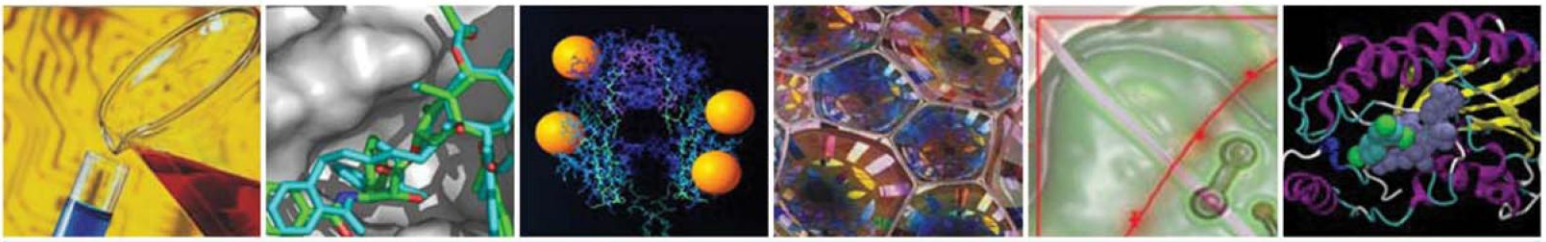
NINETEENTH ANNUAL SYMPOSIUM

ICB&DD



Institute of Chemical Biology & Drug Discovery

Drug Discovery &AI: Advances and New Directions

Thursday, October 2, 2025 ◆ Charles B. Wang Center

Distinguished Speakers

Dr. Nikolay Dokholyan, *University of Virginia*
Dr. Marta Filizola, *Icahn School of Medicine*
Dr. David Koes, *University of Pittsburgh*
Dr. Maria Wendt, *Sanofi Cambridge MA*
Dr. Patrick Walters, *OpenADMET*
Dr. Chris Sander, *Harvard Medical School*
Dr. Dima Kozakov, *UT Austin*

Poster Sessions ◆ Poster Awards

For more information, please visit
http://ws.cc.stonybrook.edu/icbdd/

Stony Brook University

From the Director

The primary objective of the Institute of Chemical Biology & Drug Discovery (ICB&DD) is to establish and sustain a world-class "Center of Excellence" in chemical biology and drug discovery at Stony Brook University. The rapid and impressive advancements in chemical biology during the last decade have clearly demonstrated that solutions for a vast majority of medical problems rely on the understanding of the molecular basis of diseases, therapeutic targets, drug actions, and drug resistance. ICB&DD promotes highly productive interdisciplinary and collaborative research among chemists, biologists, medicinal chemists, pharmacologists, and physicians to tackle major biomedical problems to find solutions including the discovery of novel therapeutic drugs and innovative diagnostic tools.

—Iwao Ojima, Director, Institute of Chemical Biology & Drug Discovery

Dr. Iwao Ojima received his B.S., M.S., and Ph.D. (1973) degrees from the University of Tokyo, Japan. He joined the Sagami Institute of Chemical Research and held a position of Senior Research Fellow until 1983. He joined the faculty at the Department of Chemistry, State University of New York at Stony Brook first as Associate Professor (1983), was promoted to Professor (1984), Leading Professor (1991), and then to Distinguished Professor (1995). He served as the Department Chair from 1997 to 2003. He has been serving as the founding Director for the Institute of Chemical Biology and Drug Discovery (ICB&DD) from 2003. He has a wide range of research interests in synthetic organic and medicinal chemistry as well as chemical biology, including discovery and development of anticancer agents, antimicrobials, and targeted drug delivery systems. His awards and honors include Arthur C. Cope Scholar Award (1994), E. B. Hershberg Award for Important Discoveries of Medicinally Active Substances (2001), the Medicinal Chemistry Hall of Fame (2006), ACS Award for Creative Work in Fluorine Chemistry (2013), and E. Guenther Award in the Chemistry of Natural Products (2019) from the American Chemical Society; the Chemical Society of Japan Award (1999); Outstanding Inventor Award (2002) from the Research Foundation of the State University of New York; Elected Fellow of J. S. Guggenheim Memorial Foundation, the American Association for the Advancement of Science, the New York Academy of Sciences, the American Chemical Society, the National Academy of Inventors and the European Academy of Sciences.

