

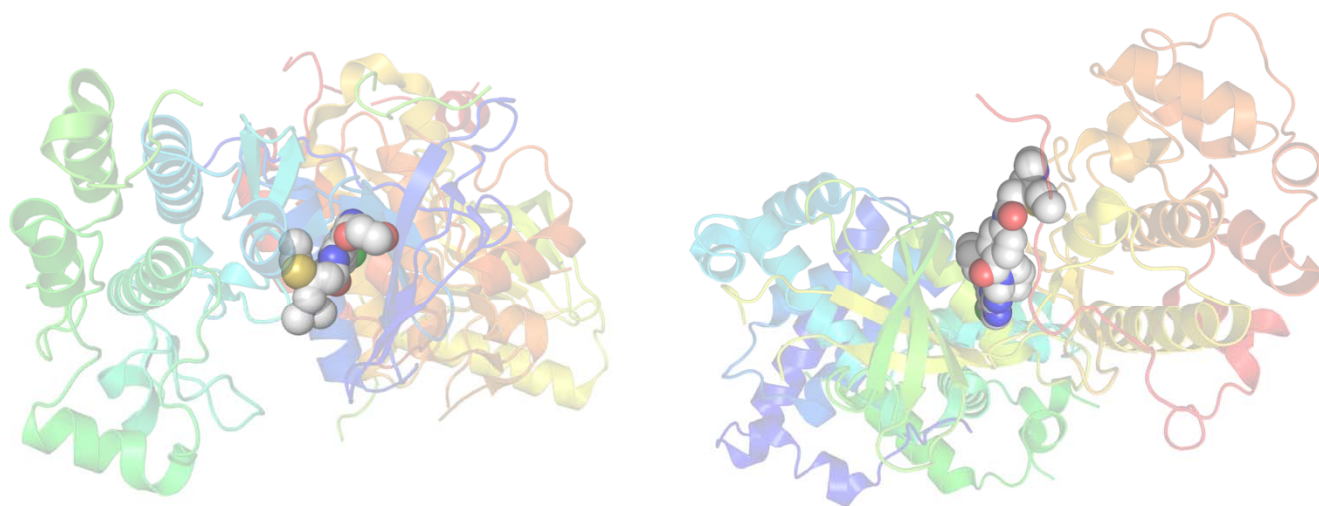


# 1<sup>st</sup> Texas Chemical Biology Conference

May 23-24, 2019

Texas A&M Hotel and Conference Center, College Station, TX

**"When Chemistry Meets Biology"**



[www.chem.tamu.edu/tcbc/](http://www.chem.tamu.edu/tcbc/)

**Organizer: Texas A&M Drug Discovery Laboratory**

*Sponsors of the  
2019 Texas Chemical Biology Conference*



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May 23-24, 2019

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## May 23, 2019 (Thursday)

6:00 – 8:00 p.m.      Registration (1<sup>st</sup> Floor Century Ballroom I & II)  
Welcome Reception (3<sup>rd</sup> Floor Pool Terrace, outdoor)

## May 24, 2019 (Friday)

7:00 – 7:50 a.m.      Coffee, Juice, Tea and Refreshment  
(Pre Function area outside of Century Ballroom I & II)

8:00 – 8:15 a.m.      *Opening Remarks* (Century Ballroom I & II)  
**Carol Fierke, Provost of Texas A&M University**  
*Welcome Remarks*  
**Professor Wenshe Liu**

8:15 – 9:00 a.m.      **Session I: Chair – Tadhg P. Begley** (Century Ballroom I & II)  
**Michelle C. Chang**, University of California, Berkeley  
*"Synthetic biology approaches to new chemistry"*

9:00 – 9:30 a.m.      **Adrian T. Keatinge-Clay**, The University of Texas at Austin  
*"An in vitro platform for engineering, studying, and harnessing modular polyketide synthases"*

9:30 – 10:30 a.m.      Coffee Break / Poster Session (Century Ballroom III & IV)

10:30 – 11:00 a.m.      **Session II: Chair – Kevin Burgess** (Century Ballroom I & II)  
**Kevin Dalby**, The University of Texas at Austin  
*"Inhibiting multifunctional ERK-protein complexes for cancer therapy"*

11:00 – 11:30 a.m.      **Thomas Meek**, Texas A&M University  
*"Rational design of inhibitors for enzymes essential to infectious diseases"*

