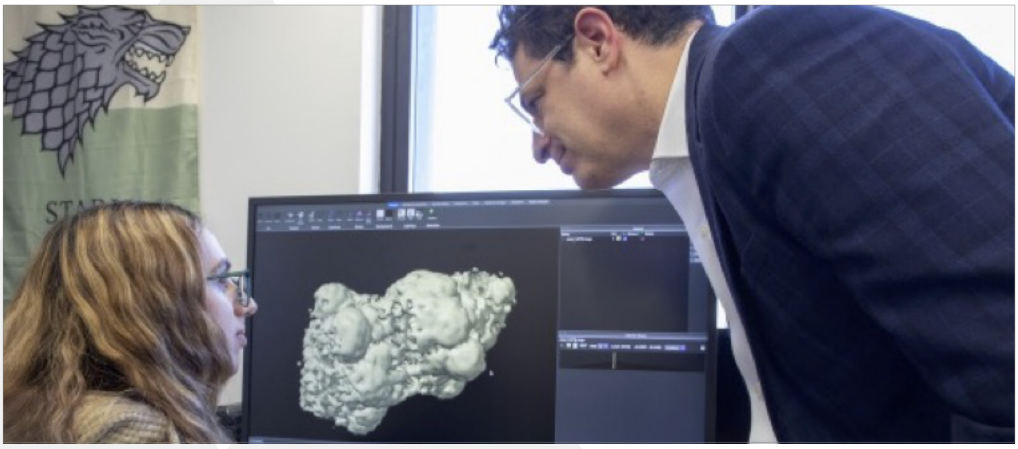
Icahn School of Medicine at Mount Sinai

Department of Pharmacological Sciences

BIA
FIRST BIANNUAL
2025

LAUNCH OF MOUNT SINAI AI SMALL MOLECULE DRUG DISCOVERY CENTER



Emma Young & Dr. Schlessinger, conduct structural analysis of a novel drug target. Credit: MSHS

We are excited to announce the launch of the **Mount Sinai AI Small Molecule Drug Discovery Center**, led by Prof. Avner Schlessinger. The Center integrates machine learning with chemical and structural biology to accelerate the design of novel small-molecule therapeutics.

One of the core challenges in drug discovery is navigating the vastness of chemical space—estimated to contain more than 1060 possible molecules. The Center aims to develop predictive models and generative algorithms that can efficiently explore this space, identify new drug targets, and rapidly design compounds to modulate them.

A key strength is access to unpublished and negative experimental data generated across Mount Sinai—resources rarely available in public datasets but highly valuable for improving model accuracy. Research efforts focus on producing pharmacologically validated probes and early-stage leads that can serve as the foundation for future translational efforts.

The Center is also launching a seminar series and a monthly discussion group to foster collaboration in AI-driven drug discovery across the department and the broader Sinai research community. The first distinguished seminar will feature Dr. Pat Walters, Chief Data Officer at Relay Therapeutics, on November 20. Stay tuned for additional events.

DPS RANKED #2 IN PHARMACOLOGY NATIONWIDE FOR 2024

We're thrilled to share that the Department of Pharmacological Sciences has been ranked **#2 in the nation for NIH funding in 2024** by the Blue Ridge Institute for Medical Research in Pharmacology—a remarkable leap from #3 in 2023. This achievement speaks volumes about the dynamic and impactful work being carried out in our department.

This success is a direct reflection of our vibrant research and education programs and the tireless dedication of every team member. Your commitment to advancing scientific discovery and innovation is truly inspiring. We look forward to building on this momentum in 2025 and beyond—here's to reaching even greater heights!

NEW CORE SCIENTIST FOR THE CRYO-EM CORE

Rampradeep Samiappan, PhD, has joined as Staff Scientist for the Cryo-Electron Microscopy (Cryo-EM) Core Facility. With over 10 years of experience in structural biology, he trains and supports researchers in preparing and analyzing biological samples at high resolution.

The Core is equipped with state-of-the-art tools, including a Vitrobot system for sample preparation and a Thermo Fisher Glacios 2 Cryo-TEM microscope with advanced detectors and software. Together, these resources enable scientists to visualize proteins and other biological structures in exceptional detail, advancing research in drug discovery and disease mechanisms.

For more information and booking details, please visit **the Cryo-EM CoRE page.**

FEATURED NEWS

Bacterial CBASS systems commonly kill virally infected cells by degrading genomic DNA. Drs. Rechkoblit (right), Aggarwal (left) from DPS, together with Dr. Gang Fang at the Department of Genomics and Genomic Sciences, have unveiled the structure of the bacterial CBASS effector Cap5, which degrades DNA and triggers bacterial self-destruction.