ICB&DD's History and Mission

The ICB&DD was established in 2004 with Stony Brook University's institutional support as well as the NYSTAR Faculty Development Award. One of ICB&DD's strengths is that it was founded by reorganizing existing exceptional talents on campus, and thus the core of the institute is a well proven entity with an excellent history. ICB&DD is open to a wide range of collaborative research programs with pharmaceutical and biotechnology industrial firms. Members of ICB&DD are from the departments of Chemistry, Biochemistry and Cell Biology, Pharmacological Sciences, Microbiology and Immunology, Physiology and Biophysics, Applied Mathematics and Statistics, Medicine, Pathology, Oral Biology and Pathology, Psychiatry and Behavioral Health, Neurobiology and Behavior, Laufer Center for Physical and Quantitative Biology, Cancer Center, and Cold Spring Harbor Laboratory. In addition, ICB&DD has two core laboratories located in the Chemistry Building: Analytical Instrumentation Laboratory and Discovery Chemistry Laboratory.

ICB&DD has three major programs: Structural and Computational Biology Program, Infectious Diseases Research Program, and Cancer Research Program. In addition, ICB&DD has been providing critical support to the Chemical Biology Training Program.

ICB&DD collaborates with the Stony Brook University Cancer Center to develop a Cancer Therapeutics Program. ICB&DD integrates the existing strengths at Stony Brook University in the basic medical sciences as well as medicinal chemistry and brings in complementary expertise from outside to explore drug discovery and development. At present, ICB&DD focuses on drug discovery in therapeutics for cancer, infectious diseases, neurodegenerative diseases, and inflammation.

Through ICB&DD connections, many collaborative research teams have been created, and research proposals have successfully acquired grants from the NIH and other funding agencies. (Total grant funding > 81M). Currently, there are nine ongoing ICB&DD-designated projects (Total funding: $23M).

ICB&DD 19th Annual Symposium

Thursday, October 2, 2025, Stony Brook Wang Center

"Drug Discovery & AI: Advances and New Directions"

9:05 am to 9:20 am	**Opening Remarks** ***Dr. Ivet Bahar,*** Louis and Beatrice Laufer Endowed Chair and Director of the Laufer Center for Physical and Quantitative Biology. Chair Symposium Organizing Committee ***Dr. Carl W. Lejuez*** *Provost, Stony Brook University* ***Dr. Iwao Ojima***, Distinguished Professor and Director, Institute of Chemical Biology and Drug Discovery (ICB&DD), Stony Brook University
9:20 am to 10:05 am	**Dr. Nikolay Dokholyan,** Professor**,** University of Virginia School of Medicine, Department of Neurology. Director, Center for Health Intelligence. *"Artificial Intelligence-Driven Drug Discovery"*
10:05 am to 10:50 am	**Dr. Marta Filizola,** Sharon & Frederick A. Klingenstein-Nathan G. Kase, MD Professor, the Icahn School of Medicine at Mount Sinai *"Advancing GPCR Drug Discovery with Integrative Modeling, Structural Dynamics, and Artificial Intelligence*"
10:50 am to 11:35 am	**Dr. David Koes,** Associate Professor, Department of Computational and Systems Biology, University of Pittsburgh *"Deep Learning for Structure-Based Drug Discovery: From Scoring to Generative Design"*
11:35 am to 12:20 pm	**Dr. Maria Wendt,** VP, Global Head of Preclinical Computational Innovation Strategy, Sanofi. Cambridge, MA *"Faster, Better, Smarter Biologics: Going for Gold with AI"*
12:20 pm to 1:30 pm	**Lunch and Poster Session** *(East Hall for faculty and Zodiac Gallery for students)*
1:30 pm to 2:15 pm	**Dr. Patrick Walters**, Chief Scientist, OpenADMET, Cambridge, MA *"There's No Free Lunch, But You Can Get a Discount – Applying Active Learning in Drug Discovery"*
2:15 pm to 3:00 pm	**Dr. Chris Sander** Professor in Residence of Cell Biology, Harvard Medical School "*Machine Learning for Hard Biological Problems"*
3:00 pm to 3:45 pm	**Coffee Break and Student Poster Session** *(Theatre Lobby)*
3:45 pm to 4:30 pm	**Dr. Dima Kozakov,** Professor, Oden Institute for Computational Engineering and Sciences, UT Austin. Member, Laufer Center for Physical & Quantitative Biology *"Modeling Disease with Atomic Resolution with Physics Aware Deep Learning"*
4:30 pm to 4:55 pm	**Dr. David LeBard**, Head of Science, EyesOpen and Cadence Molecular Science, Santa Fe, New Mexico *Drugging the Undruggable: "A Highly Accurate Method for Predicting, Detecting, and Ranking Cryptic Pockets"*
4:55 pm to **5:00 pm**	**Closing Remarks**: Dr. Ivet Bahar
5:00 pm to 6:00 pm	**Reception and Poster Session *(three poster awards)***, *(Theatre Lobby)*
6:00 pm to 6:15 pm	**Announcement of Poster Awards:** Dr. Anupam Banerjee
6:15 pm	**DINNER,** *East Hall (by invitation only)*

