

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

October 13 & 14, 2014

Edith Macy Conference Center  
550 Chappaqua Road  
Briarcliff Manor, NY 10510  
[www.edithmacy.com](http://www.edithmacy.com)



*Organizer: Cevita Webb*



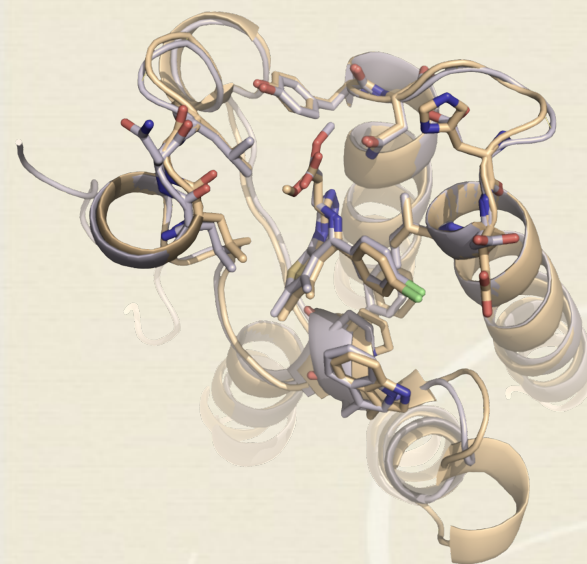
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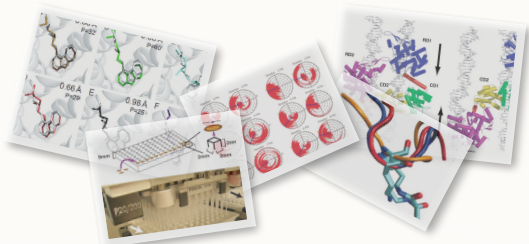
**DEPARTMENT OF STRUCTURAL  
AND CHEMICAL BIOLOGY**

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**2014 Research Retreat**  
Department of Structural  
and Chemical Biology





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://licahn.mssm.edu/departments-and-institutes/structural-and-chemical-biology>

#### On The Cover



Crystal Structures of BRD4 bromodomains bound to an inhibitor MS417 - Nicolas Babault Ph.D., Winner of the 6th SCB Annual Research Retreat 2013

#### GUEST SPEAKER



**Vivian Stojanoff, Adjunct Assistant Professor**  
A spokesperson for the NIGMS East Coast Research Facility for structural biology at the NSLS. Her research interest is focused on the characterization of bio-molecular crystals and the development of new synchrotron methods and techniques for structural biology and biological materials.

# PROGRAM

## MONDAY, OCT 13<sup>th</sup>

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

### Afternoon Session (Chair: Roman Osman)

1:15 - 1:30 Setup & Welcome  
1:30 - 2:20 Group 1 - Jian Jin  
2:20 - 2:50 Group 2 - Robert DeVita  
2:50 - 3:40 Group 3 - Michael Ohlmeyer  
3:40 - 4:00 Coffee Break  
4:00 - 4:50 Group 4 - Iban Ubarretxena  
4:50 - 5:10 Group 5 - Vivian Stojanoff  
5:10 - 6:00 Group 6 - Aneel Aggarwal  
6:00 - 7:00 Poster Session

### Evening Session

7:00 - 8:00 Wine Tasting  
8:00 - 11:30 Dinner & Evening Program

## TUESDAY, Oct 14<sup>th</sup>

8:00-9:00 AM Breakfast

### Morning Session (Chair: Martin Walsh)

9:10-10:00 Group 7 - Marta Filizola  
10:00-10:30 Group 8 - Roman Osman  
10:30-10:50 Group 9 - Mihaly Mezei  
10:50-11:10 Coffee Break  
11:10-12:00 Group 10 - Premkumar Reddy  
12:00-12:30 Group 11 - Arvin Dar  
12:30-2:15 Lunch / Nature Break

### Afternoon Session (Chair: Michael Ohlmeyer)

2:15 - 3:05 Group 12 - Martin Walsh  
3:05 - 3:55 Group 13 - Ming-Ming Zhou  
3:55 - 4:05 Awards & Closing Remarks  
4:15 PM Departure

## 2014 PRESENTING GROUPS



**Ming-Ming Zhou, Professor & Chair**  
Structural and molecular mechanisms of chromatin-based 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.



**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 interactions, gene transcription and translation, as well as structure-based small-molecule design using free energy simulations and quantum mechanical/molecular mechanical methods.



**E. Premkumar Reddy, Professor**  
The role of cell cycle and apoptotic genes in cancer progression and as target for the development of novel anticancer drugs.



**Robert DeVita, Professor**  
Small molecule drug discovery, chemical biology, target validation, organic synthesis and heterocyclic chemistry.



**Iban Ubarretxena, Associate Professor**  
Structural and molecular mechanism of regulated intramembrane proteolysis in human 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.