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
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

May 24th, 2024

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 Sczepanski
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

May 24th, 2024

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

May 25th, 2024

7:00 a.m.  Breakfast

Session 4  Creative Tools 1
Chair: Zachary Ball  
Professor, Rice University

8:00 a.m.  Discovery of Functional Peptide Macrocycles 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
May 25th, 2024

**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
May 25th, 2024

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
<table>
<thead>
<tr>
<th>Poster #</th>
<th>Presenter Name</th>
<th>Poster Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Rosemarie Elloisa Acero (Texas A&amp;M University)</td>
<td>Optimized chimeric beacon probes for live cell imaging of DNA repair</td>
</tr>
<tr>
<td>2</td>
<td>Yugendar Reddy Alugubelli (Texas A&amp;M University)</td>
<td>Discovery of First-in-Class PROTAC Degraders of SARS-CoV-2 Main Protease</td>
</tr>
<tr>
<td>3</td>
<td>Tharaka Amarasekara (Texas A&amp;M University)</td>
<td>Characterizing the Interactions between Thymine DNA Glycosylase (TDG) and RNA</td>
</tr>
<tr>
<td>4</td>
<td>Ryan Beckner (UT Southwestern Medical Center)</td>
<td>Probing hidden structure within intrinsically disordered protein domains with chiral mutagenesis</td>
</tr>
<tr>
<td>5</td>
<td>Ramesh Bista (University of Texas at Austin)</td>
<td>Combinatorial Biosynthesis of Designer Polyketides Using Engineered Modular Polyketide Synthases</td>
</tr>
<tr>
<td>6</td>
<td>Maidileyvis Castro Cabello (Southern Methodist University)</td>
<td>Mechanistic studies of the decomposition of 1,2-dioxetanes in aqueous conditions.</td>
</tr>
<tr>
<td>7</td>
<td>Ran Cheng (Baylor College of Medicine)</td>
<td>Development of a Highly Potent Covalent BTK PROTAC: Sub-stoichiometric Degradation is Dispensable</td>
</tr>
<tr>
<td>8</td>
<td>Linqi Cheng (Rice University)</td>
<td>Directed Evolution of a Cyclodipeptide Synthase to Biosynthesize Non-canonical Amino Acids-Containing Cyclodipeptides with Enhanced Efficiency and Specificity</td>
</tr>
<tr>
<td>Poster #</td>
<td>Presenter Name</td>
<td>Poster Title</td>
</tr>
<tr>
<td>---------</td>
<td>--------------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>9</td>
<td>Chia-Chuan Cho (Texas A&amp;M University)</td>
<td>Expanding viral targets for Texas A&amp;M drug discovery center.</td>
</tr>
<tr>
<td>10</td>
<td>Teck Khiang Chua (Baylor College of Medicine)</td>
<td>Inhibition and Structural Investigation of SARS-CoV-2 Main Protease</td>
</tr>
<tr>
<td>11</td>
<td>Ogonna David (University of Houston)</td>
<td>Engineering an anaerobic FRET sensor for the detection of zinc ions in live cells</td>
</tr>
<tr>
<td>12</td>
<td>Gopal K. Dubey (Texas A&amp;M University)</td>
<td>A Genetically Encoded Phage Display Technique Targeting Bromodomain Protein 9</td>
</tr>
<tr>
<td>13</td>
<td>Allison Goetz (Texas A&amp;M University)</td>
<td>Exploring Epigenetic Modification Effects on Thymine DNA Glycosylase</td>
</tr>
<tr>
<td>14</td>
<td>Weijie Guo (University of Texas at Austin)</td>
<td>Exploration of Thrombin-interactive DNA motif in Neutrophil Extracellular Traps</td>
</tr>
<tr>
<td>15</td>
<td>Xuejiao Guo (Texas A&amp;M University)</td>
<td>The Development of Small Molecule Inhibitors Selectively Targeting the ENL YEATS Domain for Treating Acute Myeloid Leukemia</td>
</tr>
<tr>
<td>16</td>
