ, Stanislowski DJ, Shekar A, Foster JD, Bahar I, Matthies HJG, Galli A. (2019) A network of phosphatidylinositol (4, 5)-bisphosphate (PIP 2) binding sites on the dopamine transporter regulates amphetamine behavior in *Drosophila Melanogaster*. *Molecular Psychiatry* 26, 4417-4430
332. Aguilar JI, Cheng MH, Font J, Schwartz AC, Ledwitch K, Duran A, Mabry SJ, Belovich AN, Zhu Y, Carter AM, Shi L, Kurian MA, Fenollar-Ferrer C, Meiler J, Ryan RM, Mchaourab HS, Bahar I, Matthies HJG, Galli A. (2021) Psychomotor impairments and therapeutic implications revealed by a mutation associated with infantile Parkinsonism-Dystonia. *ELife*, 10, e68039
J376. Hoang Nguyen, Mary Hongying Cheng, JiYoung Lee, S Aggarwal, Ole V Mortensen, **Ivet Bahar** (2024). Allosteric modulation of serotonin and dopamine transporters: New insights from computations and experiments. *Current Research in Physiology*, 10012

3. Unveiling the coupling between structural dynamics and sequence evolution, and the evaluation of the signature dynamics of protein families and the pathogenicity of variants. Evolutionary conservation patterns observed in proteins are often attributed to structural stability (e.g., core contacts), or biochemical activities (e.g., catalysis). On the other hand, conformational *dynamics* is equally important. The motions intrinsically favored by native fold often correlate with those involved in molecular machinery, allosteric regulation, responses to substrate/drug binding, pore opening, etc. suggesting that structures have evolved to favor functional dynamics [171; 189, 194, 210, 228]. We learned that residues that play a mechanical role (e.g. hinge sites) are conserved; global motions (that cooperatively embody the entire architecture of assemblies) are robust and protein families have their own signature dynamics.[287] We also learned that native structures strike a balance between *stability/specificity* and *flexibility/adaptability* to accomplish promiscuous activities and adapt to changing environment and conditions.[243] These findings guide design/intervention strategies through mutually beneficial confluence of structure-based and machine-learning/AI-based studies[361]. An important application is the prediction of the effect of missense variants on biological function, as demonstrated in our recent study of 20,000+ variants.[274]

171. Liu Y, Eyal E, Bahar I (2008) Analysis of correlated mutations in HIV-1 protease using spectral clustering *Bioinformatics* **24**: 1243-50
194. Liu Y, Gierasch LM, Bahar I (2010) Role of Hsp70 ATPase domain intrinsic dynamics and sequence evolution in enabling its functional interactions with NEFs *PLoS Comput Biol* **6**: e1000931
210. Liu Y, Bahar I (2012) Sequence evolution correlates with structural dynamics *Mol Biol Evol***29**: 2253-63
243. Haliloglu T, Bahar I (2015) Adaptability of protein structures to enable functional interactions and evolutionary implications *Curr Opin in Struct Biol* **35**: 17-23
274. Ponzoni L, Bahar I. (2018) Structural dynamics is a determinant of the functional significance of missense variants. *Proc Natl Acad Sci USA* **115**: 4164-4169
287. Zhang S, Li H, Krieger JM, Bahar I. (2019) Shared signature dynamics tempered by local fluctuations enables fold adaptability and specificity. *Mol Biol & Evol* **36**, 2053-2068, 2019
361. Banerjee A, Saha S, Tvedt NC, Yang LW, **Bahar I** (2023) Mutually beneficial confluence of structure-based modeling of protein dynamics and machine learning methods. *Current Opinion in Structural Biology* **78**, 102517

4. Implementation of computational technology for computer-aided drug discovery, chemogenomics, and quantitative systems pharmacology (QSP) using data at the proteome or transcriptome levels. Assisting the broader community to accelerate their drug discovery research by offering user-friendly tools has been a major effort in the Bahar lab. We have implemented the DruGUI and *Pharmmaker*

modules in *ProDy*[199,231] for facilitating druggability simulations[211, 281, 341] and pharmacophore modeling[295], respectively. We also developed new methods and tools for evaluating drug-target interactions, identifying repurposable drugs and side effects [223, 235], or mapping drugs to targets to pathways[301], which found usage in a broad range of applications at both molecular[281, 347] and proteome levels[329]. A recent highlight is the identification of a series of repurposable or investigational drugs against SARS-CoV-2, deduced from computational analysis of the transcriptome of infected SARS-CoV-2 A549 cells, along with the identification of immuno-modulating compounds for suppressing hyperinflammatory responses in severe COVID-19 patients.[337] A class of drug targets on which we have significantly invested are GPCRs, and in particular parathyroid hormone receptors (PTHR) as representative of class B GPCRs and an important target for curing bone diseases and regulating endocrine functions.[310, 347, 359]

223. Cobanoglu MC, Liu C, Hu F, Oltvai ZN, Bahar I (2013) Predicting drug-target interactions using probabilistic matrix factorization *J Chem Inf Model* **53**: 3399-409

211. Bakan A, Nevins N, Lakdawala AS, Bahar I (2012) Druggability assessment of allosteric proteins by dynamics simulations in the presence of probe molecules *J Chem Theory Comput* **8**: 2435-2447.

281. Lee JY, Krieger J, Herguedas B, García-Nafría J, Dutta A, Shaikh SA, Greger IH, Bahar I. (2019) Druggability Simulations and X-ray Crystallography Reveal a Ligand-binding Site in the GluA3 AMPA Receptor N-terminal Domain. *Structure* **27:** 241-252, 2019

301. Li H, Pei F, Taylor DL, Bahar I. (2020) QuartataWeb: Integrated Chemical-protein-pathway Mapping for Polypharmacology and Chemogenomics. *Bioinformatics* **36**:3935-3937.

347. Sutkeviciuta I, Lee JY, White AD, Maria CS, Peña KA, Savransky S, Doruker P, Li H, Lei S, Kaynak B, Tu C, Clark LJ, Sanker S, Gardella TJ, Chang W, Bahar I***** and Vilardaga JP*. (2022) Precise druggability of the PTH type 1 receptor. *Nature Chem Biol. Online ahead of print.*

329. Pei F, Shi Q, Zhang H, Bahar I (2021) Predicting Protein-Protein Interactions Using Symmetric Logistic Matrix Factorization. *J Chem Inf Model* **61**:1670-1682.

337. Chen F, Shi Q, Pei F, Vogt A, Porritt RA, Garcia G, Gomez AC, Cheng MH, Schurdak ME, Chan SY, Arumugaswami V, Stern AM, Taylor DL, Arditi M, **Bahar I**. (2021) A Systems-level Study Reveals Host-targeted Repurposable Drugs Against SARS-CoV2 Infection. *Molecular Systems Biol.* **17**:e10239

347. Sutkeviciuta I, Lee JY, White AD, Maria CS, Peña KA, Savransky S, Doruker P, Li H, Lei S, Kaynak B, Tu C, Clark LJ, Sanker S, Gardella TJ, Chang W, **Bahar I*** and Vilardaga JP*. (2022) Precise druggability of the PTH type 1 receptor. *Nature Chem Biol.* **18**(3):272-280.

359. Vilardaga JP, Clark LJ, White AD, Sutkeviciute I, Lee JY, **Bahar I** (2023) Molecular Mechanisms of PTH/PTHrP class B GPCR Signaling and Pharmacological Implications. *Endocrine Reviews*, **44**, 474-491.

310 Clark LJ, Krieger J, White AD, Bondarenko V, Lei S, Fang F, Lee JY, Doruker P, Böttke T, Jean-Alphonse F, Tang P, Gardella TJ, Xiao K, Sutkeviciute I, Coin I, **Bahar I***, Vilardaga JP* (2020) Allosteric interactions in the parathyroid hormone GPCR-arrestin complex formation. *Nat Chem Biol* **16**(10):1096-1104

5. Unravelling complex protein-protein/lipid interactions implicated in cell regulation and death, with focus on autophagic and ferroptotic responses. Understanding the dynamics of complex systems has been a major focus in our lab for decades, starting with stochastic (Markovian) models for *polymers*[53, 3,12,14-16,19] and protein folding kinetics,[18,120,128] and focusing on cell regulation and death in the past decade[151,233, 266] toward filling the gap between molecular and cellular dynamics. Our laboratory is involved in large-scale collaborative projects toward elucidating the role of mitochondria-mediated lipid (per)oxidation events, and in particular the interactions of PEBP1 with lipoxygenases, in the inflammatory and ferroptotic responses of the cells[222, 265, 325, 334], and inhibition of the peroxidase activity of cytochrome *c* in complexes with cardiolipin[239, 225] or ferroptotic events associated with the activities of the 15LOX/PEBP1 complex responsible for lipid peroxidation.[366]

151. Bagci EZ, Vodovotz Y, Billiar TR, Ermentrout GB, Bahar I (2006) Bistability in Apoptosis: Roles of Bax, Bcl-2, and Mitochondrial Permeability Transition Pores" *Biophys J* **90**: 1546-1559

266. Liu B, Oltvai ZN, Bayir H, Silverman GA, Pak SC, Perlmutter DH, Bahar I. (2017) Quantitative assessment of cell fate decision between autophagy and apoptosis. *Sci Rep* **7**: 17605 PMID: 29242632

222. Chu CT..., Watkins S, Bahar I, Bayir H, Kagan VE (2013) Cardiolipin externalization to the outer mitochondrial membrane acts as an elimination signal for mitophagy in neuronal cells *Nature Cell Biology* **15**: 1197-1205 PMID: 24036476; PMC3806088

265. Wenzel SE, Tyurina YY, ..., Bahar I, Bayir H, Kagan VE. (2017) PEBP1 Wardens Ferroptosis by Enabling Lipoxygenase Generation of Lipid Death Signals. *Cell* **171**: 628-641

325. Sun WY, Tyurin VA, Mikulska-Ruminska K, ..., Greenamyre TJ, Chu CT, Sadovsky Y, Bahar I, Bayir H, Tyurina YY, He RR, Kagan VE. (2021) Phospholipase iPLA$_2$ß averts ferroptosis by eliminating a redox lipid death signal. *Nat Chem Biol* **17**: 465-476.

239. Bakan A, Kapralov AA, Bayir H, Hu F, Kagan VE, Bahar I (2015) Inhibition of Peroxidase Activity of Cytochrome c: De Novo Compound Discovery and Validation *Mol Pharmacol* **88**: 421-7

366. Dar HH, Mikulska-Ruminska K, Tyurina YY, Luci DK, Yasgar A, Samovich SN, Kapralov AA, Souryavong AB, Tyurin VA, Amoscato AA, Epperly MW, Shurin GV, Standley M, Holman TR, St. Croix CM, Watkins SC, VanDemark AP, Rana S, Zakharov AV, Simeonov A, Marugan J, Mallampalli RK, Wenzel SE, Greenberger JS, Rai G, Bayir H, **Bahar I**,* Kagan VE* (2023) Discovering selective antiferroptotic inhibitors of the 15LOX/PEBP1 complex noninterfering with biosynthesis of lipid mediators. *Proc Natl Acad Sci (USA)* **120**, e2218896120

6. Discovering the superantigenic character of SARS-CoV-2 spike, hyperinflammatory reaction, and potential mechanisms of Covid-19 treatment using monoclonal antibodies or repurposable drugs. Since the emergence of Covid-19 in the Fall of 2019, our laboratory deployed significant efforts in understanding the molecular mechanisms of SARS-CoV-2 infection and associated interactions with the host cell immune system. We first focused on the Multisystem Inflammatory Syndrome in Children (MIS-C), which has been later shown to also present similar phenotypes in severely infected adults. We showed that a unique segment on the S1 subunit of SARS-CoV-2 spike possesses superantigenic sequence and structure properties highly similar to those of a bacterial toxin, staphylococcal enterotoxin B (SEB), known to elicit the same type of hyperinflammatory reaction and escalation of cytotoxic adaptive immune response[311]. Analysis of TCR repertoire in severely infected adult Covid-19 patients[311], as well as children with MIS-C[328], demonstrated the occurrence of TCR skewing consistent with the superantigenic reaction that we originally predicted[311] by computational modeling. Notably, the identified superantigenic region coincides with the polybasic S1/S2 cleavage site of the spike monomers, such that targeting this site might interfere with the proteolytic cleavage required for viral entry, thus providing a further mechanism for alleviating SARS-CoV-2 infection. Pursuing this line of thought, we examined[331] the monoclonal antibodies (mAbs) known to neutralize SEB and found that one of them, 6D3, has a higher affinity to bind SARS-CoV-2 superantigenic region and to compete with the human protease furin[331]. Experiments with live virus confirmed the inhibitory capacity of the mAb 6D3, and pointed to its potential utility for possibly treating common colds caused by human coronaviruses that possess a furin cleavage site[331]. Further machine-learning (ML)-based examination of approved and investigational drugs as repurposable compounds for Covid-19 therapy, using as input RNA-seq data SARS-CoV-2-infected A549 cells, led to the identification of a series of drug candidates, including immuno-modulating compounds, several of which exhibited antiviral activities in Vero-E6 cells[337]. Finally, more recently, we carried out an extensive study to identify which mAbs retain their neutralization power against SARS-CoV-2 variants of concerns (alpha, beta, gamma, and delta) providing a computing framework for rapid assessment of the effectiveness of existing mAbs and nanobodies for neutralizing current and future variants and potentially developing pan-sarbecovirus mAbs[346].

311. Cheng MH, Zhang S, Porritt RA, Rivas MN, Paschold L, Willscher E, Binder M, Arditi M, **Bahar I** (2020) Superantigenic character of an insert unique to SARS-CoV-2 spike supported by skewed TCR repertoire in patients with hyperinflammation. . *Proc Natl Acad Sci USA* **117**: 25254-25262 PMID: 32989130 PMCID: PMC7568239

328. Porritt RA, Paschold L, Noval Rivas M, Cheng MH, Yonker LM, Chandnani H, Lopez M, Simnica D, Schultheiß C, Santiskulvong C, van Eyk J, McCormick JK, Fasano A, **Bahar I**, Binder M, Arditi M (2021) HLA class I-associated expansion of TRBV11-2 T cells in Multisystem Inflammatory Syndrome in Children.. *J Clin Invest*. **131**(10). PMID: 33705359 PMCID: PMC8121516

331. Cheng MH, Porritt RA, Rivas MN, Krieger JM, Ozdemir AB, Garcia G Jr, Arumugaswami V, Fries BC, Arditi M, **Bahar I**. (2021) A monoclonal antibody against staphylococcal enterotoxin B superantigen inhibits SARS-CoV-2 entry in vitro.. *Structure*. **29(9)**:951-962 PMID: 33269352 PMCID: PMC7709177

337. Chen F, Shi Q, Pei F, Vogt A, Porritt RA, Garcia G, Gomez AC, Cheng MH, Schurdak ME, Chan SY, Arumugaswami V, Stern AM, Taylor DL, Arditi M, **Bahar I**. (2021) A Systems-level Study Reveals Host-targeted Repurposable Drugs Against SARS-CoV2 Infection. *Molecular Systems Biol*. **17**:e10239 PMID: 34339582 PMCID: PMC8328275

346. Cheng MH, Krieger JM, Banerjee A, Xiang Y, Kaynak B, Shi Y, Arditi M, Bahar I (2022) Impact of new variants on SARS-CoV-2 infectivity and neutralization: A molecular assessment of the alterations in the spike-host protein interactions *iScience*. 25(3):103939. PMID: 35194576

