

2024 Texas Chemical Biology Conference

**WHERE CHEMISTRY MEETS BIOLOGY :
DECODING LIFE'S LANGUAGE**



MAY 24-25, 2024

THE BIOSCIENCE RESEARCH COLLABORATIVE AUDITORIUM
RICE UNIVERSITY, HOUSTON



TEXAS A&M UNIVERSITY
Drug Discovery Center

Synth  center
at Rice University



Event Schedule

May 24th, 2024

- 11:00 a.m. Check-in
- 12:00 p.m. Lunch
- 1:00 p.m. Welcome Remarks
Wenshe Liu
Professor, Texas A&M University
- 1:05 p.m. Tribute to the Late Prof. Walter Fast
Alfred Tuley
Associate Professor of Instruction, University of Texas at Austin

Session 1

Novel Therapeutics 1

Chair: Kevin Dalby
Professor, University of Texas at Austin

- 1:10 p.m. Bring the Power of Antibodies to the Bone
Han Xiao
Associate Professor, Rice University
- 1:35 p.m. Directed Evolution of a PD-L1 Binding Peptide with Antibody-like Affinity
Steven Millward
Associate Professor, MD Anderson Cancer Center
- 2:00 p.m. Light-triggered Metallodrugs for Cancer Therapy
Sherri McFarland
Professor, University of Texas at Arlington
- 2:25 p.m. MYC-Targeting PROTACs Lead to Bimodal Degradation and N-Terminal Truncation
Damian Young
Associate Professor, Baylor College of Medicine
- 2:50 p.m. Coffee Break

Event Schedule

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Session 2

Novel Imaging Tools

Chair: Jennifer Kohler

Professor, University of Texas Southwestern Medical Center

- 3:10 p.m. Chemiluminescent 1,2-Dioxetanes for Molecular Imaging in Cells and Animals
Alexander Lippert
Professor, Southern Methodist University
- 3:35 p.m. Design of Stimuli-responsive Peptide Self-assembly for Targeted Molecular Imaging and Therapy
He Dong
Associate Professor, University of Texas at Arlington
- 4:00 p.m. DNA-Based Tools for Chemical and Biological Sensing
Devleena Samanta
Assistant Professor, University of Texas at Austin
- 4:25 p.m. Mirror Image Oligonucleotides: A New Biochemical Toolbox
Jonathan Szczepanski
Associate Professor, Texas A&M University
- 4:50 p.m. Sponsor Presentations
Chris Lunn, *Promega*
Jordon Witkop, *Shimadzu*
Madilyn Ruge, *Sino Biological*
- 5:10 p.m. Dinner
- 6:00 p.m. Poster Session (for even poster #) and Vendor Shows

Event Schedule

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Session 3 Fundamental Discoveries

Chair: Wenshe Liu
Professor, Texas A&M University

- 7:00 p.m. Discovery, Evolution, and Applications of Biological
Supramolecular Hosts for Anions
Sheel Dodani
Associate Professor, University of Texas at Dallas
- 7:25 p.m. New Directions in GPCR Signaling
Mike Robertson
Assistant Professor, Baylor College of Medicine
- 7:50 p.m. Deciphering the Chemical Basis for Low-Complexity
Domain Self-Association
Glen Liszczak
*Assistant Professor, University of Texas Southwestern Medical
Center*
- 8:15 p.m. Interrogating the Impact of Glycan Macromolecular
Structure on Recognition and Function
Cassandra Callmann
Assistant Professor, University of Texas at Austin

Event Schedule

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7:00 a.m. Breakfast

Session 4

Creative Tools 1

Chair: Zachary Ball

Professor, Rice University

8:00 a.m. Discovery of Functional Peptide Macrocyces via Multiplexed
Library Screening
Rudi Fasan
Professor, University of Texas at Dallas

8:25 a.m. Expanding the Ligandable Proteome Using Tyrosine-
Reactive Electrophiles
Ken Hsu
Associate Professor, University of Texas at Austin

8:50 a.m. An Active Site-Directed Ligand Evolution Strategy Aided by
Phage Display
Wenshe Liu
Professor, Texas A&M University