11:30 – 12:00 p.m.      **Yongcheng Song**, Baylor College of Medicine  
*"Discovery, X-ray crystallography and antiviral activity of allosteric inhibitors of flavivirus protease"*

12:00 – 13:00 p.m.      Boxed Lunch

**Session III: Chair – Shiqing Xu** (Century Ballroom I & II)

13:00 – 13:30 p.m. **Jennifer Kohler**, University of Texas Southwestern Medical Center  
*"Capturing glycan-dependent interactions with photocrosslinking sugars"*

13:30 – 14:00 p.m. **Jin Wang**, Baylor College of Medicine  
*"Small molecule induced protein degradation with PROTACs"*

14:00 – 14:30 p.m. **Zachary Ball**, The University of Texas at Austin  
*"Transition-metal approaches for selective protein modification"*

14:30 – 16:00 p.m. Coffee Break / Poster Session (Century Ballroom III & IV)

**Session IV: Chair – Wenshe Liu** (CROPS I, 2<sup>nd</sup> Floor)

14:45 – 15:15 p.m. **Michelle Bond**, NIH of General Medical Sciences  
*"Navigating the NIH funding process" - Video Lecture*

15:15 – 16:00 p.m. One-on-one Meetings with Michelle Bond (sign up in advance)

**Session V: Chair – Jonathan Szczepanski** (Century Ballroom I & II)

16:00 – 16:30 p.m. **Karen Vasquez**, The University of Texas at Austin  
*"Molecular probes to interrogate the roles of non-B DNA structures in DNA damage and genetic instability"*

16:30 – 17:00 p.m. **Chengzhi Cai**, University of Houston  
*"The effect of immobilized mannosides on biofilm formation by E. coli with type 1 fimbriae"*

17:00 – 17:30 p.m. **Blerta Xhemalce**, The University of Texas at Austin  
*"Targeting RNA interference in cancer"*

17:30 – 17:45 p.m. Conclusion Remarks and Announcement of Poster Award Winners  
**Professor Wenshe Liu**

17:45 – 18:00 p.m. Group photo

18:30 – 20:30 p.m. Banquet Dinner (Century Ballroom III & IV)

## Presenting Poster

NO.	Poster Abstract	Author & Co-Authors/Affiliation
1	Chemoenzymatic methods to map glycan-mediated interactions.	<b>Nageswari Yarravarapu</b> , Soumya Krishnamurthy, Narek Darabedian, Mathew Robert Pratt and Jennifer Kohler  University of Texas Southwestern Medical Center
2	Quantifying the Oligomeric States of Membrane Proteins in Cells through Super-resolution Localizations	<b>Xihong Xie</b> , Yu-Shan Cheng†, Meng-Hsuan Wen, Aparna Calindi, Karen Yang, Chi-Wei Chiu and Tai-Yen Chen  University of Houston
3	General Chemo-enzymatic Triketide Synthesis	<b>Alexis Cepeda</b> , Mireya Luna, Kumru Kaan, Jina Zhou and Adrian T. Keatinge-Clay  University of Texas at Austin
4	Ketoreductases as Biocatalysts in the Synthesis of Chiral Diketides	<b>Mireya Luna-Robles</b> , Zhicheng Zhang and Adrian Keatinge-Clay  University of Texas at Austin
5	An <i>in vitro</i> platform for studying, engineering, and harnessing modular polyketide synthases	<b>Melissa Hirsch</b> , Takeshi Miyazawa, Zhicheng Zhang, Shoachen You, Prachi Shah and Adrian T. Keatinge-Clay  University of Texas at Austin
6	DESIGN, SYNTHESIS, AND EVALUATION OF SMALL-MOLECULE PROTACs TO INDUCE ERK DEGRADATION	<b>Chelsea L. Massaro</b> , Tamer S. Kaoud, and Kevin N. Dalby  University of Texas at Austin
7	Chemical Synthesis and Biochemical approaches in the characterization of human cytochrome P450 8B1, the enzyme implicated in obesity and cardiovascular health	<b>Samuel D. Offei</b> and Francis K. Yoshimoto  University of Texas at San Antonio
8	Application of CRISPR-engineered Human Stem Cells for Studying Molecular Mechanisms of Copper-trafficking Proteins	<b>Meng-Hsuan Wen</b> , Xihong Xie, Aparna Calindi and Tai-Yen Chen  University of Houston
9	Biosynthesis of the O-Methyl Phosphoramidate Modification in the Capsular Polysaccharides of <i>Campylobacter jejuni</i>	<b>Zane W. Taylor</b> and Frank M. Raushel  Texas A&M University
10	Substitution of Aromatic Methyl Group with Amino: Novel Flavoenzyme Converts Vitamin into Antibiotic	<b>Isita Jhulki</b> and Tadhg P. Begley  Texas A&M University