The Cap5 tetramer, activated by a cyclic nucleotide, digests double-stranded DNA via its tetrameric HNH endonuclease domains. Two HNH domains adopt a catalytically active conformation for DNA strand cleavage, while the other two are in a topologically distinct, catalytically inactive state that mediates DNA binding. All four HNH domains track one face of the DNA, marking Cap5 as a stand-alone, non-specific nuclease.

The authors further show that chromosomally encoded CBASS Cap5 can be extrinsically activated by a cyclic nucleotide—a finding that could inform the development of potential antibiotics.

Read More on Nature Communications!

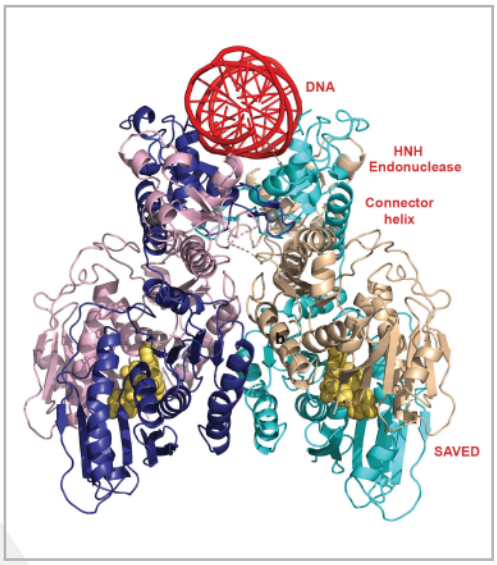


Figure | Structure of the CBASS Cap5 tetramer with DNA. CBASS Cap5 protein tetramer (shown in cyan, beige, blue and pink) formed upon binding to the cyclic dinucleotide (shown as yellow spheres) to destroy bacteria's own DNA.

PAPERS

Rechkoblit O, Sciaky D, Ni M, Li Y, Kottur J, Fang G, **Aggarwal AK**. Mechanism of DNA degradation by CBASS Cap5 endonuclease immune effector. ***Nat Commun***. 2025 Jun 5;16(1):5243.

Provasi D, **Filizola M**. Fine-Tuned Deep Transfer Learning Models for Large Screenings of Safer Drugs Targeting Class A GPCRs. ***Biochemistry***. 2025 Mar 18;64(6):1328-1337.

Qian C, Wang Z, Xiong Y, Zhang D, Zhong Y, Inuzuka H, Qi Y, Xie L, Chen X, Wei W*, **Jin J***. Harnessing the Deubiquitinase USP1 for Targeted Protein Stabilization. ***J Am Chem Soc***. 2025 Apr 30;147(17):14564-14573.

Diamant I, Clarke DJB, Evangelista JE, Lingam N, **Ma'ayan A**. Harmonizome 3.0: integrated knowledge about genes and proteins from diverse multi-omics resources. ***Nucleic Acids Res***. 2025 Jan 6;53(D1):D1016-D1028.

He Z, Tu YC, Tsai CW, Mount J, Zhang J, Tsai MF, **Yuan P**. Structure and function of the human mitochondrial MRS2 channel. ***Nat Struct Mol Biol***. 2025 Mar;32(3):459-468.

Vann KR, Sharma R, Hsu CC, Devoucoux M, Tencer AH, Zeng L, Lin K, Zhu L, Li Q, Lachance C, Ospina RR, Tong Q, **Cheung KL**, Yang S, Biswas S, Xuan H, Gatchalian J, Alamillo L, Wang J, Jang SM, Klein BJ, Lu Y, Ernst P, Strahl BD, Rothbart SB, **Walsh MJ**, Cleary ML, Côté J, Shi X, **Zhou MM***, Kutateladze TG*. Structure-function relationship of ASH1L and histone H3K36 and H3K4 methylation. ***Nat Commun***. 2025 Mar 6;16(1):2235.

GRANTS

Jinye Dai, PI, "*Investigating Glutamate Delta-type Receptors in the Synaptic Pathology of Schizophrenia*", Alkermes Pathways Research Awards. Alkermes, Inc., 04/01/2025-04/01/2027, $100,000

Jian Jin, Samir Parekh, MPI, "*Developing Lysine Methyltransferase SETD8 Selective Inhibitors for Treating Multiple Myeloma*", R01CA290791, NCI, 06/11/2025-05/31/2030, $3,506,650

Marta Filizola, PI, "*Leveraging Integrative Modeling and AI-Based Tools to Develop Safer Opioids*", R01DA063209, NIDA, 07/01/2025-03/31/2030, $3,768,530

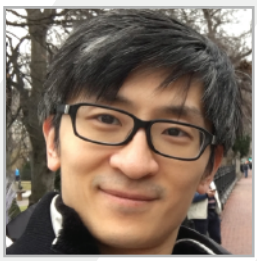
Avner Schlessinger, **Ming-Ming Zhou**, **Eric Sobie**, MPI, "*Integrated Training in Pharmacological Sciences*", T32GM154814, NIGMS, 07/15/2025-06/30/2030, $1,656,350

Sander Houten, **Robert DeVita**, **Michael Lazarus**, MPI, "*Targeting succinyl-CoA:glutarate-CoA transferase as a novel therapeutic strategy for glutaric aciduria type 1*", R01HD118270, NICHD, 08/01/2025-07/31/2030, $ 3,629,586

Tony Yuen, Weibin Zhou, **Mone Zaidi**, Ki Goosens, **Vitaly Ryu**, MPI, "*AAV-mediated Interrogation of the Brain FSH Receptor*", R61AG094602, NIA, 08/01/2025-07/31/2027, $2,129,396

View more **Publication & Grants** of 2025!