TECHNOLOGY DEVELOPMENT AND DISSEMINATION

Resource	Purpose	Publication, statistics, hyperlink
ProDy (API with multiple modules such as *Evol*,, *DruGUI*, and ESSA)	Biomolecular dynamics based on elastic network models (ENMs), comparison with sequence evolution, with applications to essential site determination and druggability	Zhang et al., Bioinformatics 2021; Bakan et al, *Bioinformatics* 2011; *Bioinformatics*, 2014; Zhang et al. *Bioinformatics* 2021 (more than 2.1 million downloads, 150,000+ unique users) http://prody.csb.pitt.edu/
ANM server	Equilibrium motions (animations) of resolved structures using the anisotropic network model	Eyal et al *Bioinformatics* 2015; ibid *Bioinformatics* 2006 http://anm.csb.pitt.edu/
DynOmics	Structural proteome scale ENM analyses of large assemblies including environment	Li et al., *Nucleic Acids Res* 2017 http://dynomics.pitt.edu/
BalestraWeb	Quantitative systems pharmacology	Cobanoglu et al *J Chem Inf Modeling* 2013 and *Bioinformatics* 2015 http://balestra.csb.pitt.edu/
iGNM	Database of protein motions	Yang et al Bioinformatics 2005; Li et al *Nucleic Acids Res* 2016 http://ignm.ccbb.pitt.edu/
Rhapsody	Prediction of the biological effect (neutral or deleterious) of point mutations in proteins	Ponzoni & Bahar, *Proc Natl Acad Sci USA* 2018; Ponzoni et al., *Bioinformatics*, 2020 http://rhapsody.csb.pitt.edu/
QuartataWeb	Integrated chemical-protein-pathway mapping for polypharmacology and chemogenomics	Li, Pei, Taylor and Bahar, *Bioinformatics* 2020.
SignDy	Signature dynamics: shared and specific features of family and subfamily members	Zhang, Li, Krieger and Bahar, *Mol Biol Evol* (2019) http://prody.csb.pitt.edu/signdy/
CryoDy	Collective dynamics of cryo-EM structures using electron density maps in the EMDataBank	Zhang et al *Prog Biophys Mol Biol* 2020 http://prody.csb.pitt.edu/cryody/
Pharmmaker	*In silico* construction of pharmacophore models for target proteins using statistical data from druggability simulations	Lee, Krieger, Li and Bahar *Protein Sci* 2020 **http://prody.csb.pitt.edu/pharmmaker/**

PUBLICATIONS

- Total number of publications: 405, listed in Supplemental Information pages 25-51, consisting of
  - 378 papers in peer-reviewed journals (see https://www.ccbb.pitt.edu/Faculty/bahar/publications.html#2021)
  - 1 textbook (Bahar, Jernigan & Dill "Protein Actions: Principles & Modeling" 2017)
  - 16 contributions (chapters) to edited books
  - 1 edited book (Cui & Bahar, Eds "Normal Mode Analysis: Theory and Applications to Biological and Chemical Systems" Chapman & Hall/CRC, 2005)
  - 8 *BiorXiv* reports
  - 1 editorial

- Total number of citations and H-index
  - 36,269 citations as of June 17, 2024 (Google Scholar_
  - H index: 93 (https://scholar.google.com/citations?user=jXWewPgAAAAJ&hl=en&oi=ao)

- 12 Selected Papers (2018-2024):

Year	Publication
2024	Banerjee A, Mathew S, Naqvi MM, Yilmaz SZ, Zacharopoulou M, Doruker P, Kumita JR, Yang SH, Gur M, Itzhaki LS, Gordon R, **Bahar I** (2024) Influence of point mutations on PR65 conformational adaptability: Insights from molecular simulations and nanoaperture optical tweezers . *Science Advances*, 10(22):eadn2208.
2022	Cheng MH, Krieger JM, Banerjee A, Xiang Y, Kaynak B, Shi Y, Arditi M, **Bahar I** (2022) Impact of new variants on SARS-CoV-2 infectivity and neutralization: A molecular assessment of the alterations in the spike-host protein interactions. *iScience* **25**(3):103939. PMID: 35194576 PMCID: PMC8851820
2021	Sutkeviciuta I, Lee JY, White AD, Maria CS, Peña KA, Savransky S, Doruker P, Li H, Lei S, Kaynak B, Tu C, Clark LJ, Sanker S, Gardella TJ, Chang W, Bahar I* and Vilardaga JP*. (2022) Precise druggability of the PTH type 1 receptor. *Nature Chem Biol.,* published online on Dec 23, 2021
2021	Chen F, Shi Q, Pei F, Vogt A, Porritt RA, Garcia G, Gomez AC, Cheng MH, Schurdak ME, Chan SY, Arumugaswami V, Stern AM, Taylor DL, Arditi M, Bahar I. (2021) A Systems-level Study Reveals Host-targeted Repurposable Drugs Against SARS-CoV2 Infection. *Molecular Systems Biol.* 17: e10239
2021	Cheng MH, Porritt RA, Rivas MN, Krieger JM, Ozdemir AB, Garcia G Jr, Arumugaswami V, Fries BC, Arditi M, Bahar I. (2021) A monoclonal antibody against staphylococcal enterotoxin B superantigen inhibits SARS-CoV-2 entry *in vitro*. *Structure* 29:951-962
2020	Cheng MH, Zhang S, Porritt RA, Rivas MN, Paschold L, Willscher E, Binder M, Arditi M*, Bahar I* (2020) Superantigenic character of an insert unique to SARS-CoV-2 spike supported by skewed TCR repertoire in patients with hyperinflammation. *Proc Natl Acad Sci USA* 117: 25254-25262
2020	Li H, Pei F, Taylor DL, Bahar I. (2020) QuartataWeb: Integrated Chemical-protein-pathway Mapping for Polypharmacology and Chemogenomics. *Bioinformatics* 36:3935-3937.
2020	Zhang S, Chen F, Bahar I**.** (2020) Differences in the Intrinsic Spatial Dynamics of the Chromatin Contribute to Cell Differentiation. *Nucleic Acids Res* 48, 1131-1145.
2019	Taylor DL, Gough A, Schurdak ME, Vernetti L, Chennubhotla CS, Lefever D, Pei F, Faeder JR, Lezon TR, Stern AM, Bahar I. (2019) "Harnessing Human Microphysiology Systems as Key Experimental Models for Quantitative Systems Pharmacology" in *Handbook Exp Pharmacol*, 260:3 27-367
2019	Cheng MH, Ponzoni L, Sorkina T, Lee JY, Zhang S, Sorkin A**,** Bahar I. (2019) Trimerization of Dopamine Transporter Triggered by AIM-100 Binding: Molecular Mechanisms and Effect of Mutations. *Neuropharmacology* 161:107676

2019	Zhang S, Li H, Krieger JM, Bahar I. (2019) Shared signature dynamics tempered by local fluctuations enables fold adaptability and specificity. *Mol Biol Evol* 36: 2053-2068.
2018	Ponzoni L, Bahar I. (2018) Structural dynamics is a determinant of the functional significance of missense variants. *Proc Natl Acad Sci USA* 115: 4164-4169

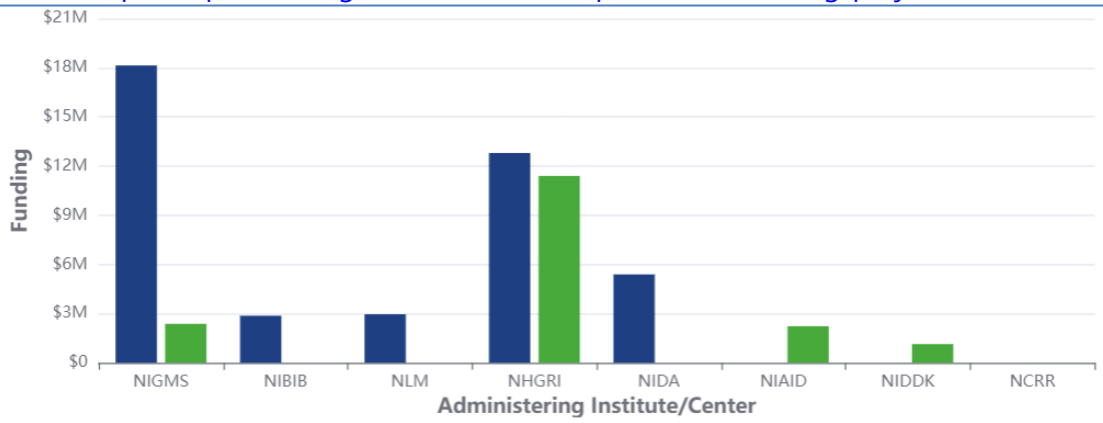
(*) equal contribution

PATENTS and INVENTION DISCLOSURES

- High Performance Biodegradable Materials from Oriented Starch Derivatives, B. Erman, J. E. Mark, B.Z. Paterson, I. Bahar & A. Kloczkowski. US Patent #6,218,532 B1 (2001).
- COMPOSITIONS AND METHODS FOR TREATING A COVID-19 INFECTION University Ref. No. 05404 and a US Nonprovisional Patent Application (MCC Ref: 10504-052US1) (Lead lab: Bahar lab) (2020) US Patent App. 17/375,601 (2022) US Patent # 11,746,144
- NOVEL APPROACH FOR THE DISCOVERY OF REPURPOSED DRUGS AND COMPOUNDS FOR TREATMENT AGAINST SARS-COV-2 INFECTION. (2) University Ref. No: 05579; Application #: PCT/US2022/013449 Lead lab: Bahar lab, with the participation of MH Cheng, Pen Fei, Qingya Shi and Fangyuan Chen) Other inventors: Moshe Arditi (Cedars Sinai), Andy Stern, Andreas Vogt, Mark Schurdak and Lans Taylor (U of Pitt Drug Discovery Institute). Filing date Jan 4, 2022. *US Patent App.* **18/273,161**
- USE OF (6,7-DIHYDROXY-2-OXO-2H-CHROMEN-4-YL) METHYL 4-OXO-3-PHENYL3,4-DIHYDROPHTHALAZINE-1-CARBOXYLATE TO ACTIVATE NCOA7 AND TREAT INFLAMMATORY CARDIOPULMONARY DISEASE (Pitt Ref No. 05948) Innovators: Stephen Yu-Wah Chan (University of Pittsburgh); Ivet Bahar (University of Pittsburgh); Lloyd David Harvey (University of Pittsburgh) (2022)
- SMALL MOLECULE ALLOSTERIC MODULATORS OF CLASS B GPCR, THE PTHR, AND METHOD TO IDENTIFY THEM" (Pitt Ref: 05559). Innovators: Jean-Pierre Vilardaga, Ivet Bahar, Ieva Sutkeviciute, Jiyoung Lee and Burak Kaynak (University of Pittsburgh) (2022) *US Patent App.* **18/277,765**

GRANT AWARDS – FUNDED PROJECTS (*)

Below we present the funding summary for Ivet Bahar accessible at the NIH reporter site as of Jan 2023, https://reporter.nih.gov/search/F_1k7L6pMkGbs6Xnuf8z2g/projects/charts



Note: Please note that if the hit list contains both a subproject and its parent grant, the subproject funding is already included in the parent project funding amount.

* Funding data available only for NIH, CDC, FDA, AHRQ, and ACF.

Administering Institute/Center	Projects	Total Funding	Sub Projects	Sub Project Funding
NIAID			10	$2,230,204
NIDDK			7	$1,139,551
NCRR			3	$1,881
NIBIB	10	$2,870,306		
NLM	8	$2,960,050		
NIDA	5	$5,390,558		
NHGRI	8	$12,799,098	20	$11,401,540
NIGMS	24	$18,142,500	9	$2,375,849
Total	**55**	**$42,162,512**	**49**	**$17,149,025**

(*) the total funding awarded to NIH projects and subcontracts in which Ivet Bahar served as Project PI/MPI or Subcontract PI, since 2002 (as of Feb 2023). The respective total amounts are $42M and $17M. The bar plot shows the distribution of the projects among NIH institutes (NIGMS, NIBIB, NIDA, NHGRI, NLM, NIAID, NIDDK and NCRR).

The table below provides information on these (NIH-funded) and additional (NSF- and HFSP-funded) projects. See more information in the Suppl Information pages 60-64.

Funding Agency	Title (PI/Role)	Years
NIH-NIDDK R01	Structure and function of PTH class B receptor (MPI: Vilardaga* and Bahar)	2023-27
NIH-NIGMS R01	Toward a deeper understanding of allostery and allotargeting by computational approaches (MPI: Bahar* and Doruker)	2021-25
HFSP RGP0027/ 2020 (Human Front in Sci Prog)	Biological springs as allosteric modulators: Information transfer across repeat-protein arrays (MPI: Bahar (Pitt), Itzhaki (University of Cambridge, UK); Reuven Gordon (Victoria U, Canada); Shang-hua Yang (National Tsing Hua U, Taiwan).	2020-23

NIH-NCI R01	Targeting posttranslational modifications of B7-H4 in carcinogenesis and therapy (PI: Yong Wan, Emory U; Role: co-I)	2021-26
NIH-NCI R01	Targeting interplay between KLF4 and PRMT5 in carcinogenesis (PI: Yong Wan, Emory U; Role: co-I)	2021-26
NIH-NIGMS - P41	NIGMS Biomedical Technology and Research Center (BTRC) on High Performance Computing for Multiscale Modeling of Biological Systems (MMBioS) (PI: Bahar 2012-21; Faeder 2021-22)	2012-22
NIH-NIBIB - T32	Integrated, Interdisciplinary, Inter-University PhD Program in Comp Biology (CPCB) (PIs: Faeder, Bahar, Bar-Joseph, Russell)	2009-23
NIH- NIGMS R01	Controlling Monolysocardiolipin/cytochrome c peroxidase complexes in Barth Syndrome (PI: Greenberg, Wayne State); co-I	2020-22
NIH- NIMH R56	Allosteric modulation of dopamine transport-functional and biochemical studies (PI: OV Mortensen, Drexel U) (Role: co-I)	2020-22
NIH-NINDS R01	Druggable Mitochondrial Targets for Treatment of Cerebral Ischemia (PIs: Clark and Bayir, UPMC) (Role: co-I)	2020-25
NIH-NIDDK – P01	New Therapies for Liver Fibrosis and Hyperproliferation in α1-AT Deficiency (PI: Perlmutter (Wash U); Role: Comp Pharm Core PI	2012-24
NIH-NHLBI-P01	Immunosuppression in acute lung injury (PI: Rama Mallampalli (Ohio State U); Role: co-I)	2019-24
NIH – NIDA- P30	NIDA Center of Excellence for Computational Drug Abuse Research (CDAR) (MPI: Xie, Bahar, and Xing)	2014-20
NIH-NIAID - U19	Signature-directed, sequential delivery of radiation mitigators (former Mitochondrial Targeting for Radiation Mitigation (PI: Greenberger (UPMC); Role: Chemoinformatics Core PI)	2010-20
NIH - NHGRI U54	BD2K (Big Data to Knowledge) Center for Causal Modeling and Discovery (CCD) (MPI: Bahar and Cooper)	2014-19
NIH-NIGMS - R01	Development of Protein Dynamics Software ProDy (PI: Bahar)	2012-16
NIH-NIGMS - R01	Structural Dynamics of Biomolecular Systems (PI: Bahar)	2009-14
NIH-CTSI-Pilot	Identification of drug candidates for PTHR (MPI: Bahar & Vilardaga	2019-20
NIH-NLM – R01	Bridging Sequence Patterns and Structural Dynamics (PI: Bahar)	2003-13
NIH-NCI – R01	Structure-based Design of Novel Small Molecule c-Myc Inhibitors (Role: co-Investigator; PI: Prochownik)	2009-14
NIH- NCRR – UL1	Clinical & Translational Science Institute (Role: Molecular and Systems Modeling Core Co-Director, with Faeder and Benos)	2011-13
NIH – NIMH – R01	Molecular Studies of Human CNS Transporters (PI: Amara; Role: co-investigator)	2007-13
NIH-NIGMS – U54	Membrane Protein Structural Dynamics Consortium (PI: Perozo; Role: Computational Core co-investigator)	2010-12
NIH-NIBIB & NSF	Bioengineering & Bioinformatics Summer Institute on Simulation & Comp Visualization of Biol Sys at Multiple Scales (PI: Bahar)	2002-10
NIH-NIGMS – R33	Computational Prediction of Biomolecular Dynamics (PI: Bahar)	2005-08
NIH-NCI – P01	Dendritic Cell Biology and Therapy (PI: Finn; role: co-I)	2004-09
NIH- NIMH – U54	Pittsburgh Molecular Libraries Screening Center (Bioinformatics PI: Lazo; Role: Cheminformatics Core PI)	2005-08
NIH-NIGMS – P20	Multiscale Dynamics of Cell Control and Apoptosis (PI: Bahar)	2003-07
NSF-ITR	Computational Learning and Discovery for Protein Sequence, Structure & Function Mapping (PI: Reddy, CMU; role: co-I)	2002-07

