The Eighth Annual Research Retreat of the **Department of Structural** and Chemical Biology Icahn School of Medicine at Mount Sinai

October 15 & 16, 2015

Edith Macy Conference Center 550 Chappaqua Road Briarcliff Manor, NY 10510 www.edithmacy.com



Organizer: Oscar Chea



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The Department of Structural and Chemical Biology applies state-of-the-art tools of experimental and computational structural biology, biophysics, and chemical biology to study fundamental problems in biomedical research with emphasis on the molecular and structural basis of human biology and disease. Major approaches include biochemistry and biophysics of proteins/nucleic acids/membranes, chemical biology of small molecules, electrophysiology, molecular biology, electron cryomicroscopy, NMR spectroscopy, X-ray crystallography, computational modeling and simulation. Topics of investigation include structure and function of membrane enzymes and receptors in cell signaling and development; and molecular mechanisms of gene transcription and translation, epigenetic regulation and DNA damage repair in stem cell biology, immunology and virology with ultimate goal to understand the molecular basis of human diseases such as cancer, Parkinson's, Alzheimer's disease and genetic disorders.

The mission of the Department is to provide a nurturing environment for discovery and innovation in basic and translational biomedical research of human biology and disease, and for advanced academic training of physicians and scientists; and to function as a scientific hub for interdisciplinary collaborations with researchers of different disciplines to tackle most challenging problems in biomedical sciences.

For more information about the exciting biomedical research and education programs being conducted in the Department of Structural and Chemical Biology, we invite you to visit the following website:

http://icahn.mssm.edu/departments-and-institutes/structural-and-chemical-biology

ON THE COVER

Alex Scopton, *PhD*, *Postdoc Fellow/The Dar Lab* Due to their central role in cellular signaling protein kinases are one of the most intensively studied drug targets across all therapeutic areas. We are interested in developing new kinase inhibitors to serve as chemical probes to study the mechanisms of cellular signaling, as well as lead compounds for the development of new cancer therapies. As one approach, we are using a fragmentation/recombination strategy, which utilizes the individual components of known kinase inhibitors to generate novel compounds.

PROGRAM

THURSDAYDAY, OCT 15th

11:00 AM	Departure from Mount Sinai
12:15 PM	Lunch

Afternoon Session (Chair: Jian Jin)

1:15 - 1:30	Setup & Welcome
1:30 - 2:15	Group I - Jian Jin
2:15 - 2:40	Group 2 - Robert DeVita
2:40 - 3:25	Group 3 - Iban Ubarretxena
3:25 - 3:45	Coffee Break
3:45 - 4:30	Group 4 - Aneel Aggarwal
4:30 - 5:15	Group 5 - Martin Walsh
5:15 - 6:00	Group 6 - Ming-Ming Zhou

6:30 - 7:30 Poster Session

Evening Session

7:30 - 11:30 Dinner & Evening Program

FRIDAY, Oct 16th

9:00-10:00 AM Breakfast		
Morning Session (Chair: Mihaly Mezei)		
10:00-10:25	Group 7 - Roman Osman	
10:25-10:50	Group 8 - Mihaly Mezei	
10:50-11:15	Group 9 - Roberto Sanchez	
: 5- :35	Coffee Break	
11:35-12:00	Group 10 - Marta Filizola	
12:00-12:25	Group II - Michael Ohlmeyer	
12:25-12:50	Group 12 - Arvin Dar	
12:50-1:05	Awards & Closing Remarks	
1:05 - 2:20	Lunch / Nature Break	

2:30 PM Departure

2015 PRESENTING GROUPS



Ming-Ming Zhou, Professor & Chair

Structural and molecular mechanisms of chromatinbased gene transcription or silencing in human biology and diseases.



Aneel Aggarwal, Professor

Protein-nucleic acid interactions in gene transcription and translation, and DNA repair with X-ray crystallography and other biophysical methods.



Arvin Dar, Assistant Professor

Exploring links between the regulation of drug targets and the system level properties of biological networks within cells and animals.



Robert DeVita, Professor

Small molecule drug discovery, chemical biology, target validation, organic synthesis and heterocyclic chemistry.



Marta Filizola, Professor

Structure-function correlation in molecular recognition and signal-transduction through the development and application of computational methods.



Jian Jin, Professor

Creating chemical probes of histone methyltransferases and functionally selective ligands of G protein-coupled receptors.



Mihaly Mezei, Associate Professor

Developing computational techniques for structural analysis of macromolecular and for small molecule design.



Michael Ohlmeyer, Associate Professor

Small-molecule drug discovery. Hit to lead and lead optimization chemistry.



Roman Osman, Professor

Molecular mechanisms of enzymatic DNA repair, receptor/ligand binding and rational drug design using molecular dynamics and simulations methods.



Roberto Sanchez, Associate Professor

Development of structural bioinformatics tools for protein structure-function relationship with emphasis on ligand recognition and disease related mutations.



Iban Ubarretxena, Associate Professor Structural and molecular mechanism of regulated intramembrane proteolysis in biology and disease. We combine biochemical methods and cryo-EM.



Martin Walsh, Associate Professor Mechanisms that regulate chromatin structure through processes that recognize and establish epigenetic information necessary to modulate gene transcription.