11	Covalent Fragments-A New Technology to Discover Covalent Probes	<b>Amit K. Gupta</b> , Sandipan Roy Chowdhury, Steven Kennedy, Alyssa Nguen and Alexander Statsyuk  University of Houston
12	Chemiluminescent Imaging Agents for Cellular Measurements and In Vivo Imaging	<b>Lucas S. Ryan</b> , Weiwei An, Jian Cao, and Alexander R. Lippert  Southern Methodist University
13	Design, Synthesis, and Biological Evaluation of Picomolar Inhibitors that Target MELK In-vitro and in Cells and Suppress Human Breast Cancer Colony Formation	<b>Ju-Hyeon Lee</b> , Juliana M. Taliaferro, Tamer S. Kaoud, Jihyun Park, Chandra Bartholomeusz and Kevin N. Dalby  University of Texas at Austin
14	Identification and Evaluation of Lysyl Hydroxylase 2 Inhibitors	<b>Juhoon Lee</b> , Eun Jeong Cho, Ashiwini K. Devkota, Masahiko Terajima, Hou-fu Guo, Mitsuo Yamauchi, Jonathan M. Kurie and Kevin N. Dalby  University of Texas at Austin
15	Syntheses of polydeuterated dihydroartemisinic acid isotopologues to study the biosynthesis of artemisinin	<b>Swapna Konda</b> ; Araceli P. Valdovinos; Valerie M. Sponsel and Francis K. Yoshimoto  University of Texas at San Antonio
16	Functional Characterization of Enzymes Involved in Synthesis of Glucuronamide Moiety of the Capsular Polysaccharide of Campylobacter jejuni NCTC11168	<b>Alexander Riegert</b> and Frank Raushel  Texas A&M University
17	Elucidating the Mechanism of Enzymes Utilized During the Bacterial Degradation of Lignin in the Protocatechuate 4,5-Cleavage Pathway	<b>Tessily N. Hogancamp</b> , Mark F. Mabanglo, Seth A. Cory, David P. Barondeau and Frank M. Raushel  Texas A&M University
18	Discovery of Featured Metabolites in Post-Traumatic Stress Disorder (PTSD) using High-Resolution Mass Spectrometry Imaging	<b>Shuli Tang</b> , Weijia Luo, Chieh Chen, Yi Liu, Shuiwang Ji, Israel Liberzon, Jiang Chang and Xin Yan  Texas A&M University
19	Antibacterial Strategy against H. pylori: Inhibition of the Radical SAM Enzyme MqnE in Menaquinone Biosynthesis	<b>Sumedh Joshi</b> , Dmytro Fedoseyenko, Nilkamal Mahanta, Rodrigo Ducati, Mu Feng, Vern Schramm and Tadhg Begley  Texas A&M University
20	The Biosynthesis of the Heptose Moeity Found in the Capsular Polysaccharide of Campylobacter jejuni NCTC 11168 (HS:2)	<b>Jamison Huddleston</b> and Frank Raushel  Texas A&M University