RECENT PLENARY LECTURES AND INVITED TALKS

The complete list of seminars and invited talks at conferences/meetings in reverse chronological order is accessible online at https://laufercenter.stonybrook.edu/Faculty/bahar/conference.html

- Keynote talks or plenary lectures (2006- 2020)
  - 2020 Protein Folding & Dynamics Webinar Lecture Series, Weizmann Institute of Science
  - 2019 Laureate Lecture Series. University of Pittsburgh School of Medicine (Dec 2019)
  - Keynote speaker. Biological Physics International Conference, Mexico City, Mexico. (Sept 2019)
  - Session Organizer and Speaker, .Inaugural International Transmembrane Transporter Society (ITTS) Symposium. Vienna, Austria. September 18-21, 2018
  - Plenary Speaker at the IV International Interdisciplinary Applied Mathematics, Modeling and Computational Science (AMMCS) Conference, Waterloo (August 2017)
  - Keynote Speaker, Workshop on Computational Biophysics and Systems Biology (CBSB2017), Cincinnati, OH (May 2017)
  - Distinguished Lecturer, 2016 Taiwan International Graduate Program, Hosted by Academia Sinica, Taiwan (Sept 2016)
  - Invited Speaker at the National Strategic Computing Initiative Anniversary Workshop. White House, Washington, DC. Invited Speaker (July 2016)
  - Invited Speaker. 8th SFB35 Transmembrane Transporters in Health and Disease Symposium, Vienna, Austria. (Sept 2015)
  - Levinthal Lecturer. CUP XV OpenEye Scientific Software's Annual Meeting, Santa Fe, (March 2015)
  - Invited Speaker. Israeli Society for Biochemistry and Molecular Biology Meeting on "Molecular Machines in Action". Weizmann Institute of Science, Rehovot, Israel. Dec 2014)
  - Speaker at the Symposium on "Computational Biology: Then and Today". Weizmann Institute of Science, Rehovot, Israel (May 2013)
  - Plenary Speaker at the GLBIO (Great Lakes Bioinformatics Conference of the International Society for Computational Biology). Carnegie Mellon U (May 2013)
  - Session Chair and Discussion Leader at the Gordon Research Conference on Stochastic Physics in Biology, Ventura, XA (Jan 13-18, 2013)
  - Featured Speaker for the Annual COB (Comp Biol) Day, NYU Courant Institute, Dec 5, 2009.
  - Keynote Speaker at ISMB Annual Satellite Meeting on Structural Bioinformatics and Computational Biophysics (3DSig 2008), Toronto. (July 18-19, 2008)
  - Plenary Lecturer at the President's Meeting of the International Society of Quantum Biology and Pharmacology (ISQBP) at the Centro Stefano Franscini, Ascona, Switzerland. (June 8-13, 2008)
  - First Main Talk at Swiss National Meeting of Biological Sciences, Symposium on "Potassium channels: molecular biology, pathophysiology and models", Basel, Switzerland.) (http://www.swissheartnet.unibe.ch/) (March 13, 2007)

- Plenary Lecture at the Annual meeting of the Society for Mathematical Biology, joint with the Society for Industrial and Applied Math (SIAM) Life Sciences at NCSU, Raleigh (North Carolina) (http://www.siam.org/meetings/ls06/invited.php (July 31-August 3, 2006).

Other invited talks at international and national meetings (2017 - 2020)

- Invited Lecturer 20th International Congress of IUPAB (International Union for Pure and Applied Biophysics), the 45th Annual SBBf (Brazilian Biophysical Society), and the 49th Annual Brazilian Biochemistry and Molecular Biology Society Meeting. Foz do Iguaco, Brazil. Oct 26-30, 2020.
- Invited Speaker at the Biophysical Society thematic meeting, "Biophysics at the Dawn of Exascale Computers". Hamburg, Germany. May 15-20, 2020
- Invited Speaker "2020 Chromatin Modeling: Integrating Mathematics, Physics, and Computation for Advances in Biology and Medicine". Research Centre of the Schrödinger International Institute for Mathematics and Physics (ESI); Vienna, Austria. March 16-20, 2020
- Invited Speaker at Jacques Monod Conference, Ligand-gated ion channels from atomic structure to synaptic transmission. Roscoff, France, Invited Speaker. May 20-24, 2019
- Seminar. National Institute of Health (NIH) National Institute on Drug Abuse (NIDA) Intramural Research Program (IRP) Seminar Series. May 13-14, 2019.
- Invited Speaker. Multiscale Modeling of Chromatin: Bridging Experiment with Theory. (Biophysical Society Thematic Meeting.) Les Houches, France March 31-April 5, 2019
- Invited Speaker at 63rd Annual Meeting of the Biophysical Society, Symposium on Glutamate Receptors. Baltimore, MD, March 2-4, 2019.
- Invited Speaker Conference on Modeling of Protein Interactions (MPI). Lawrence, Kansas. November 8-10, 2018
- Invited Speaker at CECAM (Centre European pour le Calcul Atomique et Moléculaire) Workshop, "Multiscale simulations of allosteric regulatory mechanisms in cancer-associated proteins and signaling protein networks," Lugano, Switzerland. October 15-17, 2018
- Invited Speaker at CECAM Workshop, "Normal modes of biological macromolecules: methods and applications," Paris, France, September 12-14, 2018
- Invited Speaker at "CONES2018: Frontiers of Non-Equilibrium Science" Conference, London, UK. June 25-27, 2018
- Invited Speaker, Royal Society Discussion Meeting, 'Allostery and Molecular Machines', Royal Society Headquarters, London, UK (June 2017)
- Invited Speaker at the International meeting on Molecular Perspectives on Protein-Protein Interactions (PPI2017), Eilat, Israel, Dec 3-7, 2017
- Invited Speaker at CECAM Workshop, "Computational Approaches to Investigating Allostery", Lausanne, Switzerland. Oct 30-Nov 1, 2017
- Invited Speaker at the "5th International BAU Drug Design Conference", Istanbul, Turkey, Oct 19-21, 2017
- Invited Lectures at the 5th Edition of the Brazilian Molecular Modelling School, Sao Paolo, Brazil. August 7-11, 2017
- Invited Speaker at the Gordon Research Conference (GRC) Computational Aspects - Biomolecular NMR, Grand Summit Hotel, Newry, ME. June 11-14, 2017.
- Invited Lecturer at Harvard U, Boston U and MIT (three lectures as Greater Boston Theoretical Chemistry Lecture, May 10-12, 2017.

- Invited Symposium Speaker at the 253rd National Meeting, American Chemical Society, San Francisco, CA, April 2-6, 2017.
- Seminar at UCLA Cedars Sinai Medical Center, Los Angeles, CA. March 30, 2017

See other talks in the Supplemental Information pages 52-59

MEMBERSHIPS IN PROFESSIONAL AND SCIENTIFIC SOCIETIES

International Society for Computational Biology (ISCB)	2001-present
Biophysical Society	2001-present
Protein Society	1999-present
American Association for the Advancement of Science (AAAS)	1995-present
American Chemical Society (ACS)	1987-present
International Society of Quantum Biology and Pharmacology (ISQBP)	2008-present
International Transmembrane Transporter (ITT) Society	2017-present

TEACHING

EDUCATIONAL LEADERSHIP AND ACTIVITIES

- **Founding Director of the Carnegie Mellon University/ University of Pittsburgh PhD Program in Computational Biology (CPCB)** in 2005. This is a program jointly offered between U Pitt and Carnegie Mellon University (CMU), selected for HHMI/NIBIB Interfaces Initiative Award (http://www.ccbb.pitt.edu/compbio/), and continuously funded by NIBIB T32 award since its inception. Dr. Bahar conceived and initiated this interdisciplinary program, has played a key role in designing and refining the curriculum, as well as all policies and rules for a joint cross-institutional program. This was the *first* PhD degree granting program jointly launched/offered between the two universities and served as a model for many others that followed this program.

- **Founding Director of the NSF/NIBIB funded BBSI** (Bioengineering and Bioinformatics Summer Institute; http://www.ccbb.pitt.edu/bbsi/) on "Simulation and Computer Visualization of Biological Systems at Multiple Scales", between 2002-2009, an effort in collaboration between Pitt, CMU, Pittsburgh Supercomputing Center and Duquesne University for introducing computational biology topics and methods to undergraduate students before they make career decisions. This program has been now succeeded by the NSF REU TecBio under the leadership of Dr. Joe Ayoob (PI) and has been continually funded by NSF since then. More than 90% of students attending these summer programs in the last decade have been selected from underrepresented or underserved groups.

- **Completed a graduate textbook** *Protein Actions: Principles and Modeling*, co-authored by Ivet Bahar, Robert L Jernigan and Ken A. Dill, Garland Publ, transferred to Taylor & Francis (2017), written to fill the need for a rigorous and comprehensible graduate textbook in this area.

- Invited speaker in meetings aiming at promoting interdisciplinary education and innovative research training, or **organized by graduate student**s, such as:

- Invited Lecturer at NIH/ISMB (Intelligent Systems for Molecular Biology co-organized session at the ISMB 2020 International Annual meeting, to give a talk on "Reflections and Lessons from 15 Years of Training Computational Biologists" .
- Distinguished Lecturer selected by Taiwan International Graduate Program, hosted by Academia Sinica (Sept 2016)
- ISCB Student Council Symposium Keynote Speaker at the 19th Annual Conference on Intelligent Systems for Molecular Biology (ISMB) and the 10th Annual European Conference on Comput Biology (ECCB), Vienna (June 2011)
- MERCURY National Conference on Undergraduate Computational Chemistry, Hamilton College, Clinton, NY (August 1-3, 2010)
- 22nd Annual Student Sponsored Symposium organized by NIH-funded Cell and Molecular Biology and Molecular Biophysics Programs, at the University of Illinois, Keynote Speaker (Oct 16-17, 2009)

- Teaching or co-teaching courses at all levels (undergraduate, masters and doctoral), on a broad range of topics, from statistical thermodynamics to material science, structural biology, pharmacology, in five different programs during the last three decades.

COURSES

Bogazici University; 1987-2001

Design and Simulation of Biomolecular Systems (*)
Computational Models and Methods in Structural Biology (*)
Physical Chemistry II
Thermodynamics
Advanced Fluid Mechanics. Transport Phenomena
Conformational Statistics of Macromolecules (*)
Introduction to Chemical Engineering
Introduction to Polymer Engineering
Numerical Methods in Chemical Engineering
(*) new Chem Eng elective courses initiated by I.Bahar at Bogazici University

U of Pittsburgh, 2002-

Introduction to Computational Structural Biology (joint with Camacho) (2001-2004) [(1)]
Computational Structural Biology & Molecular Biophysics II (joint with Drs. Zuckerman and Camacho) (2005-2018) [(1), (2)]
Drug Discovery and Development [(1)] (2012-17) (served as course coordinator & lecturer with the leadership of the UPDDI).
Drug Discovery—Challenges and Opportunities (fall 2014) (served as course coordinator & lecturer in Computations in Drug Discovery, and Drug Repurposing & Polypharmacology)
[(1)] *newly designed course*
[(2)] *required/core course in both Comp Bio and Struct Bio PhD programs*

PHD STUDENTS

- Completed the supervision of **20 PhD students in 5 different programs**, three institutions. Below is the list of students, with their current affiliation, thesis title and graduation year.

Chemical Engineering, Bogazici University (5 PhD students):

- Turkan **Haliloglu** (Professor at Bogazici U Chem Eng Dept, and Director of the Polymer Research Center), "Conformational Statistics and Dynamics of Polymer Chains Using the Rotational Isomeric State Formalism" (1992);
- Pemra **Doruker** (former Chair of Chemical Engineering Department at Bogazici U, Istanbul) "Molecular Dynamics Study of Macromolecular Motions and Polypeptide Helices" (1995);
- Canan (**Baysal**) **Atilgan** (Professor and Dean at Sabanci U, Istanbul; and President of the Academy of Sciences in Turkey) "Efficient Computational Models and Methods for Investigating Local Polymer Dynamics" *(co-advisor: B. Erman)* (1996);
- Ozlem **Keskin** (Professor and Department Chair at Koc University, Istanbul), "Computer-Aided Characterization of Proteins and Anticancer Agents" (1999); and
- Banu **Ozkan** (Professor and Center Director at Arizona State University, Physics Dept) "Modeling and Simulation of Protein Folding Kinetics" (2001)

Molecular Genetics & Biochemistry, School of Medicine, U of Pittsburgh (3 PhD students

- Lee-Wei **Yang** (Professor and Program Director at Tsinghua U Chemical Engineering Dept, Taiwan) "Biomolecular dynamics revealed by elastic network models and they study of mechanical key sites for ligand binding" (2005)
- Zerrin **Bagci** (Associate (tenured) Professor at Namik Kemal U, Turkey) "Mathematical Modeling and Simulation of Apoptosis and Nitric Oxide Effects) (2007)
- Basak **Isin** (Product Development and Strategy, CATALYST) "The Activation Mechanism of Rhodopsin Explored by Multiscale Methods" (2007)

Physics & Astronomy, School of Arts & Sciences, U of Pittsburgh (1 PhD student)

- Zheng **Yang** (Co-founder & CEO, Quanovate Inc., San Francisco) "Symmetry, Dynamics and Function: Biological Macromolecules Studied by Elastic Network Models" (2009)

Computational Biology, Joint Program of Carnegie Mellon U and U Pitt (10 PhD students)

- Ahmet **Bakan** (Senior Software Designer, Google) " Dynamics of Protein-Drug Interactions inferred from Structural Ensembles and Physics-Based Models: Application to MAPK phosphatases" (2009)
- Lidio **Meireles** (Research Associate II at Vertex Pharmaceuticals, Boston) "Rational Design of Small-Molecule Inhibitors of Protein-Protein Interactions: Application to Oncogenic c-Myc/Max Interaction" (2011)
- Ying **Liu** (Senior Data Analyst, Google) "Combining Sequence and Structure Information to Model Biological Systems Dynamics" (2011)
- Anindita **Dutta** (Principal Deep Learning/A Engineer, Illumina, CA) "Dynamics of ionotropic glutamate receptors: Comparison of AMPA and NMDA receptors" (2013)
- Murat Can **Cobanoglu** (UT Southwestern, Distinguished Fellow) "Probabilistic latent factor models for transformative drug discovery" (2015)
- Cihan **Kaya** (Director, Informatics and Scientific Computing, Sonic HealthcareA) "Multiscale modeling of neurobiological signal transmission: dopamine transport" (2018)
- She **Zhang** (OpenEye, Senior Software Developer) ""Elastic network models in biology: From protein mode spectra to chromatin dynamics" (2020)
- Fen **Pei** (Roivant Sciences, investigator) "Drug-Target-Pathway Mapping for Polypharmacology and Chemogenomics" (2020)
- Bentley M **Wingert** (Research Associate, New Equilibrium Biosciences) "Evaluation and Application of Computational Strategies For Exploring The Dynamics and Small-Molecule Binding Properties of Proteins" (2021)
- Yan **Zhang** (Research Associate at Illumina, San Francisco "Dynamics of Biological Systems at Molecular and Cellular Levels: (2022)

Molecular Biophysics & Structural Biology, Joint Pitt/CMU Program (1 PhD student)

- Lin **Liu** (Remegen Biosciences, Senior Scientist) (co-mentored with A. M. Gronenborn) "Conformational Dynamics of Proteins: Insights from Structure & Computations " (2011).