Speakers

Dr. Nikolay Dokholyan, Ph.D. received his PhD in Physics in 1999 at Boston University and completed postdoctoral training at Harvard University in the Department of Chemistry and Chemical Biology as a NIH NRSA Fellow. Dr. Dokholyan joined the Department of Biochemistry and Biophysics at the University of North Carolina at Chapel Hill School of Medicine as an Assistant Professor in 2002 and was promoted to (Full) Michael Hooker Distinguished Professor in 2011. Dr. Dokholyan has served as the Director of the Center for Computational and Systems Biology and the Graduate Director of the Program in Molecular and Cellular Biophysics at UNC. Dr. Dokholyan has published over 350 peer-reviewed articles and 21 book chapters. In 2018, Dr. Dokholyan moved to Penn State College of Medicine and assumed the position of the G. Thomas Passananti Professor and Vice Chair for Research in the Department of Pharmacology. Dr. Dokholyan is the Editor-in-Chief of *Proteins*. Dr. Dokholyan was elected to be a Fellow of the American Physical Society (2012), the American Association for the Advancement of Science (2019), and the American Institute for Medical and Biological Engineering (2022). Dr. Dokholyan joined Penn State Clinical and Translational Science Institute as an Associate Director in 2022. In 2024, Dr. Dokholyan joined the Editorial Board of PNAS Nexus. In 2025, Dr. Dokholyan moved to the University of Virginia School of Medicine, Department of Neurology. He will lead the Center for Health Intelligence.

"Artificial Intelligence-Driven Drug Discovery"