<td>Xuan Han (Texas A&amp;M University)</td>
<td>Cross Chiral Ligation with Alternative Substrates: A Closer Look at an Artificial Ligase Ribozyme and a More Accessible Method for Synthesizing Long L-RNAs</td>
</tr>
<tr>
<td>17</td>
<td>Adam Hillaire (Texas A&amp;M University)</td>
<td>Structural and Mechanistic Investigation of Bacterial DNA Phosphorothioation</td>
</tr>
<tr>
<td>Poster #</td>
<td>Presenter Name</td>
<td>Presenter Institution</td>
</tr>
<tr>
<td>----------</td>
<td>----------------</td>
<td>-----------------------</td>
</tr>
<tr>
<td>18</td>
<td>Chase Hutchins</td>
<td>UT MD Anderson Cancer Center</td>
</tr>
<tr>
<td>19</td>
<td>Uyen Huynh</td>
<td>University of Houston</td>
</tr>
<tr>
<td>20</td>
<td>Makena Janis</td>
<td>University of Houston</td>
</tr>
<tr>
<td>21</td>
<td>Gary Jensen</td>
<td>University of Houston</td>
</tr>
<tr>
<td>22</td>
<td>Guoqing Jin</td>
<td>Texas A&amp;M University</td>
</tr>
<tr>
<td>23</td>
<td>Kaustav Khatua</td>
<td>Texas A&amp;M University</td>
</tr>
<tr>
<td>24</td>
<td>Seungheon Lee</td>
<td>University of Texas at Austin</td>
</tr>
<tr>
<td>25</td>
<td>Xin Li</td>
<td>Baylor College of Medicine</td>
</tr>
<tr>
<td>Poster #</td>
<td>Presenter Name</td>
<td>Poster Title</td>
</tr>
<tr>
<td>----------</td>
<td>--------------------------------------</td>
<td>----------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>26</td>
<td>Hanfeng Lin (Baylor College of Medicine)</td>
<td>COOKIE-Pro: A chemoproteomics method for covalent inhibitor binding kinetics profiling</td>
</tr>
<tr>
<td>27</td>
<td>Shuya Lu (University of Texas at Austin)</td>
<td>Spatial imaging of glycoRNA in single cells with ARPLA (Sialic Acid Aptamer and RNA in situ Hybridization-mediated Proximity Ligation Assay)</td>
</tr>
<tr>
<td>28</td>
<td>Yuri Mackeyev (University of Texas Houston Houston Health Science Center)</td>
<td>[60] Fullerene: protection of normal cells across a range of tissue types and organ systems affected by oxidative stress</td>
</tr>
<tr>
<td>29</td>
<td>Lauren McGregor (Texas A&amp;M University)</td>
<td>Exploring Thymine DNA Glycosylase’s (TDG) Role in Gene Regulation by Characterization of RNA interactions</td>
</tr>
<tr>
<td>30</td>
<td>Takeshi Miyazawa (University of Texas at Austin)</td>
<td>Refactoring the pikromycin synthase for the modular biosynthesis of macrolide antibiotics in E. coli</td>
</tr>
<tr>
<td>31</td>
<td>Hazel Nguyen (University of Houston)</td>
<td>Fluorescent protein based Zn2+ sensors for tracking labile Zn2+ in aerobically and anaerobically grown Escherichia coli</td>
</tr>
<tr>
<td>32</td>
<td>Rokia Osman (Southern Methodist University)</td>
<td>Copper ion specific chemiluminescent probe</td>
</tr>
<tr>
<td>33</td>
<td>Joshua Plank (Southern Methodist University)</td>
<td>Chemiluminescence imaging of esterase activity A549 cells with a custom chemiluminescence microscope</td>
</tr>
<tr>
<td>Poster #</td>
<td>Presenter Name</td>
<td>Poster Title</td>
</tr>
<tr>
<td>---------</td>
<td>----------------</td>
<td>--------------</td>
</tr>
<tr>
<td>34</td>
<td>Moazzameh Ramezani (Texas A&amp;M University)</td>
<td>Exploring Aptamer-Based Techniques to Address the PFSE Structure of COVID-19 for Diagnosis and Treatment</td>
</tr>
<tr>
<td>35</td>
<td>Shirin Shabahang (University of Houston)</td>
<td>Expanded SAR Analysis of 3,5-Diphenyl-2-Aminopyridines as Receptor-Interacting Protein Kinase 2 and Nucleotide-Binding Oligomerization Domain Cell Signaling Inhibitors</td>
</tr>
<tr>
<td>36</td>
<td>Vishav Sharma (Texas A&amp;M University)</td>