- Currently supervising three students: Haotian (Frank) Zhang, enrolled in the CMU/Pitt PhD Program in Comp Biology; Zakaria Dahmani at the Integrative Systems Biology Program, both at the U of Pittsburgh; and Satoshi Satya at the Biochemistry and Cell Biology Program, at Stony Brook University

- Awards received by PhD advisees:
  - P. Doruker (1995), C. Baysal (1996), O. Keskin (1998) and B Ozkan (2001) received *'The Best Thesis Award'* at their graduation from Bogazici U Chemical Engineering Dept under I. Bahar supervision, awarded yearly by Bogazici U to 2-4 students among all (>500) PhD graduates.
  - Haliloglu, received TUBITAK and TUBA awards (see http://www.prc.boun.edu.tr/~turkan/).
  - Keskin http://home.ku.edu.tr/~okeskin/awards.htm received TWAS Encouragement Award (2009), TUBA Distinguished Young Scientist (2006), 2013 TUBITAK Science Award, and UNESCO L'Oreal Award (2005); 2018 NATO Science for Peace and Security Programme (SPS) Prize; and
  - Doruker http://www.prc.boun.edu.tr/cosbiom/content/view/19/) received TUBA Young Scientists Award (2002) and TUBITAK Young Scientists Encouragement Prize (2001).
  - Canan (Baysal) Atilgan received the 2005 L'Oréal Young Women Scientist Fellowship (2005), and TUBA Distinguished Young Scientist Award (2004) (see http://people.sabanciuniv.edu/canan/);
  - Banu Ozkan was elected Scialog Fellow, Research Foundation and Moore Foundation, 2014; and received Faculty Achievement Young Investigator Award, Arizona State University, 2013.
  - Lee-Wei Yang (2005) received *the 'Stephen Phillips Best Student Paper'* award of the year 2006 at U Pitt at the completion of his doctoral studies at the School of Medicine.
  - Zheng Yang received the "Best student researcher" award from the Department of Computational Biology in 2009. His paper published in *Biophys J.* has been highlighted in the 2010 brochure of *Biophysical Society* under "What is Biophysics?" section as an example study of current trends in biophysics.
  - Ahmet Bakan, Ying Liu, Anindita Dutta and Murat Can Cobanoglu (CMU-Pitt PhD Program in Computational Biology) received the '*Outstanding Research Accomplishments*" awards in 2009, 2010 and 2012 and 2013, respectively.

MASTER of SCIENCE (MS) STUDENTS

- Served as Thesis Advisor of
  - 1 MS student at Pitt *Program in Integrative Molecular Biology* (Chang Liu, 2014)
  - 20 M.S. Students in Chemical Engineering, Bogazici U (1988-2001), listed below

Piraye Yaras, 'Investigation of Local Relaxation Motions in Polymers in Dilute Solution by Dynamic Rotational Isomeric States Model' (1988); Tugce Onen, 'Thermoelastic Behavior of Polybutadiene Network' (1989); Coskun Kanberoglu, 'Fourier Transform Infrared Dichroism Study of Molecular Orientation in Polymeric Materials and Theoretical Interpretation' (1992); Bertan Badur, "Molecular Dynamics Simulation of Polymeric Systems" (1992); Turkan Haliloglu, "Segmental Orientation and Conformational Dynamics of Polymer Chains" (1989); Gokhan Sakrak, "Computer Simulation of 2-D Trifunctional Bimodal Networks" (1993); Zeynep Sarac, "Characterization of Biaxially Oriented Polypropylene Films"' (1993) ; Toprak

Serhatkulu "Experimental and Theoretical Investigation of Thermo-mechanical Properties of Polymer Blends" (1995); Mine Kaplan "Sequence-Structure Relationships in Globular Proteins" (1995); Seda Erdal, "Swelling of Sodium Chloride Filled Polybutadiene Networks in Aqueous Environment" (*co-advisor:* B. Erman) (1996); Banu Ozkan "Identification of Native Structure of Proteins Using a Low Resolution Model" (1997); Basak Samur "Determination of Protein Structures Using Distance Constraints" (1998); Taner Zafer Sen "Comparison of Local Chain Dynamics of *cis*-Polybutadiene and *cis*-Polyisoprene Based on Cooperative Kinematics Theory" (*co-advisor: B. Erman*) (1998); Zeynep Nevin Gerek 'Dynamics of Protein-DNA Complexes Examined by Gaussian Network Model' (*co-advisor: A. R. Atilgan*) (1999); Haluk Konyali "Thermal and Mechanical Characterization of Star-Branched and Linear Polybutadiene Networks" (*co-advisor: N. Nugay*) (1999); Alpay Temiz "NMR Relaxation Behavior of Proteins Predicted by Analytical Approaches" (*co-advisor: T, Haliloglu*) (2001); Zerrin Bagci "Knowledge-Based Study of Packing Characteristics of Amino Acids in Folded Proteins" (2000); Basak Isin "Stability of Folded and Molten Globule States of Proteins Examined by Differential Scanning Calorimetry" (*co-advisor: P. Doruker*) (2000); Safak Kirca "Structure-Based Analysis of Immunoglobulins: Functional Motions and Antigen Recognition" (2001)

POSTDOCTORAL FELLOWS AND RESEARCH ASSOCIATES

APostdoctoral Fellows and Research Associates	Name	Background	Current Position
	JiYoung Lee*	PhD in Physics, Pohong U of Sci & Technol, S Korea	Staff Scientist at the Laufer Center, Stony Brook U
	Antony Bogetti*	PhD in Chemistry, U of Pittsburgh	Postdoctoral fellow at the Laufer Center, Stony Brook U
	Xiao Bogetti*	PhD in Chemistry, U of Pittsburgh	Postdoctoral fellow at the Laufer Center, Stony Brook U
	Mary H Cheng*	PhD in Chemical Engineering, Rensselaer Polytechnic Inst	Senior Scientist at the Laufer Center, Stony Brook U
	Anupam Banerjee*	PhD in Bioinformatics from Indian Institute of Technol, Kharagpur	Senior postdoctoral fellow at the Laufer Center, Stony Brook U
	James Krieger	PhD in Neurobiology, Cambridge U, UK	Marie Curie Fellow for Postdoc studies, Research Associate at the U of Madrid
	Karolina Mikulska-Ruminksa	PhD in Physics, N Copernicus U, Poland	Associate Prof, Dept of Biophysics, Institute of Physics, Nicolaus Copernicus U, Torun, Poland
	Burak T Kaynak	PhD in Physics, Bogazici U, Istanbul, Turkey	Research Scientist, Salk Institute for Biol Studies, Comp Neurobiology lab
	Bing Liu	PhD in Comp Systems Biol, Nat U of Singapore	(*) *deceased*
	Luca Ponzoni	PhD in Physics, ICTP International Center for Physics, Trieste, Italy	Postdoctoral scholar, Institute for Neurodegenerative Diseases, UCSF

	Elia Zomot	PhD in Biology, Hebrew U, Jerusalem, Israel	Research Associate, Department of Biochemistry, Technion, Israel
	Mert Gur	PhD in Science and Engineering, Koc U	Associate Prof, Istanbul Technical U, Mechanical Engineering Department
	Ignacio General	PhD in Physics, North Carolina State U	Assistant Professor, U Nacional de San Martin, Buenos Aires, Argentina
	Timothy Lezon	PhD in Physics, Penn State	Principal Scientist, Applied Math USA
	Divesh Bhatt	PhD in Chem Eng, UC Berkeley	Senior Scientist, Kimberly Clark, Roswell, Georgia
	Kristina Paris	PhD in Chemistry, Rutgers U	Research Assoc, Dept of Comp & Systems Biol, U of Pittsburgh
	Jason DeChancie	PhD in Chemistry, UCLA	Biomedical Research Analyst at American Systems, Washington D.C.
	Indira H. Shrivastava	PhD in Physics, Puna University, India	Research Assist Prof at the Dept of Environ & Occupational Heath, Pitt
	Eran Eyal	PhD in Bioinformatics Ben Gurion U, Israel	Senior Algorithm Developer, Evogene, Israel
	Dror Tobi	PhD in Biochemistry, Hebrew U, Jerusalem	Associate Professor, Dept of Comp Sci, and Dept of Mol Biology, Ariel University Center of Samaria, Israel
	AJ Rader	PhD in Physics & Chem, Michigan State U	Director of Data Science, DMC Insurance, Inc., Indianapolis, IN
	Amutha Ramaswamy	PhD in Physics, U of Madras, India	Assistant Professor, Pondicherry U, Center for Bioinformatics, India
	Chakra Chennubhotla	PhD in Computer Science, Toronto U	Assoc Professor, Dept of Comput and Systems Biology, Pitt and CEO and co-Founder, SpIntellx, Pittsburgh
	Lucy (Chunyan) Xu	PhD in Biological Sci, U of Pittsburgh	Associate Director, Global Quality, Clinical Biomarker Res, Eisai, Inc. NY
	Rajan Munshi	PhD in Biology, U of Mississippi	Deputy Director, Scientific Program Management, Stanford University
Predoctoral Fellows	Zakaria Dahmani*	PhD in Bioinformatics and Molecular Modeling, Sorbonne University, Paris	Predoctoral fellow in the Bahar lab t the U of Pittsburgh
	Gan Yu	BS in Comp Biology, China U of Sci & Technol	PhD student in Comput Biology, China U of Science & Technology, China
	Enrique Marcos	Inst of Chemistry, Barcelona, Spain	Postdoctoral fellow at U of Washington
	Shann-Ching Chen	PhD in Biomed Eng Carnegie Mellon U	Senior Scientist, Compal, San Francisco

(*) Current members of the Bahar lab

PROFESSIONAL SERVICE

SCIENTIFIC REVIEW BOARDS (*)

2022	US National Academy of Sciences (NAS) Alexander Hollaender Award in Biophysics, Selection Committee
2018-2025	European Research Council (ERC) Scientific Review Board, Synthetic Chemistry and Materials Review Panel (Brussels, Belgium)
2021-2023	Department of Quantitative and Computational Biology (QCB) EAB, U of Southern California, External Advisory Board Member
2021-2022	National Institutes of Health Common Funds Illuminating the Druggable Genome (IDG) Program Face-to-Face Committee. External Program Consultant (EPC), Arlington, VA
2021	NIGMS Early-Stage Investigator Maximizing Investigator Research Award (ESI MIRA) Grant Review Board. Panel Member
2016-2020	NIH NLM Biomedical Informatics, Library and Data Sciences (BILDS) Review Panel, Chartered Member (Bethesda, Maryland)
2020	The Heidelberg Institute for Theoretical Studies (HITS), HITS gGmbH Scientific Advisory Board "Molecular and Cellular Modeling (MCM)" Research Group Review Board. Heidelberg, Germany.
2011-2016	Human Frontier Science Program (HFSP) Scientific Review Board (Strasbourg, France)

NIH REVIEW PANELS AND OTHER NIH-RELATED ACTIVITIES

2016-2020

- NIH NLM Biomedical Informatics, Library and Data Sciences Review Committee (BILDS) Chartered Member of Review Panel (2016-2020)
- March 8-9, 2018: BILDS Study Section
- February 27, 2018: National Institute of Mental Health, Invited Speaker
- Oct 1-4, 2017: Nov 2-3: BILDS study section.
- Jun 15-16, 2017: BLIRC study section
- March 7-10, 2017: BLIRC study section
- July 11-12, 2016: NIBIB Training Program Directors Meeting. Natcher Conf Center, NIH
- March 13-15, 2016: NIH BTRR P41 Directors Meeting, Bethesda, MD. Invited Speaker.

2013-2015

- March 30-31, 2015: **Chair** of the NIH IMST-R, Pilot Centers for Precision Disease Modeling (U54) study section. Washington, DC.
- April 23-23, 2015: NIH Director's New Innovator Award Review, Editorial Review Panel
- Sept 20-22: NIH-NINDS (National Institute of Neurological Disorders and Stroke) Board of Scientific Counselors, *Ad-hoc* member
- Nov 17-18, 2015: NIH P01 "Molecular structure, dynamics, and mechanism of key membrane transporters & enzymes in cellular metabolism". Online Review Panel **Chair**.
- March 5-7, 2014: NIH Review Panel member for National Biomedical Computation Resource (P41-BTRC) Program, UCSD, San Diego, CA.

- April 7, 2014. NIH Library of Integrated Network-Based Cellular Signatures (LINCS) Centers (U54) Review panel **Chair**
- March 18-19, 2013: NIH BTRC P41 Directors Meeting, Bethesda, MD. Invited Speaker.
- July 1-3, 2013: NIH site visit/review meeting for IMST Program at the U of Wisconsin
- October 20-22, 2013: NIH Advisory Board member. U of Illinois Urbana-Champaign, IL
- Dec 9-10, 2013: NIH R15 Area Review. Washington, DC. Review Panel Member.

2009-2011

- March 9-10, 2009: NIH Study Section member for National Technology Centers for Networks and Pathways (TCNP), NIH Director's Roadmap for Medical Res, San Francisco.
- Sept 30-Oct 2, 2009: NIBIB-HHMI Interdisciplinary Training Workshop, Bethesda.
- May 6-7, 2010: NIGMS Glue Grant Membrane Proteins Consortium Meeting, Chicago.
- June 24-25, 2010: NIBIB T32 Training Grant PIs Meeting, Bethesda, MD.
- July 21, 2010: NIH IMST Study Section **Chair**, Bethesda MD
- March 2011, NIH Eureka Proposals Review, Pittsburgh, PA
- Nov 17, 2011: NIBIB MSM Review Panel on 'Development of Multiscale Models"

2007-2008

- NIH MABS (Modeling & Analysis of Biological Systems) Study Section **Chair** and chartered member, 2007-2008
- Dec 18, 2007: NIH CSR Chairs meeting, CSR Biomol Chartered Study Section, **Chair**, MD
- Jan 28-29, 2008: NIH MABS Study Section, Bethesda, MD
- June 1-2, 2008: NIH MABS Study Section, Bethesda, MD
- April 17, 2008: BBSI Annual Meeting organized by NSF and NIH/NIBIB, Washington DC
- June 1-2, 2008: NIH MABS Study Section, Bethesda, MD

2004-2006

- NIH MABS (Modeling & Analysis of Biological Systems) Study Section Member, 2004-2006
- March 9-11: Site Visit (as reviewer) at NIH Research Resource at Scripps on "Multiscale Modeling Tools in Structural Biology"
- July 28-29: NIH MABS (Modeling and Analysis of Biological Systems) Study Section
- March 2-3: NIH MABS Study Section, Bethesda MD.
- March 17-18: NIH/NSF BBSI Grantees Meeting, Bethesda, MD.
- June 26-28: HMMI-NIBIB Awardees meeting, NIH, Bethesda, MD
- October 23-24: NIH MABS Study Section, Bethesda, MD

RECENT SCIENTIFIC SERVICE, ADVISORY AND EDITORIAL ACTIVITIES

- *Bioinformatics Advances*, Oxford U Press, Associate Editor 2021-
- *Quarterly Reviews of Biophysics Discovery* International Journal, Assoc Editor 2020 -
- Biophysical Society, Awards Committee 2017 - 2018
- Biophysical Society, Executive Board 2009 – 2011
- Biophysical Society, Council 2008 – 2011
- International Society of Quantum Biology & Pharmacology, Council 2008 – 2012
- Associate Editor, *Proteins: Structure, Function and Bioinformatics* (Wiley) 2017-
- Editorial Board, *Proteins: Structure, Function and Bioinformatics* (Wiley) 2008 - 2017
- Editorial Board, *Structure* (Cell Press) 2014-
- Editorial Board *Scientific Reports* (*Nature* Publishing Group) 2014-