We will describe a new generation of computational approaches to drug discovery that integrate physics-based modeling with artificial intelligence to accelerate the identification of novel therapeutics. At the foundation is MedusaDock, a physics-driven docking platform for accurate prediction of ligand–protein binding. To scale this capability, we developed MedusaNet, a machine-learning framework that prioritizes candidate compounds for docking, and NeuralDock, a deep-learning tool that bypasses physical docking altogether, enabling virtual screening of up to a billion compounds per day. While these platforms accelerate discovery, rational design remains central to creating effective therapies. To this end, we developed YuelDesign, an AI-guided platform for *de novo* drug design. YuelDesign integrates structural biology, medicinal chemistry principles, and generative AI models to design novel compounds with optimized binding affinity, selectivity, and drug-like properties. YuelDesign opens frontiers beyond screening existing chemical space into the proactive design of molecules tailored to specific therapeutic needs, expanding the frontier of molecular innovation. To ensure that drug candidates are not only potent but also safe, we established the Drug–Receptor Interaction Fingerprinting Technology (DRIFT), an AI-powered platform designed to systematically map drug–protein interactions and predict off-target effects. DRIFT represents a paradigm shift: it not only accelerates drug repurpose and novel therapeutic discovery but also provides a roadmap for ensuring safety and efficacy earlier in the development process. By enabling *silico* pharmacology at scale, DRIFT extends discovery beyond traditional small molecules to natural products, botanicals, and new molecular modalities, opening opportunities for breakthroughs in diseases long considered untreatable. Taken together, MedusaDock, MedusaNet, NeuralDock, YuelDesign, and DRIFT form a comprehensive and transformative ecosystem that unites physics, data-driven learning, and artificial intelligence into a coherent vision for the future of medicine. This integrated approach moves beyond incremental advances in efficiency—it redefines the scale, speed, and imagination with which we can explore chemical and biological space. Finally, we will discuss our ongoing efforts to incorporate quantum computing into this ecosystem, with the potential to capture molecular complexity at levels unimaginable with classical computation. These advances mark the beginning of a new era in drug discovery, one in which computation does not merely aid discovery, but fundamentally drives it.

David LeBard, Ph.D., is a Director of Scientific Software and the Head of Target Exploration at OpenEye. He has a background in both theoretical and computational modeling of complex biological systems and works to foster industrial and academic collaborations that find solutions to problems in drug discovery, including modeling of passive permeability of drug-like molecules, rare-event sampling of biomolecules, and cryptic pocket detection in proteins thought undruggable.

"Drugging the Undruggable: "A Highly Accurate Method for Predicting, Detecting, and Ranking Cryptic Pockets"

An unfortunate truth is that many proteins involved in the most prolific life-threatening diseases remained elusive as therapeutic targets for decades simply because a binding pocket for a molecular inhibitor could not be found. One classic example is the KRAS protein, which is a GTPase involved in more than 25% of all human cancers, yet persisted as an undruggable target for over 30 years despite immense efforts by academic and industrial researchers to find a viable pocket. To help expand the druggable proteome to include difficult-to-drug targets like KRAS, we present an automated computational workflow that allows anyone to validate a protein for its ligandability. With only a protein structure (X-Ray, Cryo-EM, Al-generated, etc.), our workflow uses a Weighted Ensemble path sampling strategy using intrinsic normal modes as progress coordinates to sample rare protein conformational states, which are analyzed with a set of Markov state models to identify residues that cooperatively form pockets. Furthermore, the workflow also ranks detected pockets by their ligandability using a neural network model estimator of the potential to bind a ligand in the pocket. The automated workflow is performed entirely with elastic cloud computing inside the Orion® platform and can uncover pockets that form either by conformational selection of rare protein states or through an induced-fit mechanism by a probe molecule. In this work, we present a proof-of-concept study of KRASG12D to illustrate that our methodology can predict known cryptic pockets, including the Switch-II pocket that remained hidden for decades. Finally, a validation of our automated protein sampling and cryptic pocket detection workflow on a set of proteins that represent several dozen unique pocket types will also be presented.

Speakers

Marta Filizola, Ph.D. is the Sharon & Frederick A. Klingenstein-Nathan G. Kase, MD Professor at the Icahn School of Medicine at Mount Sinai, with appointments in the Departments of Pharmacological Sciences, Neuroscience, and Artificial Intelligence and Human Health. She also serves as Dean of the Graduate School of Biomedical Sciences, where she oversees accreditation of all PhD and Master's degree programs, directs training for postdoctoral fellows, and contributes to institution-wide strategic planning in graduate education. Dr. Filizola's research focuses on uncovering mechanistic insights into the structure, dynamics, and function of key membrane proteins, such as G Protein-Coupled Receptors, transporters, channels, and β3 integrins, using a wide range of computational approaches, including molecular modeling, molecular dynamics and metadynamics simulations, free-energy calculations, cheminformatics, and AI/ML-driven drug design. A native of Italy, Dr. Filizola earned her bachelor's and master's degrees in chemistry from the University of Naples Federico II, a PhD in Computational Chemistry from the Second University of Naples and completed postdoctoral training in Computational Biophysics at the Molecular Research Institute in California.