9:15 a.m. Advancing Metallomics, Glycomics and Gene Therapy using
DNAzymes and Aptamers
Yi Lu, Professor
University of Texas at Austin

9:40 a.m. Coffee Break

Event Schedule

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Session 5

Novel Therapeutics 2

Chair: Jin Wang

Professor, Baylor College of Medicine

- 10:00 a.m. Building Better Antioxidants: Fighting Neurodegenerative Disease with a Multi-tactical Approach
Kayla Green
Professor, Texas Christian University
- 10:25 a.m. Natural Leads for Precision Antibiotics
Chad Johnston
Assistant Professor, Baylor College of Medicine
- 10:50 a.m. From Drug Screen to Therapeutic Target: The Potential of Statins as B7-H3-Dependent Immune Modulators
Margie Sutton
Instructor, MD Anderson Cancer Center
- 11:15 a.m. Discovery of First-in-Class PROTAC Degraders of SARS-CoV-2 Main Protease
Shiqing Xu
Assistant Professor, Texas A&M University
- 11:40 a.m. Sponsor Presentations
David Li, *MedChemExpress*
Scott Hutto, *Beckman Coulter*
Clifford Stephan, *IBT Cores*
- 12:00 p.m. Lunch
- 1:00 p.m. Poster Session (for odd poster #) and Vendor Shows

Event Schedule

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Session 6 Creative Methodologies 2

Chair: Shiqing Xu

Assistant Professor, Texas A&M University

- 2:00 p.m. From Early Chemical Probes to Clinical Compounds: Small Molecule Tools from MD Anderson's Therapeutics Discovery Division
Michael Soth
Institutional Director, MD Anderson Cancer Center
- 2:25 p.m. Stronger Together: Condensates Promote Cancer Signaling
Juan Guan
Assistant Professor, University of Texas at Austin
- 2:50 p.m. Use Forward Genetics for Small Molecule Target Identification
Deepak Nijhawan
Associate Professor, University of Texas Southwestern Medical Center
- 3:15 p.m. Coffee Break
- 3:35 p.m. Poster Pitches
- 3:50 p.m. The 2024 SynthX Texas Chemical Biology Young Investigator Lecture:
Microdroplet Mass Spectrometry for In-depth Lipidomics and Drug-Protein Interactions
Xin Yan
Assistant Professor, Texas A&M University
- 4:20 p.m. Award Presentation and Closing Remarks from the Meeting Chair
Wenshe Liu
Professor, Texas A&M University

Poster Session

Poster #	Presenter Name	Poster Title
1	Rosemarie Elloisa Acero (Texas A&M University)	Optimized chimeric beacon probes for live cell imaging of DNA repair
2	Yugendar Reddy Alugubelli (Texas A&M University)	Discovery of First-in-Class PROTAC Degraders of SARS-CoV-2 Main Protease
3	Tharaka Amarasekara (Texas A&M University)	Characterizing the Interactions between Thymine DNA Glycosylase (TDG) and RNA
4	Ryan Beckner (UT Southwestern Medical Center)	Probing hidden structure within intrinsically disordered protein domains with chiral mutagenesis
5	Ramesh Bista (University of Texas at Austin)	Combinatorial Biosynthesis of Designer Polyketides Using Engineered Modular Polyketide Synthases
6	Maidileyvis Castro Cabello (Southern Methodist University)	Mechanistic studies of the decomposition of 1,2-dioxetanes in aqueous conditions.
7	Ran Cheng (Baylor College of Medicine)	Development of a Highly Potent Covalent BTK PROTAC: Sub-stoichiometric Degradation is Dispensable
8	Linqi Cheng (Rice University)	Directed Evolution of a Cyclodipeptide Synthase to Biosynthesize Non-canonical Amino Acids-Containing Cyclodipeptides with Enhanced Efficiency and Specificity