- Editorial Board *Protein Science* (*Wiley-Blackwell*) 2014-
- Editorial Board, *Biophysical Journal* (Cell Press) 2004- 2007

- *Program Committee and Symposium Chair*. 17th European Conference on Computational Biology (ECCB) 2018; Athens, Greece. September 8-12, 2018
- *External Review Board Member*. Computational Biology Program, College of Liberal Arts and Sciences, University of Kansas, Nov 19-21, 2017.
- *External Advisory Board Member* for BCM Structural and Computation Biology and Molecular Biophysics Graduate Program, Baylor College of Medicine, Jan 20-21, 2016
- *External Advisory Board Member* for NIH Biomedical Technology and Research Resource (BTRR) Center for Biomolecular NMR Data Processing and Analysis, (PI: Hoch, UConn), (2016 – present)
- *Conference Chair* and *Organizer*. Gordon Research Conference (GRC) on Biopolymers. Chair. Salve Regina, Rhode Island. (June 2014)
- *Organizer/Chair*, Biophysical Society Thematic Meeting on Modeling Biomolecular Systems Interactions (co-organizer: O. Keskin), Istanbul, Turkey, (Sept 2014)
- *Program Committee and Symposium or Session Chair*. ISMB/ECCB 2005, 2007 and 2008 (15th Annual International Conf on Intelligent Systems for Molecular Biology (ISMB) & 6th European Conference on Computational Biology (ECCB), Vienna; and ISMB2008, Toronto; Computational Structural Bioinformatics Workshop in IEEE BIBM 2009, Washington, DC)
- *Keynote Symposium Organizer*. 2009 Keystone Symposium on Protein Dynamics, Allostery and Function, (co-organizer: Lila M. Gierasch) Keystone, Colorado (June, 2009)
- *External Advisory Board*: NIH National Center for Macromolecular Imaging (Director: W. Chiu) Baylor College of Medicine (2004);
- *External Advisory Board*: Beckman Institute, M & ENS (Mol and Electronic Nanostructures) Division, U of Illinois, Urbana-Champaign (2004; March 2008; April 2009; Nov 2013)
- *Executive Board* - Great Lakes Bioinformatics Consortium (2004); University of Kansas, Center for Bioinformatics, 2008
- Dickson Prize Committee member at the U of Pittsburgh (2013 -2019)

SCIENTIFIC PAPERS REVIEWS

for *Science*, *Nature*, *Cell*, *Proceedings of the National Academy of Science USA*, *eLife*, *Philosophical Transactions of the Royal Society B*; *Proteins: Structure, Function & Bioinformatics*, *Physical Review Letters, Biophysical Journal, Bioinformatics, J. Chemical Physics, Journal of Chemical Theory and Computation; European Polymer J, Macromolecules, Biophys. Biochim. Acta, Comput & Theor Polymer Science, Structure, Biochemistry, Protein Science, Phys Rev E, J Mol. Biology, BMC Bioinformatics, PLoS Computational Biology, Molecular Systems Biology* and *Proceedings of the National Academy of Sciences USA*.

SUPPLEMENTAL INFORMATION (SI)

Topics	Main pages	SI pages
Publications	9	25-51
Invited talks and seminars	13-14	52-59
Grants, funded projects	11 -12	60-64

PUBLICATIONS

JOURNALS (*)

(*) includes 378 papers published in refereed journals, 1 editorial, and 8 BioRxiv reports.

2024

J380. Banerjee A, Mathew S, Naqvi MM, Yilmaz SZ, Zacharopoulou M, Doruker P, Kumita JR, Yang SH, Gur M, Itzhaki LS, Gordon R, **Bahar I** (2024) Influence of point mutations on PR65 conformational adaptability: Insights from molecular simulations and nanoaperture optical tweezers . *Science Advances*, 10(22):eadn2208.

J379. A Banerjee, S Zhang, **I Bahar** (2024) Genome structural dynamics: insights from Gaussian network analysis of Hi-C data . *Briefings in Functional Genomics*, elae014

J378. Lloyd D Harvey, Mona Alotaibi, Hee-Jung Janice Kim, Yi-Yin Tai, Ying Tang, Wei Sun, Wadih El Khoury, Chen-Shan C Woodcock, Yassmin Al Aaraj, Claudette M St. Croix, Donna B Stolz, Jiyoung Lee, Mary Hongying Cheng, Tae-Hwi Schwantes-An, Ankit A Desai, Michael W Pauciulo, William C Nichols, Amy Webb, Robert Lafyatis, Mehdi Nouraie, Haodi Wu, Jeffrey G McDonald, Caroline Chauvet, Susan Cheng, **Ivet Bahar**, Thomas Bertero, Raymond L Benza, Mohit Jain, Stephen Y Chan (2024) Genetic regulation and targeted reversal of lysosomal dysfunction and inflammatory sterol metabolism in pulmonary arterial hypertension . *BioRxiv*, 2024.02. 26.582142

J377. Andreia CK Fontana, Adi NR Poli, Jitendra Gour, Yellamelli VV Srikanth, Nicholas Anastasi, Devipriya Ashok, Apeksha Khatiwada, Katelyn L Reeb, Mary Hongying Cheng, **Ivet Bahar**, Scott M Rawls, Joseph M Salvino (2024) Synthesis and Structure¿Activity Relationships for Glutamate Transporter Allosteric Modulators . *Journal of Medicinal Chemistry*, 67, 8, 6119¿6143

P4. I Sutkeviciute, JP Vilardaga, J Lee, **I Bahar**, B Kaynak (2024) Small molecule allosteric modulators of class B GPCR, the PTHR, and method to identify them. *US Patent App.* **18/277,765**

P3. Mark E Schurdak, Andreas Vogt, Andrew Michael Stern, Douglass Lansing Taylor, CHEN Fangyuan, PEI Fen, Hongying Cheng, **Ivet Bahar**, SHI Qingya, Moshe Arditi (2024) Compounds for the treatment of a disease or disorder, methods for identifying said compounds . *US Patent App.* **18/273,161**

J376. Hoang Nguyen, Mary Hongying Cheng, JiYoung Lee, S Aggarwal, Ole V Mortensen, **Ivet Bahar** (2024). Allosteric modulation of serotonin and dopamine transporters: New insights from computations and experiments. *Current Research in Physiology*, 10012

J375. Yueming Zhu, Anupam Banerjee, Ping Xie, Andrey A Ivanov, Amad Uddin, Qiao Jiao, Junlong J Chi, Lidan Zeng, Ji Young Lee, Yifan Xue, Xinghua Lu, Massimo Cristofanilli, William J Gradishar, Curtis J Henry, Theresa W Gillespie, Manali Ajay Bhave, Kevin Kalinsky, Haian Fu, **Ivet Bahar**, Bin Zhang, Yong Wan (2024) A Pharmacological suppression of the OTUD4-CD73 proteolytic axis revives antitumor immunity against immune-suppressive breast cancers. *Journal of Clinical Investigation,* 134(10): e176390.

J374. JiYoung Lee, Emma Gebauer, Markus A. Seeliger, **Ivet Bahar** (2024) Allo-targeting of the kinase domain: Insights from in silico studies and comparison with experiments. *Curr Opin Struct Biol* Volume 84, 102770

J373. Carlos Ventura, Anupam Banerjee, Maria Zacharopoulou, Laura S Itzhaki, **Ivet Bahar** (2024) Tandem-repeat proteins conformational mechanics are optimized to facilitate functional interactions and complexations. *Curr Opin Struct Biol* 84, 102744

J372. Svetlana N Samovich, Karolina Mikulska-Ruminska, Haider H Dar, Yulia Y Tyurina, Vladimir A Tyurin, Austin B Souryavong, Alexander A Kapralov, Andrew A Amoscato, Ofer Beharier, S Ananth Karumanchi, Claudette M St Croix, Xin Yang, Theodore R Holman, Andrew P VanDemark, Yoel Sadovsky, Rama K Mallampalli, Sally E Wenzel, Wei Gu, Yuri L Bunimovich, **Ivet Bahar**, Valerian E Kagan, Hülya Bayir (2024) Strikingly High Activity of 15-Lipoxygenase Towards Di-Polyunsaturated Arachidonoyl/Adrenoyl-Phosphatidylethanolamines Generates Peroxidation Signals of Ferroptotic Cell Death. *Angewandte Chemie International Edition,* e202314710

J371. MGS Costa, M Gur, JM Krieger, **Bahar I** (2024) Computational biophysics meets cryo-EM revolution in the search for the functional dynamics of biomolecular systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science* 14, e1689

J370. MP Dalton, MH Cheng, **Bahar I**, JA Coleman (2024) Structural Mechanisms for VMAT2 inhibition by tetrabenazine . *Elife* **Mar 22:12:RP91973**

2023

J369. Valerian E Kagan, Yulia Y Tyurina, Karolina Mikulska-Ruminska, Deena Damschroder, Eduardo Vieira Neto, Alessia Lasorsa, Alexander A Kapralov, Vladimir A Tyurin, Andrew A Amoscato, Svetlana N Samovich, Austin B Souryavong, Haider H Dar, Abu Ramim, Zhuqing Liang, Pablo Lazcano, Jiajia Ji, Michael W Schmidtke, Kirill Kiselyov, Aybike Korkmaz, Georgy K Vladimirov, Margarita A Artyukhova, Pushpa Rampratap, Laura K Cole, Ammanamanchi Niyatie, Emma-Kate Baker, Jim Peterson, Grant M Hatch, Jeffrey Atkinson, Jerry Vockley, Bernhard Kühn, Robert Wessells, Patrick CA van der Wel, **Bahar I**, Hülya Bayir, Miriam L Greenberg (2023) Anomalous peroxidase activity of cytochrome c is the primary pathogenic target in Barth syndrome. *Nature Metabolism* **5**, 2184-2205

J368. Denys Bondar, Olga Bragina, Ji Young Lee, Ivan Semenyuta, Ivar Järving, Volodymyr Brovarets, Peter Wipf, **Bahar I**, Yevgen Karpichev (2023) Hydroxamic Acids as PARP-1 Inhibitors: Molecular Design and Anticancer Activity of Novel Phenanthridinones. *Helvetica Chimica Acta* 106 (10), e202300133

J367. Yan Zhang, Xiaojie Qiu, Jonathan S Weissman, **Ivet Bahar**, Jianhua Xing (2023) Graph-Dynamo: Learning stochastic cellular state transition dynamics from single cell data. *BioRxiv,* 2023.09.24.559170

P2. **Bahar I**, H Cheng, S Zhang, R Porritt, M Arditi (2023) Compositions and methods for treating a COVID-19 infection . *US Patent* **11,746,144**

J366. Dar HH, Mikulska-Ruminska K, Tyurina YY, Luci DK, Yasgar A, Samovich SN, Kapralov AA, Souryavong AB, Tyurin VA, Amoscato AA, Epperly MW, Shurin GV, Standley M, Holman TR, St. Croix CM, Watkins SC, VanDemark AP, Rana S, Zakharov AV, Simeonov A, Marugan J, Mallampalli RK, Wenzel SE, Greenberger JS, Rai G, Bayir H, **Bahar I***, Kagan VE* (2023) Discovering selective antiferroptotic inhibitors of the 15LOX/PEBP1 complex noninterfering with biosynthesis of lipid mediators. *Proc Natl Acad Sci (USA)* **120**, e2218896120

J365. Zhang C, Zhang X, Weiß T, Cheng MH, Chen S, Ambrosius CK, Czerniak AS, Li K, Feng M, **Bahar I**, Beck-Sickinger AG (2023) Structural basis of CMKLR1 signaling induced by chemerin9. *BioRxiv* , 2023.06. 09.544295

J364. Amoscato AA, Anthonymuthu T, Kapralov O, Sparvero LJ, Shrivastava IH, Mikulska-Ruminska K, Tyurin VA, Shvedova AA, Tyurina YY, **Bahar I**, Wenzel S, Bayir H, Kagan VE (2023) Formation of protein adducts with hydroperoxy-PE electrophilic cleavage products during ferroptosis. *Redox Biology* **63**, 1-17, 102758

J363. Banerjee A, **Bahar I** (2023) Structural Dynamics Predominantly Determine the Adaptability of Proteins to Amino Acid Deletions. *International Journal of Molecular Sciences* **24 (9)**, 8450

J362. Kaynak BT, Dahmani ZL, Doruker P, Banerjee A, Yang SH, Gordon R, Itzhaki LS, **Bahar I** (2023) Cooperative mechanics of PR65 scaffold underlies the allosteric regulation of the phosphatase PP2A. *Structure* **31**, 607-618.

J361. Banerjee A, Saha S, Tvedt NC, Yang LW, **Bahar I** (2023) Mutually beneficial confluence of structure-based modeling of protein dynamics and machine learning methods. *Current Opinion in Structural Biology* **78**, 102517

J360. Shekar A, Mabry SJ, Cheng MH, Aguilar JI, Patel S, Zanella D, Saleeby DP, Zhu Y, Romanazzi T, Ulery-Reynolds P, **Bahar I**, Angela M Carter, Heinrich JG Matthies, Aurelio Galli (2023) Syntaxin 1 Ser14 phosphorylation is required for nonvesicular dopamine release *Science Advances*, **9**(2), eadd8417

J359. Vilardaga JP, Clark LJ, White AD, Sutkeviciute I, Lee JY, **Bahar I** (2023) Molecular Mechanisms of PTH/PTHrP class B GPCR Signaling and Pharmacological Implications. *Endocrine Reviews*, **44**, 474-491. https://doi.org/10.1210/endrev/bnac032

2022

J358. Smith IN, Dawson JE, Krieger J, Thacker S, **Bahar I**, Eng C (2022) Structural and Dynamic Effects of PTEN C-Terminal Tail Phosphorylation. *J Chem Inf Model*. **62**(17):4175-4190. PMID: 36001481

J357. Noval Rivas M, Porritt RA, Cheng MH, **Bahar I** M Arditi (2022) Multisystem inflammatory syndrome in children and long COVID: the SARS-CoV-2 viral superantigen hypothesis. *Frontiers in Immunology*, 3480

J356. Abram A, Jakubiec M, Reeb K, Cheng MH, Gedschold R, Rapacz A, Mogilski S, Socala K, Nieoczym D, Szafarz M, Latacz G, Szulczyk B, Kalinowska-Tluscik J, Gawel K, Esguerra CV, Wyska E, Müller CE, Bahar I, Fontana ACK, Wlaz P, Kaminski RM, Kaminski K (2022) Discovery of (R)-N-Benzyl-2-(2,5-dioxopyrrolidin-1-yl)propanamide [(R)-AS-1], a Novel Orally Bioavailable EAAT2 Modulator with Drug-like Properties and Potent Antiseizure Activity In Vivo. *J. Med. Chem.* **65, 17,** 11703-11725

J355. Todd NK, Huang Y, Lee JY, Doruker P, Krieger JM, Salisbury R, MacDonald M, **Bahar I**, Thathiah A (2022) GPCR kinases generate an APH1A phosphorylation barcode to regulate amyloid-β generation *Cell Reports* **40** (3), 111110

J354. Wingert B, Doruker P, **Bahar I** (2022). Activation and Speciation Mechanisms in Class A GPCRs. *J Mol Biol*. 2022 Jun 18:167690. doi: 10.1016/j.jmb.2022.167690.