<td>Phosphomethylpyrimidine synthase (ThiC): A “Radical Dance” in bacterial thiamin biosynthesis</td>
</tr>
<tr>
<td>37</td>
<td>Ge Shi (University of Texas at Arlington)</td>
<td>Optimizing the phototherapy effects of metallodrug photosensitizers for cancer treatment</td>
</tr>
<tr>
<td>38</td>
<td>Dylan Snider (University of Texas at Austin)</td>
<td>DNA-Locked Peptide Beacons for CRISPR-Amplified Sensing of Protease Activity</td>
</tr>
<tr>
<td>39</td>
<td>Tripti Midha (Rice University)</td>
<td>Resolving discrepancies in the error and speed estimates from the copolymerization and enzyme-kinetics approaches</td>
</tr>
<tr>
<td>40</td>
<td>Chia-Lung Tsai (Texas A&amp;M University)</td>
<td>Bifunctional Tagging for Charge Inversion and Characterization of Glycerophospholipid Isomers in Tandem Mass Spectrometry</td>
</tr>
<tr>
<td>Poster #</td>
<td>Presenter Name</td>
<td>Poster Title</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>41</td>
<td>Kalista Vanden Berge (Texas A&amp;M University)</td>
<td>Utilizing L-Aptamers for the Detection of Cross-Chiral RNA Interactions</td>
</tr>
<tr>
<td>42</td>
<td>Tianlu Wang (Texas A&amp;M University - IBT/CTCR)</td>
<td>Repurposing salicylic acid as a versatile inducer of proximity for biomedical applications</td>
</tr>
<tr>
<td>43</td>
<td>Zhenyu Xi (Texas A&amp;M University)</td>
<td>Elucidating Liraqustide Oligomerization by Ion Mobility Mass Spectrometry and Molecular Dynamics Simulation</td>
</tr>
<tr>
<td>44</td>
<td>Shudan Yang (Rice University)</td>
<td>NIR-II pH-Responsive BODIPY Probes for Breast Cancer Bone Metastases Imaging</td>
</tr>
<tr>
<td>45</td>
<td>Chen-Hsu Yu (Texas A&amp;M University)</td>
<td>The Influence of Chirality on the Behavior of Oligonucleotides Inside Cells: Revealing the Potent Cytotoxicity and Cellular Interactome of G-rich L-RNA</td>
</tr>
<tr>
<td>46</td>
<td>Sangho Yun (Texas A&amp;M University)</td>
<td>Capturing Ras Oligomerization on a Membrane</td>
</tr>
<tr>
<td>47</td>
<td>Mengxi Zhang (Rice University)</td>
<td>Creation of Sticky Proteins and Bacteria with A Nature-Inspired Non-Canonical Amino Acid</td>
</tr>
<tr>
<td>48</td>
<td>Zihan Ann Zhang (Texas A&amp;M University)</td>
<td>Chemo-genetic Chimeric Antigen Receptor (CAR) T Cells</td>
</tr>
<tr>
<td>49</td>
<td>Baiyu Zhu (Texas A&amp;M University)</td>
<td>Investigating the molecular interactions between R-loops and TDG</td>
</tr>
</tbody>
</table>
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: SynthX center at Rice University
Travel Award Winner

Takeshi Miyazawa
University of Texas at Austin

Weijie Guo
University of Texas at Austin

Moazzam Ramezani
Texas A&M University

Ge Shi
University of Texas at Arlington

Adam Hillaire
Texas A&M University

Rokia Osman
Southern Methodist University
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 μmol – 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)
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.

Web: SynthX.rice.edu
Scan Here
Established as a free-standing unit by Texas A&M Board of Reagents in Houston in 1986 and a founding member of the Texas A&M health

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

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

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
Sponsors

Silver Sponsors

- Texas A&M Health Institute of Biosciences and Technology
- MCE
- Beckman Coulter Life Sciences
- Sino Biological
- Promega
- Shimadzu Excellence in Science

Bronze Sponsors

- Vazyme
- Agilent

Core Support