

AGENDA (DAY 1)

APRIL 15, 2024 (MONDAY)

07:30 - 08:30 am **Registration and breakfast**
08:30 - 08:50 am **Welcome Address and Introduction to day 1 events**
Hendrik Luesch, Ph.D., *Director CNPD3, Department of Medicinal Chemistry, University of Florida*
Thomas Kodadek, Ph.D., *Department of Chemistry, UF Scripps*
Peter Swaan, Ph.D., M.Pharm., *Dean, College of Pharmacy, University of Florida*
Jon Licht, M.D., *Director, UF Health Cancer Center*

SESSION 1: Induced Proximity Drug Discovery

Conveners: Ciaran Seath (UF Scripps) and Xingui Liu (UF)

08:50 - 09:30 am **How PROTAC Degraders Work: Molecular Recognition and Design Principles (Keynote 1)**
Alessio Ciulli, Ph.D., Professor, *School of Life Science, University of Dundee*

09:30 - 09:50 am **Chemical Manipulation of Protein Post-Translational Modifications**
Thomas Kodadek, Ph.D., Professor, *Department of Chemistry, UF Scripps*

09:50 - 10:10 am **Chemical Tools to Study Biological Systems**
Monika Raj, Ph.D., Associate Professor, *Winship Cancer Institute, Emory University*

10:10 - 10:30 am **Leucine Rich Repeat Kinase 2 PROTACs**
Xingui Liu, Ph.D., Assistant Professor, *Department of Medicinal Chemistry, University of Florida*

10:30 - 10:50 am **Altering the H3 Methylation Landscape through Degradation of Methyl-Lysine Reader Proteins**
Lindsay James, Ph.D., Assistant Professor, *Eshelman School of Pharmacy, University of North Carolina*

10:50 - 11:05 am **BREAK**

SESSION 2A: Emerging Voices in Drug Research (Postdoctoral Fellows)

Convener: Gustavo Seabra (UF)

11:05 - 11:35 am Sam Afoullouss, Ph.D., *Department of Chemistry, University of South Florida*
Sofia Kokkaliari, Ph.D., *Department of Medicinal Chemistry, University of Florida*
Andrés Cumsille, Ph.D., *Department of Microbiology and Cell Science, University of Florida*
Dake Liu, Ph.D., *Department of Medicinal Chemistry, University of Florida*

11:35 - 12:35 pm **LUNCH BREAK**

SESSION 3: Drug Discovery for Infectious Diseases

Conveners: Robert Huigens (UF) and Luiz Carvalho (UF Scripps)

12:35 - 01:15 pm **Using Complex-and-Diverse Small Molecules to Explore Drug-Resistant Bacteria and Develop Novel Antibiotics (Keynote 2)**
Paul Hergenrother, Ph.D., Professor, *Department of Chemistry, University of Illinois Urbana-Champaign*

01:15 - 01:35 pm **Targeting Klebsiella pneumoniae Extracellular Polysaccharides Facilitates Capsular Loss and Biofilm Matrix Collapse**
Renee Fleeman, Ph.D., Assistant Professor, *Burnett School of Biomedical Sciences, University of Central Florida*

01:35 - 01:55 pm **Nature-Inspired Strategies to Overcome Mycobacterial Drug Resistance and Tolerance**
Kyle Rohde, Ph.D., Associate Professor, *Burnett School of Biomedical Sciences, University of Central Florida*

01:55 - 02:15 pm **A Multidisciplinary Approach to Developing a Targeted Therapy to Eliminate a Keystone Dental Pathogen from Oral Biofilms**
Jose Lemos, Ph.D., Professor, *College of Dentistry, University of Florida*

02:15 - 02:35 pm **Repurposing of Type II Human Kinase Inhibitors: Discovery of Resistance-Refractory Prophylactic and Therapeutic Antimalarial**
Debopam Chakrabarti, Ph.D., Professor, *Burnett School of Biomedical Sciences, University of Central Florida*

02:35 - 02:50 pm **BREAK**

SESSION 4: Natural Products and Synthetic Biology

Conveners: Marc Chevrette (UF) and Matthew Disney (UF Scripps)

02:50 - 03:30 pm **The Structure-based Design of Modern Hsp90 Inhibitors and their Biological Opportunities (Keynote 3)**
Brian Blagg, Ph.D., Professor, *Department of Chemistry and Biochemistry, University of Notre Dame*