Poster Session

Poster #	Presenter Name	Poster Title
9	Chia-Chuan Cho (Texas A&M University)	Expanding viral targets for Texas A&M drug discovery center.
10	Teck Khiang Chua (Baylor College of Medicine)	Inhibition and Structural Investigation of SARS-CoV-2 Main Protease
11	Ogonna David (University of Houston)	Engineering an anaerobic FRET sensor for the detection of zinc ions in live cells
12	Gopal K. Dubey (Texas A&M University)	A Genetically Encoded Phage Display Technique Targeting Bromodomain Protein 9
13	Allison Goetz (Texas A&M University)	Exploring Epigenetic Modification Effects on Thymine DNA Glycosylase
14	Weijie Guo (University of Texas at Austin)	Exploration of Thrombin-interactive DNA motif in Neutrophil Extracellular Traps
15	Xuejiao Guo (Texas A&M University)	The Development of Small Molecule Inhibitors Selectively Targeting the ENL YEATS Domain for Treating Acute Myeloid Leukemia
16	Xuan Han (Texas A&M University)	Cross Chiral Ligation with Alternative Substrates: A Closer Look at an Artificial Ligase Ribozyme and a More Accessible Method for Synthesizing Long L-RNAs
17	Adam Hillaire (Texas A&M University)	Structural and Mechanistic Investigation of Bacterial DNA Phosphorothioation

Poster Session

Poster #	Presenter Name	Poster Title
18	Chase Hutchins (UT MD Anderson Cancer Center)	Membrane Dynamics and Druggability of Rheb and RhoA
19	Uyen Huynh (University of Houston)	Elucidating zinc requirements and transport mechanisms in intestinal <i>Lactobacillaceae</i>
20	Makena Janis (University of Houston)	Improving Cofactor Incorporation of Slr1393g3 from <i>Synechocystis</i> sp. PCC6803 for Metal Sensing Applications in Bacteria
21	Gary Jensen (University of Houston)	Utilizing Native and Mutant Phycoerythrobilin- Binding Proteins as Florescent Zinc Sensors
22	Guoqing Jin (Texas A&M University)	β -Difluoropyrrolyl-Cysteine SNAr Chemistry Enabling Functional Porphyrin Bioconjugation
23	Kaustav Khatua (Texas A&M University)	Aza peptides with unique covalent warheads as SARS-CoV-2 main protease inhibitors
24	Seungheon Lee (University of Texas at Austin)	Chemical and Biological Detection in Cells using DNA-Based Nanostructures
25	Xin Li (Baylor College of Medicine)	Small molecule inhibitor of the protein-protein interactions between AF9/ENL and DOTIL/AF4/AFF4 or degrader of ENL suppresses malignant gene expression and tumor growth

Poster Session

Poster #	Presenter Name	Poster Title
26	Hanfeng Lin (Baylor College of Medicine)	COOKIE-Pro: A chemoproteomics method for covalent inhibitor binding kinetics profiling
27	Shuya Lu (University of Texas at Austin)	Spatial imaging of glycoRNA in single cells with ARPLA (Sialic Acid Aptamer and RNA in situ Hybridization-mediated Proximity Ligation Assay)
28	Yuri Mackeyev (University of Texas Houston Houston Health Science Center)	[60]Fullerene: protection of normal cells across a range of tissue types and organ systems affected by oxidative stress
29	Lauren McGregor (Texas A&M University)	Exploring Thymine DNA Glycosylase's (TDG) Role in Gene Regulation by Characterization of RNA interactions
30	Takeshi Miyazawa (University of Texas at Austin)	Refactoring the pikromycin synthase for the modular biosynthesis of macrolide antibiotics in E. coli
31	Hazel Nguyen (University of Houston)	Fluorescent protein based Zn ²⁺ sensors for tracking labile Zn ²⁺ in aerobically and anaerobically grown Escherichia coli
32	Rokia Osman (Southern Methodist University)	Copper ion specific chemiluminescent probe
33	Joshua Plank (Southern Methodist University)	Chemiluminescence imaging of esterase activity A549 cells with a custom chemiluminescence microscope