"Advancing GPCR Drug Discovery with Integrative Modeling, Structural Dynamics, and Artificial Intelligence"

A comprehensive understanding of drug efficacy in G Protein-Coupled Receptor (GPCR)-mediated signaling requires atomic-level insights into the conformational dynamics and kinetics that govern ligand-specific GPCR–G protein activation. Such details cannot yet be achieved with a single method; instead, it demands the integration of data from multiple experimental and computational approaches. At the same time, the field urgently needs chemical probes with defined pharmacological profiles, tools that can both illuminate GPCR function and guide the development of safer, more effective therapeutics. Artificial intelligence (AI), when coupled with high-resolution GPCR structures and ultra-large chemical libraries, offers transformative opportunities to accelerate this discovery process. In this talk, time permitting, I will highlight our recent advances in this area, including: (a) a Bayesian integrative modeling framework that recalibrates conformational ensembles of ligand-bound GPCR–G protein complexes from enhanced molecular dynamics (MD) simulations using kinetic insights into G protein conformational dynamics obtained from single molecule-imaging; (b) long-timescale MD simulations of experimentally derived conformational states of GPCR-G protein complexes along the G-protein activation pathway, revealing how ligands with distinct safety and efficacy profiles shape GPCR signaling; (c) robust network analyses of allosteric communication pathways across experiment-informed conformational ensembles to generate testable hypotheses about the molecular basis of safer drug action; and (d) innovative AI/machine learning strategies designed to accelerate and refine GPCR-targeted therapeutic discovery.

David Koes, Ph.D. is an Associate Professor in the Department of Computational and Systems Biology at the University of Pittsburgh. He develops and applies innovative computational methods to accelerate drug discovery by combining machine learning, discrete algorithms, and structural modeling. A key focus of his work is the creation of open-source, easy-to-use software platforms that lower the barrier to entry for drug discovery, such as the Pharmit online virtual screening resource and the GNINA molecular docking software. He received his PhD in computer science from Carnegie Mellon University in 2009.

"Deep Learning for Structure-Based Drug Discovery: From Scoring to Generative Design"

Structure-based drug discovery has been transformed by the integration of deep learning, enabling more accurate modeling of protein–ligand interactions and the scalable exploration of chemical space. In this talk, I will present our work developing and applying deep convolutional neural networks (CNNs) for protein–ligand scoring, docking, and virtual screening, with a focus on our open-source docking software GNINA. These models have demonstrated strong performance in both retrospective benchmarks and prospective applications, including results from the CACHE community wide assessment. I will then discuss how these CNN architectures form the foundation for LiGAN, an early generative model that learns to propose 3D ligand structures directly within a protein binding site. Extending beyond CNNs, I will describe more recent efforts using graph-based deep generative models for both unconditional molecule generation and conditional design with a focus on our state-of-the-art FlowMol flow matching model. Finally, I will introduce SPRINT, a novel embedding method that leverages learned latent spaces for ultrafast virtual screening, enabling rapid prioritization of large compound libraries with minimal loss of accuracy. Together, these approaches illustrate a unified deep learning pipeline for structure-based drug discovery—spanning docking, screening, and generative design.

Speakers

Maria Wendt, Ph.D. is VP, Global Head of Preclinical Computational Innovation Strategy for R&D at Sanofi in Cambridge, MA. With 25 years of experience bridging computation and biology, Maria oversees AI and computational strategies across all therapeutic areas, research platforms, precision medicine, translational sciences and CMC units. Prior to this, she was Global Head of Digital Biologics Strategy and Innovation, focusing on smart biologics and AI-driven discovery. From 2019-2023, Maria was Head of Biologics Research US covering the biologics portfolio for immunology and inflammation, immuno-oncology and rare and neurological diseases. Before Sanofi, Dr. Wendt spent 18 years at Genedata AG, in Basel, Switzerland, rising to Head of Science. She was the Founding Principal Scientist of Genedata Biologics® and Bioprocess® platforms, widely used in the pharmaceutical industry. Early in her career, she specialized in -omics Big Data and led part of the EU InnoMed Predictive Toxicology consortium from 2004-2008. Dr. Maria Wendt holds a Ph.D. in Chemical Engineering from Iowa State University.