J353. Lefever DE, Miedel MT, Pei F, DiStefano JK, Debiasio R, Shun TY, Saydmohammed M, Chikina M, Vernetti LA, Soto-Gutierrez A, Monga SP, Bataller RA, Behari J, Yechoor VK, **Bahar I**, Gough A, Stern AM, Taylor DL (2022) A Quantitative Systems Pharmacology Platform Reveals NAFLD Pathophysiological States and Targeting Strategies. *Metabolites* **12**(6), 528

J352. Acar O, Zhang S, **Bahar I**, Carvunis AR (2022) Elastic Network Modeling of Cellular Networks Unveils Sensor and Effector Genes that Control Information Flow. *PLOS Computational Biology* **18** (5), e1010181. PMID: 35639793

J351. Krieger JM, Sorzano COS, Carazo JM, **Bahar I** (2022) Protein dynamics developments for the large scale and cryoEM: case study of ProDy 2.0. *Acta Crystallographica Section D: Structural Biology* **78** (4) PMID: 35362464 PMCID: PMC8972803

J350. Colas C, **Bahar I**, Shi L, Font Sadurni J (2022) Editorial: Targeting Membrane Proteins: Structure-Function-Dynamics Relationships. *Front Chem.* Mar 3;10:862802. PMID: 35308796

J349. Refai O, Aggarwal S, Cheng MH, Gichi Z, Salvino JM, Bahar I, Blakely RD, Mortensen OV (2022) Allosteric Modulator KM822 Attenuates Behavioral Actions of Amphetamine in *Caenorhabditis elegans* through Interactions with the Dopamine Transporter DAT-1. *Molecular Pharmacology* **101** (3) 123-131.

J348. Sang Z, Xiang Y, **Bahar I**, Shi Y. (2021) *Llamanade*: an open-source computational pipeline for robust nanobody humanization.. *Structure*, **30**(3):418-429.e3. PMID: 34373858 PMCID: PMC8351782

J347. Sutkeviciuta I, Lee JY, White AD, Maria CS, Peña KA, Savransky S, Doruker P, Li H, Lei S, Kaynak B, Tu C, Clark LJ, Sanker S, Gardella TJ, Chang W, **Bahar I*** and Vilardaga JP*. (2021) Precise druggability of the PTH type 1 receptor. *Nature Chem Biol.* **18**(3):272-280. PMID: 34949836 PMCID: PMC8891041

J346. Cheng MH, Krieger JM, Banerjee A, Xiang Y, Kaynak B, Shi Y, Arditi M, **Bahar I** (2022) Impact of new variants on SARS-CoV-2 infectivity and neutralization: A molecular assessment of the alterations in the spike-host protein interactions. *iScience* **25**(3):103939. PMID: 35194576 PMCID: PMC8851820

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81. Bahar I, Atilgan AR, Erman B (1997) Direct evaluation of thermal fluctuations in protein *Folding & Design* **2**: 173-181.

80. Bahar I, Jernigan RL (1997) Inter-residue potentials in globular proteins and the dominance of highly specific hydrophilic interactions at close separations *J Mol Biol* **266**: 195-214.

The publications (1-79) are accessible on the Bahar lab website or Google Scholar page.

BOOK AND EDITED BOOK

Protein Actions: Principles & Modeling. Bahar I, Jernigan R, Dill K. (2017) New York, NY: Garland Science, Taylor & Francis Group ISBN: 9780815341772 (**Recipient of 2018 Prose Award in Textbook, Biol and Life Sciences**)

Normal Mode Analysis. Theory and Applications to Biological and Chemical Systems" Eds Qiang Cui and I Bahar (2006) Chapman & Hall / CRC Mathematical and Computational Biology Series, CRC Press, Taylor & Francis Group. See review in http://bib.oxfordjournals.org/cgi/reprint/bbm010v1

CHAPTERS IN EDITED BOOKS

1. Bahar, I. Thermodynamics of Compatibility in Binary Polymeric Mixtures. In: **Polymer Blends and Mixtures**, NATO ASI Series E: No.89, Martinus Nijhoff Publ, Dordrecht: 1985. p. 349.

2. Erman B, Bahar I, Kloczkowski A, Mark JE. Stress-strain and segmental orientation in networks with semirigid chains. In: Mark JE, Erman B, editors**. Elastomeric Polymer Networks**" Ed. Prentice Hall Polymer Science and Engineering Series, New Jersey: Prentice Hall, Inc; 1992 p. 142.

3. Erman B, Bahar I. Local dynamics of polymers in restrictive environment. In: Noda I, Rubingh DN, editors. **Polymer Solution, Blends, and Interfaces** Elsevier Science Publishers; 1992. p. 197-208.

4. Erman B, Bahar I, Yang Y, Kloczkowski A, Mark JE. Novel orientation techniques for the preparation of high-performance materials from semi-flexible polymers such as cellulosics. In: Noda I, Rubingh DN, editors. Polymer Solution, Blends and Interfaces; Elsevier Science Publishers; 1992. p. 209-220.

5. Kloczkowski A, Mark JE, Erman B, Bahar I. Isotropic-nematic phase transitions in polymer networks deformed in the dry and swollen states. In Noda I, Rubingh DN, editors. **Polymer Solution, Blends and Interfaces**, Elsevier Science Publishers; 1992. p. 221-233.

6. Erman B, Bahar I, Kloczkowski A, Mark JE. Networks with semi-flexible chains. In: Aharoni, SM, editor. **Synthesis, Characterization, and Theory of Polymeric Networks and Gels**" New York: Plenum Press; 1992. p. 113-126.

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8. Jernigan RL, Bahar I. Coarse grained searches over protein conformations. In: Schleyer PR, Allinger NL, Clark T, Gasteigen J, Kollman P A, Schaefer III H F, Schreiner PR. editors. **The Encyclopedia of Computational Chemistry**. Chichester: John Wiley & Sons; 1998.

9. Erman B, Bahar I. Simulations of polymeric systems. In: Inan E, Markov KZ, editors**. Continuum models and discrete systems**. World Scientific Publishing; 1998. p. 297-303.

10. Jernigan RL, Bahar I. Geometric regularities among bonded and nonbonded residues in proteins. In: Vijayan M, Yathindra N, Kolaskar AS, editors. **Perspectives in Structural Biology** (GN Ramachandran Volume) Indian Academy of Sciences, Universities Press, Hyderabad, 1999. p. 209-225.

11. AJ Rader. Chakra Chennubhotla, Lee-Wei Yang, and Ivet Bahar "The Gaussian Network Model: Theory and Applications" by, *in* "**Normal Mode Analysis. Theory and Applications to Biological and Chemical Systems**" Eds Qiang Cui and I Bahar, Chapman & Hall / CRC *Mathematical and Computational Biology Se*ries, CRC Press, Taylor & Francis Group, 41-64, 2006.

12. Lezon TR, Shrivastava IH, Yang Z and Bahar I. *Elastic network models for biomolecular dynamics: Theory and application to membrane proteins and viruses*, in **Handbook on Biological Networks**. Edited by Boccaletti S, Latora V and Moreno Y. World Scientific, 2009.

13. Zomot E, Bakan A, Shrivastava IH, DeChancie J, Lezon TR, Bahar I. *Sodium-coupled Secondary Transporters: Insights from Structure-based Computations*, in **Molecular Machines**. Edited by Roux B. World Scientific, 2011.

14. Doruker P, Liu Y, Yang Z, Bahar I *In Silico Coarse-Grained Approaches to Structural Dynamics and Function of Proteins and their Assemblies* in **Comprehensive Biophysics**. Editor-in-Chief: EH Egelman, vol 9, chapter 9.3, pp 27-52, Academic Press, Elsevier, 2012.

15. Taylor DL, Gough A, Schurdak ME, Vernetti L, Chennubhotla CS, Lefever D, Pei F, Faeder JR, Lezon TR, Stern AM, **Bahar I**. (2019) "Harnessing Human Microphysiology Systems as Key Experimental Models for Quantitative Systems Pharmacology" in Handbook of Experimental Pharmacology book series, Springer.

16. Shrivastava IH, Liu C, Dutta A, Bakan A, **Bahar I**. (2020) Allostery as Structure-Encoded Collective Dynamics: Significance in Drug Design. Structural Biology in Drug Discovery: Methods, Techniques, and Practices. *Eds Jean-Paul Renaud*. Chapter 6, p125-141, John Wiley & Sons, NY.

INVITED TALKS AND SEMINARS (2004 - 2016)

2004

- International Workshop on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, March 17-20; 2004; Granlibakken, Lake Tahoe, CA (Invited Speaker)
- 12th International Conference on Intelligent Systems for Molecular Biology (ISMB) (ISMB/ECCB2004 July 31 – August 4, 2004, Glasgow, Scotland (Invited Speaker)
- Modeling Protein Stability, Flexibility and Motions workshop, July 17-July 22, 2004, Banff, Alberta, Canada (Invited Speaker)
- Seminar at Michigan State U, Biochemistry and Biophysics Dept., May 2004.

2005

- January 27, 2005: Seminar at Dept of Materials Science & Engineering at Rensselaer Polytech Inst
- February 12-16, 2005: Biophysical Society Annual Meeting - Long Beach California (http://www.biophysics.org/meetings/annmtg/) (Invited Speaker)
- April 25, 2005: Seminar at Department of Chemistry and Biochemistry and Institute for Physical Science and Technology at the University of Maryland (Invited Speaker)
- April 30 - May 1, 2005: Midwest Computational Structural Biology Workshop in Augusta, Michigan (Invited Speaker)
- May 15-18, 2005: Workshop on Flexibility in Biomolecules (Tempe Arizona) (http://biophysics.asu.edu/workshop_2005/) (Invited Speaker)
- June 27-30, 2005: International Conference on Computational Science and Engineering (Istanbul, Turkey) (Scientific Committee Member and Session Chair) (http://www.iccse.org/about.php)
- July 7-13, 2005: 5th International Discussion Meeting on Relaxations in Complex Systems (Lille, France). (http://www-ldsmm.univ-lille1.fr/meeting.html) (Invited Speaker)
- August 14-19, 2005: 40th IUPAC Congress - Innovation in Chemistry (Beijing, China) (http://www.ccs.ac.cn/IUPAC2005.htm) (Invited Speaker)
- November 1-3, 2005: Paul Flory Colloquium: Modeling and Simulation Fall 168th Technical Meeting (David L. Lawrence Convention Center Pittsburgh, Pennsylvania) ACS Rubber Division (http://www.rubber.org/meetings/fall.htm) (Invited Speaker)
- International Conference on Multiscale Modeling in Biological Systems, Imperial College, London October 5-7, 2005, (Invited Speaker)
- Dec 27, 2005: Seminar at Department of Chemical and Biological Engineering, Koc University, Istanbul, Engineering Seminar Series. Title: "A Markov Model for Allosteric Communication in Biomolecular Systems"

2006

- February 23, 2006: Seminar at the Department of Biochemistry and Molecular Genetics, University of Virginia
- March 25, 2006: Natural Sciences Technical Session of Second Annual Conference of TASSA, Philadelphia, PA. (Invited Speaker)
- April 19-20, 2006: Seminar at Notre Dame, Department of Computer Science and Engineering. Computational Biophysics Seminar Series
- April 24, 2006: Seminar at the Department of Biophysics, Johns Hopkins University, invited by the institute of Multi-scale Modeling of Biological Interactions (http://webapps.jhu.edu/eventslist/eventDetail.cfm?eventID=16403&profile=undefined)
- April 27, 2006: Seminar at the University of Akron, invited by the Department of Polymer Science (http://www2.uakron.edu/cpspe/DPS/SeminarSchedule.htm)

- May 18-21, 2006: Symposium on Protein Dynamics - Invited Speaker University of Wisconsin-Madison (http://www.biochem.wisc.edu/steenbock/symposium32/)
- May 22-26, 2006: IPAM Cell and Materials Workshop on Systems Biology and Molecular Modeling at UCLA, and the Institute for Pure and Applied Mathematics (IPAM) - Invited Speaker (http://www.ipam.ucla.edu/programs/cmws4)
- June 11-16, 2006: Biopolymers Gordon Research Conference, Salve Regina University Newport, RI - Invited Speaker (http://www.grc.uri.edu/programs/2006/biopolym.htm)
- July 26-29, 2006: "Modeling elastic manifolds, from soft condensed matter to biomolecules" at ICTP (Abdus Salam International Center for Theoretical Physics), Trieste, Italy, invited speaker
- July 31 - August 3, 2006: Annual meeting of the Society for Mathematical Biology, joint with the Society for Industrial and Applied Math (SIAM) Life Sciences at NCSU, Raleigh (North Carolina). (Plenary Lecture) (http://www.siam.org/meetings/ls06/invited.php)
- September 7, 2006: Systems Biology Symposium, organized at Pennsylvania State University, sponsored by the Huck Life Science Institute and College of Science and Engineering, College Park (PA). (Invited Speaker) (http://www.esm.psu.edu/~mcd18/sysbiol.htm)
- October 5, 2006: "Science 2006: Feel the Power" University of Pittsburgh Annual Science Meeting, Pittsburgh (Spotlight speaker) (http://www.science2006.pitt.edu/)
- December 8, 2006: Molecular Biophysics Seminar Series, organized at Rutgers University. "Understanding biomolecular machinery and allostery using network models for structures." (Invited Speaker). (http://rutchem.rutgers.edu/~mbcenter/)
- December 11-12, 2006: Workshop on the Future of BioMolecular Simulations: From Ab Initio to Nano-molecular Machines at the Oak Ridge National Laboratory (ORNL). (Invited speaker) (http://nccs.gov/news/workshops/biomolecular06/index.html)

2007

- March 13, 2007: Swiss National Meeting of Biological Sciences, Symposium on "Potassium channels: molecular biology, pathophysiology and models", Basel, Switzerland. (First Main Talk) (http://www.swissheartnet.unibe.ch/)
- April 20-21, 2007: 3rd CAPRI (Critical Assessment of PRedicted Interactions) meeting in Toronto. (Invited speaker)
- April 24, 2007: Seminar at Systems Biology Interest Group at Integrative Computational Biology Lab (http://tango01.cit.nih.gov/sig/home.taf?_function=main&SIGInfo_SIGID=124) CRIIT, NHLBI, NIH.
- April 29 - May 1, 2007: Molecular Libraries Screening Centers Network (MLSCN) Steering Committee meeting in Philadelphia. (Invited Participant)
- June 17-22, 2007: Gordon Research Conference, Proteins Session, Holderness School, Plymouth, NH. - Invited Speaker (http://www.grc.uri.edu/programs/2007/proteins.htm)
- July 8, 2007: EURO Working Group on Operational Research in Computational Biology, Bioinformatics and Medicine, Invited talk, Prag. (http://euro2007.vse.cz/)
- July 29- Aug 3, 2007: Gordon Research Conference on Computer Aided Drug Design, at Tilton School in New Hampshire (Invited Speaker) http://www.grc.org/programs.aspx?year=2007&program=cadd
- August 19-23, 2007: 234th Annual ACS meeting in Boston (Invited Speaker) I
- Dec 6, 2007: McGowan Institute for Regenerative Medicine Seminar Series. Invited Speaker. www.mirm.pitt.edu/events/seminarseries.asp
- Dec 7, 2007: Duke University. Seminar

- December 18, 2007: NIH Center for Scientific Review (CSR) Open House meeting, Chair of a CSR Biomolecular Chartered Study Section

2008

- Jan 14-18, 2008: Institute for Mathematics and its Applications (IMA) workshop on "Mathematics of Molecular and Cellular Biology", University of Minnesota, Invited Speaker. (www.ima.umn.edu)
- February 1, 2008: Seminar at Carnegie Mellon University, School of Computer Science
- April 6-10, 2008: International Symposium on "Multiscale Modeling in Biophysics", Spring 2008 National Meeting of the American Chemical Society in New Orleans, Louisiana. Invited Speaker. (http://aiche.confex.com/aiche/s08/computation.htm)
- April 30, 2008: Case Western Reserve University, Center for Proteomics and Spectrometry, Cleveland, Ohio, Invited Speaker.
- June 8-13, 2008: President's Meeting of the International Society of Quantum Biology and Pharmacology (ISQBP) at the Centro Stefano Franscini, Ascona, Switzerland. Plenary Lecturer
- July 18-19, 2008: ISMB Annual Satellite Meeting on Structural Bioinformatics and Computational Biophysics (3DSig 2008), Toronto. Keynote Speaker
- July 19-23, 2008: ISMB-2008 16th International Conference on Intelligent Systems for Molecular Biology, Toronto, Canada. Program Committee and Highlights Session Chair.
- August 26- Sept 20, 2008: Weizmann Institute of Science, Rehovot, Israel, Visiting Professor and Invited Speaker, Department of Structural Biology
- September 2 and 9: Seminars at Weizmann Institute, Structural Biology Department, Rehovot, Israel.
- September 18, 2008: Seminar at Hebrew University, Biological Sci Dept, Jerusalem, Israel
- October 2-4 , 2008: 2008 BMES (Biomedical Engineering Society) Fall Meeting, "Gateway to Innovation", St Louis. Invited Speaker
- October 9 – 11, 2008: 8th KIAS-Yonsei Protein Conference, Seoul, Korea, Invited Speaker
- October 17 – 20, 2008: RiMed Foundation Fellowship Interviews, Invited Speaker and Interviewer, Member, Palermo, Italy, RiMed Foundation Scientific Committee.