Poster Session

Poster #	Presenter Name	Poster Title
34	Moazzameh Ramezani (Texas A&M University)	Exploring Aptamer-Based Techniques to Address the PFSE Structure of COVID-19 for Diagnosis and Treatment
35	Shirin Shabahang (University of Houston)	Expanded SAR Analysis of 3,5-Diphenyl-2-Aminopyridines as Receptor-Interacting Protein Kinase 2 and Nucleotide-Binding Oligomerization Domain Cell Signaling Inhibitors
36	Vishav Sharma (Texas A&M University)	Phosphomethylpyrimidine synthase (ThiC): A "Radical Dance" in bacterial thiamin biosynthesis
37	Ge Shi (University of Texas at Arlington)	Optimizing the phototherapy effects of metallodrug photosensitizers for cancer treatment
38	Dylan Snider (University of Texas at Austin)	DNA-Locked Peptide Beacons for CRISPR-Amplified Sensing of Protease Activity
39	Tripti Midha (Rice University)	Resolving discrepancies in the error and speed estimates from the copolymerization and enzyme-kinetics approaches
40	Chia-Lung Tsai (Texas A&M University)	Bifunctional Tagging for Charge Inversion and Characterization of Glycerophospholipid Isomers in Tandem Mass Spectrometry

Poster Session

Poster #	Presenter Name	Poster Title
41	Kalista Vanden Berge (Texas A&M University)	Utilizing L-Aptamers for the Detection of Cross-Chiral RNA Interactions
42	Tianlu Wang (Texas A&M University - IBT/CTCR)	Repurposing salicylic acid as a versatile inducer of proximity for biomedical applications
43	Zhenyu Xi (Texas A&M University)	Elucidating Liraglutide Oligomerization by Ion Mobility Mass Spectrometry and Molecular Dynamics Simulation
44	Shudan Yang (Rice University)	NIR-II pH-Responsive BODIPY Probes for Breast Cancer Bone Metastases Imaging
45	Chen-Hsu Yu (Texas A&M University)	The Influence of Chirality on the Behavior of Oligonucleotides Inside Cells: Revealing the Potent Cytotoxicity and Cellular Interactome of G-rich L-RNA
46	Sangho Yun (Texas A&M University)	Capturing Ras Oligomerization on a Membrane
47	Mengxi Zhang (Rice University)	Creation of Sticky Proteins and Bacteria with A Nature-Inspired Non-Canonical Amino Acid
48	Zihan Ann Zhang (Texas A&M University)	Chemo-genetic Chimeric Antigen Receptor (CAR) T Cells
49	Baiyu Zhu (Texas A&M University)	Investigating the molecular interactions between R-loops and TDG

2024
SynthX Texas
Chemical Biology
Young
Investigator Award



Xin Yan

Assistant Professor, Texas A&M University

Honoring Outstanding Achievement in Reactive Microdroplet
Mass Spectrometry for in-depth Lipidomics

Sponsored By:

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at Rice University



Travel Award Winner

Takeshi Miyazawa
University of Texas at Austin

Weijie Guo
University of Texas at Austin

Moazzameh Ramezani
Texas A&M University

Ge Shi
University of Texas at Arlington

Adam Hillaire
Texas A&M University

Rokia Osman
Southern Methodist University



TEXAS A&M UNIVERSITY

Drug Discovery Center

The primary focus of the Texas A&M Drug Discovery Center is to guide targets identified by investigators through the drug discovery process and to facilitate the transition from basic research studies to drug discovery. In the past five years, we have acquired over \$2 million in instrumentation to aid in drug discovery research. By consolidating resources within Texas A&M, services or consultations are available for nearly all preclinical applications in drug discovery. There are three main areas of focus within the center:

1. Facilities to support the identification and optimization of peptide therapeutics are available including phage selections, synthesis, and a variety of characterization techniques.
2. We have a customizable automated screening platform made up of the largest Access Workstation in Texas and will aid in all stages of the high throughput screening process, from assay development to lead identification.
3. A core focused on small molecule drug development is targeted to provide resources and consultations for synthetic methods, assay design, and computer-aided drug design.

Small Molecule Drug Development

- Structure-Based Drug Design
 - Consultations
 - Large Scale Synthesis
- Assay Design and Probe Synthesis
- Molecular Modeling
 - Virtual Screening/Docking
 - Early prediction of PK/PD and ADMET

Automated Screening Platforms

- Access Workstation – Largest Unit in Texas!
 - Echo 650 Liquid Handler
 - Microplate Washer
 - Cytomat 10C Incubator
 - Neo2 Plate Reader
- Integra Assist Liquid Handler
- Customizable Assay Development Services