"Faster, Better, Smarter Biologics: Going for Gold with AI"

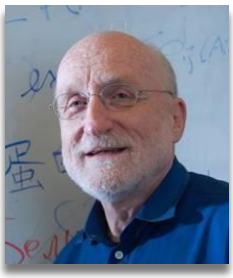
I will be discussing the revolution in biologics, novel mechanisms (incl. how it is changing the landscape of cancer), complex modalities and the need and applications of AI. The biopharmaceutical industry is entering its fourth wave of innovation, marked by the emergence of multi-targeting therapeutics that are transforming our approach to complex diseases, particularly in immunotherapy and cancer treatment. I will present how artificial intelligence is revolutionizing our ability to design sophisticated biological molecules that can simultaneously engage multiple disease pathways. Through our Biologics x AI Moonshot program at Sanofi, we've achieved significant breakthroughs in protein engineering and molecular design, moving beyond traditional single-pathway interventions to engineer more effective immune responses. Our comprehensive Digital Biologics Strategy has yielded remarkable results, including the first successful demonstration of virtual screening for complex biologics, achieving approximately 80% accuracy in predicting protein expression and activity. I will showcase how our innovative use of Protein Language Models (PLMs) and deep learning approaches are accelerating the development of "smart biologics" that can tackle previously undruggable targets. This transformation in drug discovery represents a pivotal moment in medicine, where AI-driven multi-specific antibodies and sophisticated therapeutic platforms are enabling us to address unmet medical needs with unprecedented precision. For patients, this means potential access to more effective, precisely targeted treatments that could revolutionize outcomes in cancer and other challenging diseases.

Patrick Walters, Ph.D. is the Chief Scientist at OpenADMET in Cambridge, MA. an open science initiative that combines insights from high-throughput experimentation, structural biology, and machine learning to improve the prediction of drug absorption, metabolism, excretion, and toxicity. Before his current role, Pat spent thirty years in leadership positions at Relay Therapeutics and Vertex Pharmaceuticals. Pat is the 2023 recipient of the Herman Skolnik Award for Chemical Information Science from the American Chemical Society. He is a member of the editorial advisory boards for the Journal of Chemical Information and Modeling and Artificial Intelligence in the Life Sciences and previously held a similar role with the Journal of Medicinal Chemistry. Pat is co-author of the book "Deep Learning for the Life Sciences", published in 2019 by O'Reilly and Associates. He received his Ph.D. in Organic Chemistry from the University of Arizona where he studied the application of artificial intelligence in conformational analysis. Prior to obtaining his Ph.D., Pat worked at Varian Instruments as both a chemist and a software developer. He received his B.S. in Chemistry from the University of California, Santa Barbara.

"There's No Free Lunch, But You Can Get a Discount – Applying Active Learning in Drug Discovery"

While computational methods have become a mainstay in drug discovery programs, many calculations take too long to be used with large datasets. Active learning (AL), a machine learning technique that guides searches iteratively, can make it possible to use computationally intensive methods like relative binding free energy (RBFE) on datasets with thousands of molecules. Additionally, AL can be applied to virtual screening, allowing for the rapid analysis of billions of molecules. This presentation will offer an overview of two practical uses of AL in drug discovery.