HONORS & AWARDS



KA LUNG (WILLIAM) CHEUNG, PhD
Assistant Professor

JIAN JIN, PhD
Professor

MONE ZAIDI , MD, PhD, MACP
Professor

The exceptional accomplishments of our students, postdocs and faculty are reflected in the prestigious honors they have received from peers. We are proud to announce that Dr. Ka Lung (William) Cheung received the Mount Sinai Faculty Council Award for Academic Excellence by a Junior Faculty Member, Dr. Jian Jin was honored with The Pharmaceutical Society of Korea Distinguished Lectureship Award, and Dr. Mone Zaidi received the 2025 William F. Neuman Award from the American Society of Bone and Mineral Research. Please join us in congratulating our esteemed colleagues for their achievements.

UPCOMING EVENT

THE 18TH ANNUAL RESEARCH RETREAT OF THE DEPARTMENT OF PHARMACOLOGICAL SCIENCES
THE 18TH JACK PETER GREEN LECTURESHIP

Brian T. Chait, D.Phil.
Camille and Henry Dreyfus Professor
Laboratory for Mass Spectrometry
and Gaseous Ion Chemistry
The Rockefeller University

"Towards a Molecular Microscope"

Thursday, September 11th, 2025
9 AM - 5 PM

Goldwurm Auditorium, Icahn Building
1425 Madison Avenue, New York NY 10029

Registratrion Required:
https://bit.ly/dps_retreat

THE 25TH IRVING L. SCHWARTZ LECTURE

The Department continues its proud tradition of hosting lectures at the forefront of science. On May 29, 2025, Carol Robinson, DBE, FRS, FMedSci FRSC, Dr. Lee's Professor of Chemistry from the University of Oxford (UK), delivered the 25th Irving L. Schwartz Lectureship in Structural & Chemical Biology. Her lecture, titled "Isolation of Metabotropic Glutamate Receptors from Human Brain Uncovers Remodeling in Depression", was held in Hatch Auditorium of the Guggenheim Pavilion, followed by a reception.

DPS NETWORKING

The Department kicked off 2025 with a successful Networking Hour in Annenberg 19-79, hosted by Lakshmi Devi, PhD and Eric Sobie, PhD. They curated a delightful spring-themed event with a fantastic spread of food and refreshing beverages, providing a wonderful opportunity for faculty, staff, and students to connect and relax.

PHD STUDENTS SUPPORTED BY THE NEWLY AWARDED T32

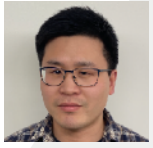
We are excited to introduce the inaugural cohort of PhD students supported by the newly awarded T32 in Pharmacological Sciences. This prestigious training grant supports six outstanding candidates engaged in innovative, multidisciplinary research at the interface of drug discovery, pharmacology, and disease mechanisms.

The cohort includes Jesus Ayala (Lazarus), Olivia Cullen (Schlessinger), Abigail Daily (Azeloglu/Satlin), Anna Mortari (Wacker), Christian Valade (Dai), and Emma Young (Slesinger/Schlessinger). Together, they represent diverse areas of expertise and backgrounds, with research interests spanning receptor pharmacology, chemical biology, AI, neuropharmacology, and translational systems pharmacology.

These trainees were selected for their academic excellence, scientific potential, and commitment to advancing impactful translational research. We look forward to the groundbreaking discoveries this next-generation cohort will contribute to the field.

MEMBERS UPDATE

NEW MEMBERS



Ci Chu, PhD
Postdoctoral Fellow
Wacker Lab

Laxmi Tiwari, PhD
Assistant Scientist
DeVita Lab

ALUMNI

Alexander Lachman, PhD
Assistant Professor
Ma'ayan Lab

Lauren Qiu
Associate Researcher
Yazawa Lab

PROMOTIONS

Kaixiu Luo, PhD
Associate Scientist
Jin Lab

Maryam Mansoori, PhD
Associate Scientist
Hadri Lab

View All

EXTERNAL PAGES

Visit our other pages for more notable news from our department!

PUBLICATIONS GRANTS AND AWARDS MEMBERS DPS WEBSITE