2009

- February 1 - 3, 2009: NSF's Awardees conference, "Building Connections within the Engineering Education Research Community," Reston, VA. Hosted by the NSF's Division of Engineering Education and Centers and Virginia Tech's Department of Engineering Education, invited participant.
- March 22-27, 2009: 2009 Spring ACS National meeting Phys. Chem. Symposium on Functional Motions in Enzyme Catalysis, Salt Lake City. Invited Speaker
- April 14, 2009. John K. Vries Inaugural Lecture, University of Pittsburgh
- April 24, 2009. Seminar, Center for Simulations and Modeling, University of Pittsburgh.
- April 28, 2009. Seminar, University of Pittsburgh Cancer Institute.
- April 30, 2009. Seminar, Department of Environmental and Occupational Health, Graduate School of Public Health, University of Pittsburgh
- June 5-10, 2009: 2009 Keystone Symposium on Protein Dynamics, Allostery and Function, Keystone, Organizer and Speaker, co-organizer: Lila M. Gierasch.
- September 7-10: CECAM Workshop on 'Coarse-graining Biological Systems: Towards Large-Scale Interactions and Assembly" Lausanne, Switzerland, Invited Speaker.
- October 16-17, 2009: 22nd Annual Student Sponsored Symposium organized by NIH-funded Cell and Molecular Biology and Molecular Biophysics Programs, at the University of Illinois, Keynote Speaker

- October 21, 2009: Blue Knot Initiative, United Jewish Federation of Greater Pittsburgh, University of Pittsburgh School of Medicine, Pittsburgh, PA; Speaker.
- October 29, 2009: MB/SB Seminar Series, Department of Structural Biology, University of Pittsburgh.
- November 11, 2009: City College of New York (CCNY); Seminar Speaker
- December 5, 2009: NYU Courant Institute, Annual COB (Computational Biology Research) Day. Featured Speaker.

2010

- January 4-8, 2010: Pacific Symposium on Biocomputing Modeling of Biological Macromolecules, Big Island of Hawaii, Invited Speaker
- January 10-15, 2010: 5th Gordon Research Conference on Protein Folding Dynamics, Ventura Beach, CA; Invited Speaker
- April 29-30, 2010: Biological Interfaces: A TYC Computational Modelling Workshop, King's College London Guy's Campus, New Hunt's House, London, UK. Invited Speaker
- June 6-11, 2010: Gordon Research Conference on Biopolymers, Session on binding, allsotery and dynamics, Salve Regina University in Newport, RI. Invited Speaker
- July 5-9, 2010: TSRC, Telluride Workshop on Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, Colorado. Invited Speaker
- July 21, 2010: NIH Interdisciplinary Molecular Sciences and Training Review Panel on Computational Biology, Image Processing, and Data Mining. Panel Chair, Washington, DC
- August 1-3, 2010: MERCURY National Conference on Undergraduate Computational Chemistry, Hamilton College, Clinton, NY. Invited Speaker
- September 7-8, 2010: Workshop on 'Coarse-Grained Modelling of Biological Systems', Kavli Royal Society Center, Organized by UK Royal Society to celebrate its 350th anniversary. Kavli, Milton Keynes, UK, Invited Speaker
- September 25-28, 2010: 24th Annual Gibbs Conference in Biothermodynamics, Touch of Nature Conference Center in Carbondale Illinois. Invited Speaker
- October 14-16, 2010: Chemical Physics IX Congress, Cesme, Izmir, Turkey. Invited Speaker
- October 20-23, 2010: PPS2010 - Polymer Processing Society Istanbul Regional Meeting, Istanbul, Turkey, Invited Speaker
- October 23-27, 2010: RiMed Foundation Fellowship Interviews, Member, Palermo, Italy, RiMed Foundation Scientific Committee, Palermo, Italy. Scientific Committee Member
- December 1, 2010: University of Rochester, Biochemistry and Biophysics Seminar Series, Rochester, NY, Seminar Speaker
- December 4-7, 2010: The Zing Conference on Structural Biology and Drug Discovery, The Ocean Coral, Puerto Morelos, Cancun, Mexico, Invited Speaker

2011

- January 3-7, 2011: Pacific Symposium on Biocomputing 2011, PSB Session on Multi-scale Modeling of Biosystems: From Molecular to Mesoscale, Kona, Big Island of Hawaii, Invited Speaker
- March 5-9, 2011: Biophysical Society 55th Annual Meeting, Executive Board Meeting and Session Co-Chair on Molecular Dynamics, Baltimore DC
- May 18-25, 2011: The International Congress on Bioinformatics and Biomics, Pine Bay Holiday Resort, Kusadasi, Turkey, Invited Speaker
- June 9, 2011: Membrane Protein Structural Dynamics Consortium (MPSDC), Annual Meeting, Chicago, IL; Invited Speaker and Consortium Member.
- June 13, 2011: Biophysical Society, Austin, TX, Spring Executive Board Meeting

- June 14-18, 2011: Albany 2011: The 17th Conversation, at the State University of New York at Albany, Invited Speaker
- July 4-7, 2011: International Conference on Mathematical Biology, Institute Mathematics Initiative (IMI), at IISc, Bangalore, India, Invited Speaker
- July 14-19, 2011: 19th Annual Conference on Intelligent Systems for Molecular Biology (ISMB) and the 10th Annual European Conference on Computational Biology (ECCB), Program Committee Member, and ISCB Student Council Symposium Keynote Speaker, Vienna, Austria.
- September 16, 2011: Biochemistry Colloquium, Department of Chemistry & Biochemistry, University of Arizona, Invited Speaker
- October 14, 2011: Seminar, University of Akron, Department of Polymer Engineering, Akron, Ohio
- December 3-7, 2011: The Zing Conference on Protein and RNA Structure Prediction, The Ocean Coral, Puerto Morelos, Cancun Mexico, Invited Speaker

2012

- February 25-29, 2012: 56th Biophysical Society Annual Meeting. San Diego, CA. Executive Committe Member, Council Member and Panelist
- March 7-9. 2012: EMBO Workshop VIZBI 2012 on Visualizing Biological Data, Visualization of Proteins & Complexes Session, European Molecular Biology Laboratory. Heidelberg, Germany, Invited Speaker
- April 24, 2012: Seminar at SUNY Buffalo, NY.
- May 2-4, 2012: Membrane Protein Structural Dynamics Consortium (MPSDC), Chicago, IL. Invited Speaker and Discussion Panel member.
- June 3-8, 2012: Gordon Research Conference on Biopolymers, Salve Regina, Newport, RI, Vice Chair
- September 6, 2012: Seminar at the Ohio State University, Children's Hospital.
- October 8-10, 2012: CECAM Workshop "Signalling pathways: Interplay between microscopic changes and global behavior of biological systems." Ecole Normale Supérieure de Cachan, France, Invited Speaker.
- December 3-7, 2012: Zing Conference on Mathematical and Computational Medicine, Mexico. Plenary Speaker.

2013

- January 13-18, 2013: Gordon Research Conference (GRC) on Stochastic Physics in Biology. Ventura, CA. Invited Session Chair.
- January 21-23, 2013: Review Committee Meeting for The International Human Frontier Science Program Organization. Strasbourg, France, Committee Member.
- March 7-8, 2013: Tetralateral Symposium Tsinghua University, Hong Kong University of Science and Technology, and the Chinese University of Hong Kong. Invited Speaker.
- March 18-19, 2013: NIH Biomedical Technology & Research Centers (P41) Directors Meeting, Bethesda, MD. Invited Speaker.
- April 15-19, 2013: Conference on "Protein Dynamics and Function" Collingwood College, Durham University, UK, and workshop on Protein Dynamics and Function at the Durham Institute of Advanced Study, organized jointly between Durham Biophysics Sciences Institute and the EU Network SoftComp. Invited Speaker.
- May 6-9, 2013: Symposium on "Computational Biology: Then and Today". Weizmann Institute of Science, Rehovot, Israel, Keynote Speaker.
- May 14-16, 2013: GLBIO (Great Lakes Bioinformatics, a conference of the International Society for Computational Biology). Carnegie Mellon University, Pittsburgh, PA, Keynote Speaker.

- May 21, 2013: UPCI Basic and Translational Seminar Series. University of Pittsburgh Cancer Institute, PA. Invited Seminar Speaker.
- June 3-6, 2013: "In-silico Drug Design and In-silico Screening" track in Drug Discovery & Therapy World Congress 2013 International Conference. Boston, MA, Invited Speaker.
- June 10-14, 2013: Theoretical and Computational Biophysics Group Computational Biophysics Workshop, Pittsburgh, PA, Lecturer.
- July 1-3, 2013: NIH-Interdisciplinary Molecular Science and Training (IMST) Program Review Panel-Site Visit for P41 Application. University of Wisconsin, Madison. Review Panel.
- July 21-26, 2013: 7th International Discussion Meeting on Relaxations in Complex Systems (7th IDMRCS). Session: Amorphous pharmaceuticals and biopharmaceuticals - physical and chemical stability. Barcelona Spain. Invited Speaker.
- October 4, 2013: Science 2013 Symposium. Pittsburgh, PA. Invited Speaker.
- October 20-22. 2013: NIH Advisory Board Meeting. University of Illinois Urbana-Champaign, IL. Advisory Board Member.
- October 25, 2013: Publications Committee Meeting. Rockville, MD. Committee Member.
- December 9-10, 2013: NIH R15 Area Review. Washington, DC. Review Panel (Study Section) Member.

2014

- January 14, 2014: Laufer Center Seminar Series. Stony Brook University, New York. Invited Seminar Speaker.
- January 20-22, 2014: The International Human Frontier Science Program Research Grant Review Committee. Strasbourg, France. Review Committee Member.
- February 15-19, 2014: Biophysical Society 58th Annual Meeting on "Bridging the Sciences to Explore Biology". Moscone Center in San Francisco, California. Invited Speaker at the Mid Career Luncheon.
- Febuary 19, 2014: Biophysical Society Publications Committee Meeting. San Francisco, California. Publications Committee Member.
- March 5-7, 2014: NIH Review Panel for National Biomedical Computation Resource (P41-BTRC) Program. UCSD, San Diego, CA. Review Panel Member.
- March 24-25, 2014: National Institute of Biomedical Imaging and Bioengineering (NIBB) and National Institute for General Medicine Sciences (NIGMS) Biomedical Technology Research (P41) Centers Principal Investigator Meeting. Rockville, Maryland. P41 Principal Investigator.
- April 4, 2014: Saint Francis University Seminar Series. Invited Seminar Speaker.
- April 7, 2014: NIH Library of Integrated Network-Based Cellular Signatures (LINCS): Perturbation-Induced Data and Signature Generation Centers (U54) Area Review. Washington, DC. Review Panel Chair.
- May 7-9, 2014: Membrane Protein Structural Dynamics Consortium Frontiers in Membrane Protein Structural Dynamics. Chicago, IL. Invited Speaker.
- May 11-19, 2014: Collaborative book writing meeting at Stony Brook University. Stony Brook, NY.
- May 19-23, 2014: Hands-on Workshop on Computational Biophysics. Pittsburgh Supercomputing Center, Pennsylvania. Instructor.
- June 2-6, 2014: Gordon Research Conference on Biopolymers. Salva Regina, Chair of the Conference.
- June 15-19, 2014: Coarse-graining as a Frontier of Statistical Mechanics Conference. Santa Fe, New Mexico, Invited Speaker.
- July 16-19, 2014: Zing Conference on Protein Folding. Punta Cana, Dominican Republic, Invited Speaker.
- August 11-14, 2014: IUPAP Conference for Computational Physics (CCP 2014). Boston, MA, Invited Speaker.

- September 10-14, 2014: Biophysical Society Thematic Meeting "Modeling of Biomolecular Systems Dynamics, Allostery and Regulation: Bridging Experiments and Computations." Istanbul, Turkey. Organizing Committee Member.
- September 30, 2014: Children's Hospital of Pittsburgh of UPMC, Molecular Medicine Research Seminar Series. Pittsburgh, PA. Seminar Speaker.
- October 20-21, 2014: Biophysical Publications Committee Meeting. Rockville, Maryland. Committee Member.
- October 30-31, 2014: MMBioS National Center for Multiscale Modeling of Biological Systems External Advisory Board Meeting. Pittsburgh, PA. Principal Investigator.
- November 11, 2014: Seminar Series, Department of Chemistry and Biochemistry. University of Maryland, Baltimore, Maryland. Invited Speaker.
- December 4, 2014: Israeli Biochemistry Society Meeting on "Molecular Machines in Action". Weizmann Institute of Science, Rehovot, Israel. Keynote Lecturer.

2015

- January 12-16, 2015: Collaborative book writing meeting at Stony Brook University. Stony Brook, New York.
- January 26-28, 2015: The International Human Frontier Science Program Research Grant Review Committee. Strasbourg, France. Review Committee Member.
- February 5, 2015: Inaugural Lecture for your appointment as Distinguished Professor of Computational and Systems Biology in the School of Medicine, University of Pittsburgh. Pittsburgh, PA.
- February 7-11, 2015: In Vivo Biophysics Subgroup Symposium in conjunction with the Bridging the Sciences: Computation and Experiment, Biophysical Society 59th Annual Meeting. Baltimore, Maryland. Invited Speaker.
- February 15-20, 2015: 22nd International Molecular Medicine Tri-Conference. San Francisco, CA. Featured Speaker.
- March 9-11, 2015: Cup XV OpenEye Scientific Software's Annual Meeting, Santa Fe, CA. Levinthal Lecturer.
- March 22-26, 2015: ACS National Meeting Symposium, "Progress and Challenges in Molecular Simulations of Biomolecules". Denver, Colorado. Invited Presenter and Speaker.
- March 30-31, 2015: Chair of the NIH IMST-R, Pilot Centers for Precision Disease Modeling (U54) study section meeting. Washington, DC. Chair.
- April 16, 2015: Bioengineering Department Seminar Series, University of Pittsburgh, PA. Invited Seminar Speaker.
- April 23-24, 2015: NIH Director's New Innovator Award Review, Bethesda, Maryland. Editorial Review Panel Member.
- June 1-5, 2015: Hands-on Workshop on Computational Biophysics. Pittsburgh Supercomputing Center, Pennsylvania. Instructor.
- June 29-July 1, 2015: The International Human Frontier Science Program Selection Committee, Strasbourg, FR. Selection Committee Member.
- August 9-10, 2015: P01DK096990 External Advisory Board Meeting, Pittsburgh, PA. Computational Pharmacology Core PI.
- September 7-9, 2015: 8th SFB35 Transmembrane Transporters in Health and Disease Symposium, Vienna, Austria. Invited Speaker.
- September 17-18, 2015: MMBioS National Center for Multiscale Modeling of Biological Systems External Advisory Board Meeting. Pittsburgh, PA. Principal Investigator.