Peptide Therapeutics

- Selections using phage-displayed peptide libraries ($>10^9$ sequences per library)
 - Option for insertion of noncanonical amino acids within libraries
 - Linear and Macrocyclic peptides
- Customizable peptide synthesis
 - 25 μ mol – 1.2 mmol scale
- Peptide Characterization Techniques
 - Biolayer Interferometry
 - Surface Plasmon Resonance
 - AlphaScreen/AlphaLISA
 - Fluorescence Polarization

Director: Wenshe Ray Liu (wsliu2007@tamu.edu)

Manager: J. Trae Hampton (jhampton1@tamu.edu)

Pioneering Precision in Molecule Synthesis for Translational Excellence

The mission of Rice Synthesis X (SynthX) is to develop groundbreaking cancer drugs and technologies by leveraging innovations in the synthesis of molecules and materials from the fields of organic chemistry, chemical biology, nanomaterial synthesis, and artificial intelligence drug discovery in collaboration with cancer programs at the Texas Medical Center (TMC). We collaborate with our strategic TMC allies, to facilitate the synthesis of next-generation drugs with atomic precision at any scale, addressing the overarching cancer treatment challenges posed by the National Cancer Institute (NCI), Cancer Prevention and Research Institute of Texas (CPRIT), and the Department of Defense (DoD). The initiative aims to propel the development of innovative approaches for cancer prevention and early detection through the enhancement of minimally invasive techniques, thereby reducing the global cancer burden. Additionally, it seeks to optimize immunotherapy and personalized medicine to improve patient response rates and treatment efficacy. Moreover, the initiative seeks to transform cancer treatment strategies, especially for advanced stages and metastatic cases, by devising holistic approaches that minimize side effects and ensure durable treatment effects.

Rice SynthX is leading the way in synthesizing and designing molecules with exceptional precision at various length scales. Through advanced techniques and the integration of AI, we are now able to manipulate and engineer macromolecular and supramolecular structures at an atomic level, surpassing the constraints of natural biological processes. This breakthrough paves the way for groundbreaking advancements and novel prospects in multiple fields.



Leveraging Rice's extensive knowledge in organic and biological synthesis, nanomaterials, and computational biology, and connections with the TMC, the research conducted at Rice SynthX will primarily focus on four key areas: 1) Innovative Drug Design, collaborating with TMC to create synthetic and natural drugs using cutting-edge methods; 2) Precision Protein Modification, synthesizing advanced biologics in collaboration with clinical researchers; 3) Advancing Biomedical Materials through interdisciplinary efforts in biomaterial creation; and 4) AI in Drug Discovery, accelerating drug discovery through virtual screening and improving clinical trials for personalized medicine and healthcare advancement.

By establishing a robust and interconnected network of collaborations, SynthX serves as a catalyst for scientific breakthroughs, laying the foundation for continued innovation.





TEXAS A&M HEALTH

Institute of Biosciences
and Technology

FOUR RESEARCH CENTERS OF EXCELLENCE:

- Epigenetics & Disease Prevention
- Genomic & Precision Medicine
- Translational Cancer Research
- Infectious & Inflammatory Diseases

TRAINING PROGRAMS

- Houston Graduate Program in Medical Sciences
- Houston Postdoctoral Training Program
- 39 Current Students
- 130 Former Students
- 15 Postdoctoral Fellows



SUMMARY STATS

- \$86M in Extramural Funding
- 432 Proposals Submitted Since 2019
- 124 Proposals Awarded
- 3 Active Clinical Trials
- 1 Precision Medicine Clinic
- 60 Active Patents with Leading Industry Partners

NINE ADVANCED TECHNOLOGY CORES & COLLABORATIVE INITIATIVES:

- Antibody & Biopharmaceuticals Core (ABC)
- Center for Advanced Imaging
- High Throughput Flow Cytometry Analysis and Cell Sorting
- High Throughput Research and Screening
- Microphysiological Lead Optimization Screening (MLOTS)
- Pre-Clinical Imaging Core
- Protein Production, Characterization and Molecular Interaction (PPCMI)
- Rigor and Reproducibility Core
- Texas A&M Clinicogenomics

Established as a free-standing unit by Texas A&M Board of Regents in Houston in 1986 and a founding member of the Texas A&M health



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Trusted Answers

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Notes



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