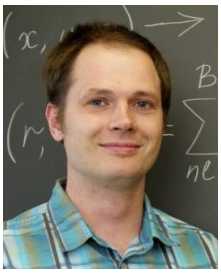
Speakers



Chris Sander, Ph.D was trained as a theoretical physicist and as postdoc switched to theoretical biology. He founded two computational biology departments, at the European Molecular Biology Laboratory and Memorial Sloan Kettering Cancer Center. He co-founded the research branch of the European Bioinformatics Institute and built a center for computational biology at Dana-Farber Cancer Institute. At Harvard Medical School his group and collaborators focus on solving hard biological problems using AI and statistical learning at the level of molecules, cells and humans. (1) EVcouplings: Protein structure and function from natural and experimental evolution – building on the concept of co-evolution developed by him for the first successful protein folding in 2011 (EVfold) and now a key ingredient in the latest AI methods for protein structure prediction. (2) CancerRiskNet: Identifying high risk of cancer from real-world clinical records using machine learning. They analyze real-world clinical records to define patient groups at high risk for aggressive cancers and collaborate with clinicians to design screening programs aimed at catching cancer early. (3) Perturbation Biology & CellBox: after developing the foundational concept of perturbation biology, they derive computational models of cell biological processes from large-scale and single cell perturbation-response experiments, especially using mass spec protein profiling, and the design of anti-resistance cancer combination therapy. As a service to the research community, they build tools for the research and clinical communities, such as the EVcouplings server for highlighting co-evolution patterns in protein sequences and 3D structures and mutation effects of genetic variation, with focus on human genomes; the Pathway Commons knowledge resource; and the cBioPortal for Cancer Genomics in collaboration with the Knowledge Systems Groups at MSKCC and DFCI.

Machine Learning for Hard Biological Problems

AI and statistical learning can generate quantitatively predictive and actionable predictions at the level of molecules, cells and humans. (1) EVcouplings: protein structure from experimental evolution; design of proteins for sustainability of life. (2) Perturbation Biology: designing targeted intervention from large-scale perturbation-response proteomics experiments. (3) CancerRiskNet: Identifying high risk of pancreatic cancer from real-world clinical records for early detection and therapeutic or preventive intervention. On the biomedical applications of perturbation biology: Cells and organisms have evolved as robust to external perturbations and adaptable to changing conditions. This capacity poses severe problems for cancer patients. Some targeted anti-cancer drugs work remarkably well, yet resistance is almost certain to emerge. We use experimental perturbation biology (systematic perturbation coupled with rich observation of response, such as changes in protein levels and protein modifications by protein mass spectrometry) to derive executable network models for cancer cells that guide the development of combination therapy, especially combination of targeted compounds rather than general chemotherapeutics.



Dima Kozakov, Ph.D received an MS in Applied Mathematics and Physics at the Moscow Institute of Physics and Technology, and PhD in Biomedical Engineering at Boston University. Currently, he is the W. A. "Tex" Moncrief, Jr. Chair in Computational Life Sciences and Biology, and Center Director for AI/Physics in Drug Discovery at UT Austin. He is also a Research Professor at Stony Brook University. Dr. Kozakov is interested in method development for modeling of biological macromolecules, with emphasis on molecular interactions and drug design. Dr. Kozakov's approaches, ClusPro for protein docking and FTMap for hotspot identification, are heavily used in academia and the pharmaceutical industry and are consistently top-performing in blind molecular modeling completions.

"Modeling and Modulation of Disease with Atomic Resolution with Physics Aware Deep Learning"

Understanding disease mechanisms requires connecting molecular interactions to cellular and organismal outcomes. We present an integrative framework that combines state-of-the-art deep learning with physics-based modeling to achieve atomic-resolution insights into macromolecular interactions at the proteome scale. Our approach enables structural modeling of protein–protein, protein–ligand, and post-translationally modified complexes in both healthy and diseased contexts. By mapping these interaction networks, we aim to uncover the organizational principles that drive disease progression and identify actionable targets for therapeutic intervention. We follow up with therapeutic development through the modeling of antibodies, PROTACs, and molecular glues, providing a path toward engineering-driven strategies for drug discovery and precision medicine.

NOTES_____

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Acknowledgments

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