- September 20-22, 2015: NINDS Board of Scientific Counselors meeting. Bethesda, MD. Ad Hoc Reviewer.
- October 1-2, 2015: Center for Causal Discovery (CCD) External Advisory Board Meeting. University of Pittsburgh, PA. Principal Investigator.
- November 11, 2015: University of Pittsburgh Drug Discovery Institute (UPDDI) External Advisory Board (EAB) meeting. Speaker.
- November 17-18, 2015: NIH P01 Program Project application "Molecular structure, dynamics, and mechanism of key membrane transporters and enzymes in cellular metabolism". Review Panel Chair.
- December 4, 2015: CATER Seminar Series. Invited Seminar Speaker.
- December 7, 2015: University of Maryland Biophysics Program, Seminar Series. Invited Seminar Speaker.

2016

- January 19-20, 2016: Structural and Computational Biology and Molecular Biophysics (SCBMB) program, Baylor College of Medicine, Houston, TX. Review Board Member.
- January 25-27, 2016: The International Human Frontier Science Program Selection Committee, Strasbourg, FR. Selection Committee Member.
- February 9, 2016: External Advisory Board Meeting for P41 NIGMS Center for Biomolecular NMR Processing and Analysis, UConn Health, Farmington, CT. Invited EAB Member.
- February 10,2016: Arizona State University in the Center for Biological Physics Seminar Series, Tempe, AZ. Invited Speaker.
- March 13-15, 2016: NIH BTRR P41 Directors Meeting, Bethesda, MD. Invited Speaker.
- March 15-17, 2016: "Landscapes, Pathways, and Kinetics in Biomolecular Simulations" Symposium, 251st ACS National Meeting & Exposition. San Diego, California. Invited Speaker.
- June 6-10, 2016: Hands-on Workshop on Computational Biophysics. Pittsburgh Supercomputing Center, Pennsylvania. Instructor.
- June 13-16, 2016: The Center for Causal Discovery from Biomedical Data, Summer Short Course. Instructor.
- June 21, 2016: Webinar to SBGrid members on software application, ProDy. Presenter.
- July 11-12, 2016: NIBIB Training Grantees Meeting. Natcher Conference Center, NIH Main Campus, Bethesda, MD. Invited NIBIB Training Program Director.
- July 18-20, 2016: 4th International Conference on Integrative Biology, "Innovation, Insight and Integration of Future Science". Courtyard Berlin City Centre, Germany. Invited Speaker.
- August 31-September 2, 2016: 9th SFB35 Symposium, "Transmembrane Transporters in Health and Disease". Vienna, Austria. Invited Chairperson.
- September 20, 2016: Academia Sinica, Seminar Series. Taiwan. Taiwan International Graduate Program Distinguished Lecturer.
- September 22, 2016: Institute of Bioinformatics and Structural Biology, National Tsing Hua University. Taiwan. Invited Lecturer.

GRANTS – FUNDED PROJECTS

ACTIVE

See the table on pages 11-12.

COMPLETED (2002- 2020)

NIDA Center of Excellence for Computational Drug Abuse Research (CDAR)
P30DA035778-01A1 (Multiple PI: Bahar, Xie, Xing) 8/1/14-7/31/20
NIH-NIDA $200,000 (Bahar Lab)
Recent years have seen a significant increase in the number of structurally characterized membrane proteins, including those implicated in drug abuse and addiction. We will take advantage of the rapidly accumulating structural data as well as advances in biocomputing technology to generate data and develop and disseminate software that will facilitate the design, discovery and development of structure-based computer-aided strategies against DA. (Role: co-PI and Project 2 Leader)

Center for Causal Modeling and Discovery of Biomedical Knowledge from Big Data
U54HG007934-01(Multiple PI: Cooper and Bahar) 9/15/14-9/14/19
NIH-NHGRI $131,607 (Bahar Lab)
We will establish our Center for Causal Modeling and Discovery (CCMD) of Biomedical Knowledge from Big Data as collaboration among the University of Pittsburgh (Pitt; lead institution), Carnegie Mellon University (CMU), and Yale University (Yale). The CCMD will develop, validate, and disseminate methods, tools, and software based on Causal Bayesian Networks, which will enable the broader scientific community to effectively interrogate large imaging, genomic, and clinical (phenotype) data and derive knowledge on the causality of observed phenomena.

Mitochondrial Targeting Against Radiation Damage
2U19AI68021-11 (PI: Greenberger) 9/1/2015-8/31/2020
NIH-NIAID $114,348 (Bahar Lab)
The Bahar lab is leading the Chemoinformatics/computational pharmacology core (Core F) of this NIAID-funded Center (Center for Medical Countermeasures against Radiation, CMCR). The Core is performing the following tasks: (1) assist in the design, screening, validation, and optimization of novel inhibitors using pharmacophores modeling, docking simulations and QSAR techniques, (2) screen and validate project-designed drugs for potential or expected side effects based on known structure and binding characteristics in close coordination with Core B, and (3) screen for predicted or expected drug polypharmacological effects and interactions as the "cocktail" of a multi-drug regimen is being formulated. (Role: Chemoinformatics Core PI)

Continued Development of Protein Dynamics Software ProDy
5R01 GM099738-02 (PI: Bahar) 3/26/2012-12/31/2016
NIH-NIGMS $174,483
Our lab has developed software and servers to enable the examination of the collective motions accessible to proteins under physiological conditions. In view of the growing recognition of the significance of protein dynamics in defining the mechanisms of biomolecular function, and the rapidly growing experimental data on protein structures in multiple forms, we extended our protein dynamics software into an integrated suite, ***ProDy***, with an easily modifiable and versatile programming interface

(API). *ProDy* provides the community with insights into the dominant motions and accessible conformers selected by families of proteins, and how they differentiate among subfamilies.

Structural Dynamics of Biomolecular Systems
5R01GM086238-04 (PI: Bahar) 1/1/2009-12/31/2014
NIH-NIGMS $191,881/yr (Bahar lab)
We are building on our previous work on biomolecular systems dynamics to further explore the structure -> dynamics -> function mapping of allosteric and/or multimeric/multisubunit proteins using physically-based and computationally efficient models, in collaboration with the NCBC Simbios group at Stanford U.

Supplement to BTRC on High Performance Computing for Multiscale Modeling
1P41GM103712 01S1 (PI: Bahar) 9/24/2012-7/31/2014
NIH-NIGMS $49,425/yr (Bahar lab)
This supplement aims at establishing aims at enabling the broad use of cutting-edge technology for performing molecular dynamics simulations software. This service will essentially be provided by the Pittsburgh Supercomputing Center, in coordination with D.E. Shaw for making accessible to selected group Anton supercomputing facilities, and providing adequate training and computing service.

Bridging Sequence Patterns and Structural
5R01LM07994-07 (PI: Bahar) 9/30/2003-9/29/2013
NIH-NLM $213,174/yr (Bahar lab)
Dynamics (former title: Alignment Independent Analysis of Sequence). The goal of this project is to analyze sequence conservation and co-evolution patterns with regard to the dynamic correlations inferred from elastic network models and the physical constraints imposed by structure. Our goal is to further our understanding of sequence-function relationships by investigating the couplings between sequence evolution and structural dynamics, with focus on a widely studied systems such as molecular chaperones, selected enzyme families and membrane proteins, along with their multimerization, assembly and intermolecular interactions.

Structure-based design of novel low molecular weight c-Myc inhibitors
5R01CA140624-05 (PI: Prochownik) 7/1/2009-5/31/2014
NIH-NCI $20,725 (Bahar lab)
c-Myc bHLH-ZIP oncoprotein is over-expressed by many cancers and in some cases is directly pathogenic. All known functions of c-Myc, including transformation, are dependent on its ability to heterodimerize with another bHLH-ZIP protein, Max. This project proposes studies that promise new insights regarding the rational design of Myc compounds and the mechanisms by which they disable this critical oncoprotein. (Role: Co-investigator)

Development of Multiscale Methods for Simulating Neurosignaling Systems Dynamics
Ri.MED Foundation (PI: Bahar) 9/1/2012-4/13/2013
Ri.MED (Italy) $50,684/yr
This is a fellowship award by the Italian government, aiming at supporting the work of a postdoctoral fellow, Dr. Filippo Pulara, working in Bahar lab on multiscale modeling of neurobiological transport and signaling events. (Role: PI/advisor)

Clinical & Translational Science Institute-Molecular and Systems Modeling (MSM) Core
5UL1RR024153-05 (PI: Reis) 7/1/2011-6/30/2013

NIH-NCRR $54,882/yr (Bahar lab)

The project aims at establishing the MSM Core as a new organizational structure that will (a) bring together a multi-disciplinary team of computational biologists to respond to the growing need of providing modeling expertise or assistance to life science researchers affiliated with, or supported by, the CTSI, (b) provide the environment and infrastructure to advance and integrate the tools that will promote the interaction between basic and clinical researchers in the broader Pittsburgh area, (c) generate new computational methods and tools, and (d) assist in the dissemination and efficient usage of these tools. (Role: Core co-Director).

Molecular Studies of Human CNS Glutamate Transporters

5R01NS033273-09 (PI: Amara) 4/1/2007-2/28/2013

NIH-NIMH $50,000/yr (Bahar lab)

This competing renewal builds upon the initial project and includes assessing the proximity of different residues during the transport cycle using introduced cysteine pairs and cross-l inking reagents; emphasizing kinetic, biochemical, pharmacological and electro-physiological aspects of excitatory amino acid transport. (Role: Co-investigator)

Membrane Protein Structural Dynamics Consortium-Core

U54GM087519 (PI: Perozo, U of Chicago) 8/15/2010-9/30/2012

NIH-NIGMS $30,000/yr (Bahar lab)

This is a large scale collaborative project, with the goal of developing experimental and computational methods that will help understanding the mechanism of function of membrane proteins implicated in neurotransmission, regulation and signaling activities, the malfunction of which entails significant neurodegenerative diseases. A molecular understanding of the machinery of membrane proteins, is a first step towards developing rational therapeutics against these diseases. Role: Co-investigator

Integrated, Interdisciplinary Inter-University PhD Program in Computational Biology

NIBIB 5T32EB009403-02 (PI: Bahar - transferred in 2009 to Benos) 1/4/2009-3/31/2011

NIBIB $ 295,725/yr (fellows)

This proposal supports the interdisciplinary graduate training program in Computational Biology that has been built under a grant from HHMI in Phase I of the HHMI-NIBIB Interfaces Initiative. It is a truly joint program between Carnegie Mellon University (CMU) and the University of Pittsburgh (Pitt), with a single point of admissions for students and equal representation of the two universities in all committees and administration. A guiding principle is that all students receive deep training in both computational and natural sciences, and, that they be fully versed in its principles and paradigms.

Bioengineering and Bioinformatics Summer Institute on Simulation and Computer Visualization of Biological Systems at Multiple Scales

EEC 0609139 and 0234002 (PI: Bahar) 9/15/2002-8/31/2006 and 1/1/2007-1/1/2010

NSF-NIBIB

This educational program jointly offered between the University of Pittsburgh, Pittsburgh Supercomputing Center, Duquesne University and Carnegie Mellon University aims at exposing students to the current state-of-the-art in the field of molecular to cellular simulations, both in terms of biological advances and computational methods

Computational Prediction of Biomolecular Dynamics

1R33 GM068400 01A2 (PI: Bahar) 9/15/2005-8/31/2008

NIH – NIGMS $220,000/yr

The goal of this project is to develop both computationally efficient and physically realistic models and methods for estimating the collective dynamics of large structures and assemblies, and in particular to assess the cooperative motions that are relevant to key biological functions. Collaborators include Pitt Faculty (Co-PI Hassan Karimi, School of Information Sci.,) and Faculty from Cornell U (Ron Elber; Co-PI), and from the Pittsburgh Supercomputing Center.

In silico screening strategies for identifying small molecule inhibitors of PUMA mediated apoptosis
U19AI68021-05 (PI-Greenberger) 9/1/2009-8/31/2010
NIH-NIAI $62,476/yr (Bahar lab)
The goal of the proposed studies is to utilize computational methods and high throughput *in silico* screens to identify potential lead compounds that disrupt the interaction between PUMA and Bcl-2 proteins. Compounds resulting from this screening process will be tested in enzymatic inhibition assays to evaluate the abilities of these newly identified compounds to inhibit PUMA. (Role: Co-investigator)

Building Better Predictive Computational Models of Complex Biological Processes
MPC 09-01-1 (PI: Benos) 1/1/2009-6/30/2010
MPC Corporation $28,932/yr (Bahar Lab)
The purpose is to develop efficient computational models and methods to study the interactions of DSPs with small molecules toward developing selective and potent inhibitors. (Role: Co-investigator)

Dendritic Cell Biology and Therapy
2P01 CAO73743-06 (PI: Finn) 7/1/2004-6/30/2009
NIH – NCI $14,300/yr (Bahar lab)
The goals of this program project are 1) to understand the roles of different dendritic cells (DC) subsets in vitro and in vivo to affect customized responses to distinct antigens and pathogens; 2) to understand which DC subsets function in different tissues and how they mediate aberrant immune responses that lead to disease; 3) to understand if their in vivo function can be modulated to prevent or cure disease in animal models. Role: Co-Investigator

Comprehensive, Inter-University Ph.D. Program in Computational Biology
HHMI 56005679 (PI: Murphy) 1/1/2006-12/31/2008
HHMI-NIBIB $166,200/yr (Pitt)
This is a multi-track Ph.D.-granting program in computational biology, offered jointly by the University of Pittsburgh and Carnegie Mellon University. The primary goal of that support has been the careful development and evaluation of new curriculum and procedures for the program. Role: Co-PI

Pittsburgh Molecular Libraries Screening Center
1U54MH074411 (Lazo) 7/1/05-6/30/08
NIH $112,820/yr (Bahar Lab)
The goals of the MLSC will be to (1) validate assays for use in high throughput screening, (2) use these assays with secondary assays and informatics to identify active small molecules from chemical libraries, (3) facilitate the use of these assays nationally, (4) disseminate information about compound activity, and (5) assist in the further optimization of the lead compounds. Role: Director, Bioinformatics Core

Multiscale Dynamics of Cell Cycle Control and Apoptosis
Pre-NPEBC Program, P20 (PI: Bahar) 8/1/2003-8/14/2007
NIH-NIGMS $250,000/yr (Bahar lab)

This is a multi-institutional planning grant that is intended to lay the groundwork for the establishment of a National Program of Excellence in Biomedical Computing at the University of Pittsburgh, School of Medicine in partnership with Carnegie Mellon University, Duquesne University and the Pittsburgh Supercomputing Center. The objective is to develop and integrate new tools for understanding molecular-to-cellular dynamics, with focus on the interactions involved in cell cycle regulation and signaling. http://www.health.pitt.edu/pcbc/

Computational Learning and Discovery for Protein Sequence, Structure & Function Mapping

EIA-0225636 (PI: Raj Reddy, CMU) 09/15/02-08/31/07

NSF – ITR $81,743/yr (Bahar lab)

This is a multi-institutional, large scale collaborative project between the University of Pittsburgh (Judith Klein-Seetharaman, Ivet Bahar, Hagai Meirovitch), Carnegie Mellon University (Raj Reddy, Jaime Carbonell, Roni Rosenfeld, Yiming Yang, Chien Ho), Massachusetts Institute of Technology (Jonathan King, H. Gobind Khorana), Canadian National Research Council (Michele Loewen); and Boston University (Cathy Costello). The goal is to understand organism-specific protein sequence-structure-function mapping relations and develop novel statistical natural language models for predicting structure, folding/misfolding and function. Role: co-PI and Executive Committee Member