03:30 - 03:50 pm **Advancing the Palmerolides**
Bill Baker, Ph.D., Professor, *Department of Chemistry, University of South Florida*

03:50 - 04:10 pm **Genome Mining for Bacterial Terpenoids**
Jeff Rudolf, Ph.D., Assistant Professor, *Department of Chemistry, University of Florida*

04:10 - 04:30 pm **Unveiling and Engineering Nature's Tools for Diketopiperazine Assembly**
Amy Lane, Ph.D., Professor, *Department of Chemistry and Biochemistry, University of North Florida*

04:30 - 04:50 pm **Heterologous Expression of Nutraceuticals, Antibiotics, and Anticoagulants for Use in Space**
Amor Menezes, Ph.D., Assistant Professor, *Department of Mechanical and Aerospace Engineering, University of Florida*

04:50 - 06:30 pm **POSTER SESSION**

AGENDA (DAY 2)

APRIL 16, 2024 (TUESDAY)

- 07:30 - 08:30 am **Registration and breakfast**
08:30 - 08:40 am **Introduction to day 2 events**
Hendrik Luesch, Ph.D., *Director CNPD3, Department of Medicinal Chemistry, University of Florida*
Thomas Kodadek, Ph.D., *Department of Chemistry, UF Scripps*

SESSION 5: AI-driven Drug Discovery

Conveners: Yanjun Li (UF) and Chenglong Li (UF)

- 08:40 - 09:20 am **Virtual Screening with GNINA and Pharmit (Keynote 4)**
David Koes, Ph.D., Associate Professor, *School of Medicine, University of Pittsburgh*
- 09:20 - 09:40 am **Rational Enzyme Engineering via AI for Therapeutic Development**
Wenjun Xie, Ph.D., Assistant Professor, *Department of Medicinal Chemistry, University of Florida*
- 09:40 - 10:00 am **Learning the Language of Life from DNA and Proteins**
Yana Bromberg, Ph.D., Professor, *Department of Biology, Emory University*
- 10:00 - 10:20 am **Exploring Vast Molecular Spaces with Instant Similarity**
Ramon Alain Miranda Quintana, Ph.D., Assistant Professor, *Department of Chemistry, University of Florida*
- 10:20 - 10:40 am **A Machine Learning Framework for Cancer Drug Sensitivity Estimation Using Time-lapse Microscopy Imaging**
Wei Zhang, Ph.D., Associate Professor, *Department of Computer Science, University of Central Florida*

10:40 - 10:55 am **BREAK**

SESSION 2B: Emerging Voices in Drug Research (Graduate Students)

Conveners: Gustavo Seabra (UF)

- 10:55 - 11:35 am Alexis R. Smith, *Department of Medicinal Chemistry, University of Florida*
Ridhwana Appiah, *Burnett School of Biomedical Sciences, University of Central Florida*
Corey M. Perkins, *Department of Pharmaceutics, University of Florida*
Nick McKee, *Center for Inflammation Science and Systems Medicine, UF Scripps*
Yuzhao Zhang, *Department of Medicinal Chemistry, University of Florida*

11:35 - 12:35 pm **LUNCH BREAK WITH SPONSOR PRESENTATIONS**

SESSION 6: Synthesis-driven Drug Discovery

Conveners: Justin Lopchuk (Moffitt) and Jane Aldrich (UF)

- 12:35 - 01:15 pm **Adventures in Drug Hunting (Keynote 5)**
Wendy Young, Ph.D., *former SVP, Drug Discovery, Genentech*
- 01:15 - 01:35 pm **Accelerating Drug Discovery Through Innovation in Asymmetric S(VI) Reagents and Methods**
Justin Lopchuk, Ph.D., Associate Professor, *Moffitt Cancer Center*
- 01:35 - 01:55 pm **Late-Stage C-H Functionalization of Bioactive Compounds**
Masayuki Wasa, Ph.D., Associate Professor, *Department of Chemistry, UF Scripps*
- 01:55 - 02:15 pm **Terpene-Inspired Mevalonate Pathway Inhibitors**
James Frederick, Ph.D., Associate Professor, *Department of Chemistry and Biochemistry, Florida State University*
- 02:15 - 02:35 pm **Diversity-Oriented Synthesis and MS/MS-Based Analysis of Brain Glycosphingolipids**
Zhongwu Guo, Ph.D., Professor, *Department of Chemistry, University of Florida*
- 02:35 - 03:00 pm **Closing Remarks and Awards**
Hendrik Luesch and Thomas Kodadek