21	Light Promoted Cyclohexene-Tetrazine IEDDA reactions	<b>Axel Lored</b> and Han Xiao Rice University
22	A noncanonical amino acid-based relay system for site-specific protein labeling	<b>Yuda Chen</b> , Axel Lored, Aviva Gordon, Juan Tang and Han Xiao Rice University
23	Halopyridines As Switchable Electrophiles: Covalent DDAH Inhibitors	<b>Alfred Tuley</b> , Christopher Schardon, Yeong-Chan Ahn, Valerie May, Sean Patel, Pamela Horton, Jake Swartzel and Walter Fast University of Texas at Austin
24	Glucocorticoids Inhibit Oncogenic RUNX1-ETO in Acute Myeloid Leukemia with Chromosome Translocation t(8;21)	<b>Lianghao Lu</b> , Yefei Wen, Yuan Yao, Fengju Chen, Guohui Wang, Fangrui Wu, Jingyu Wu, Padmini Narayanan, Michele Redell, Qianxing Mo and Yongcheng Song Baylor College of Medicine
25	Epigallocatechin Gallate Inhibits Hepatic Glucose Production in Primary Hepatocytes via Downregulating PKA Signaling Pathways and Transcriptional Factor FoxO1.	<b>Xiaopeng Li</b> , Yunmei Chen, James Zheng Shen, Quan Pan, Wanbao Yang, Hui Yan, Huimin Liu, Weiqi Ai, Wang Liao and Shaodong Guo Texas A&M University
26	Single-Atom Fluorescence Switch: A General Approach towards Visible Light-Activated Dyes for Biological Imaging	<b>Juan Tang</b> , Michael Robichaux, Jingqi Pei, Kuan-Lin Wu, Theodore G. Wensel and Han Xiao Rice University
27	Structural determinants for accurate dephosphorylation of RNA polymerase II by its cognate CTD phosphatase during eukaryotic transcription	<b>Seema Irani</b> , Yan Zhang University of Texas at Austin
28	Modulation of Restrictive Element 1 Silencing transcription factor REST/NRSF activity through allosteric covalent inhibition of Small CTD Phosphatase 1.	<b>Medellin, B.P.</b> , Konduri S., Lin B., Wu H., Irani S.I., Matthews W.L., Siegel D. and Zhang Y. University of Texas at Austin
29	Utilizing a Thioester Intermediate Capture Strategy in the Characterization of the Azinomycin Biosynthetic Pathway	<b>Lauren Washburn</b> , Vasudha Sharma, Gilbert T. Kelly and Coran Watanabe Texas A&M University
30	Transthyretin Disassembly Mechanism and Metal-Induced Oxidation Degradation Pathway Studied via Native Mass Spectrometry and Surface-Induced Dissociation	<b>Mehdi Shirzadeh</b> , Michael Poltash, Christopher D. Boone, Arthur Laganowsky and David H. Russell

		Texas A&M University
31	Methods for Incorporating Two Different Non-Canonical Amino Acids	<b>Chia-Chuan Cho</b> and Wenshe Liu Texas A&M University
32	The Development of Small Molecule Inhibitor of Human ENL YEATS Domain as a Potential Drug Candidate for Acute Leukemia Treatment	<b>Xinyu Ma</b> , Shiqing Xu, Sukant Das and Wenshe Liu Texas A&M University
33	Selective Binding of a Toxin and Phosphatidylinositides to a Mammalian Potassium Channel	<b>Yang Liu</b> , Catherine E. LoCaste, Wen Liu, Michael L. Poltash, David H. Russell and Arthur Laganowsky Texas A&M University
34	Metabolic pathway engineering for algal hydrocarbons	<b>Ivette Cornejo-Corona<sup>1</sup></b> , Hem R. Thapa and Timothy P. Devarenne Texas A&M University
35	Studying the in vitro kinetics and in cellulo stability of mirror-image: DNA strand displacement reactions	<b>Brian Young</b> and Jonathan Sczepanski Texas A&M University
36	Heterochiral DNA Nanotechnology	<b>Adam M. Kabza</b> , Brian E. Young and Jonathan T. Sczepanski Texas A&M University
37	Targeted therapeutic drug discovery program (TTP) for integrated, collaborative, high-throughput drug development at The University of Texas-Austin	<b>Eun Jeong Cho</b> , A.K. Devkota, R. Edupugant, T.S. Kaoud, J. Lee, R. Sammons, J. Lee, C. Zhang, P. Ren and K.N. Dalby University of Texas at Austin
38	Glucagon regulates hepatic mitochondrial function and biogenesis through Foxo1	<b>Wanbao Yang</b> , Hui Yan, Quan Pan, James Zheng Shen, Fenghua Zhou, Chaodong Wu, Yuxiang Sun and Shaodong Guo Texas A&M University
39	The role of zinc in the growth, metal uptake, and biofilm formation of <i>Lactobacillus plantarum</i>	<b>Uyen Huynh</b> and Melissa L. Zastrow University of Houston
40	An Optimal “Click” Formulation Strategy for the Antibody-Drug Conjugate Synthesis	<b>Erol C. Vatansever</b> , Jeffrey Kang, Alfred Tuley, E. Sally Ward, and Wenshe Ray Liu Texas A&M University
41	Oxygen Uptake in Complexes Related to [NiFeS] and [NiFeSe] Hydrogenase Active Sites	<b>Xuemei Yang</b> , <b>Lindy Elrod</b> , Trung Le, Michael B. Hall and Marcetta Y. Darensbourg Texas A&M University



42	Analysis of KRAS GTPase activity using high resolution native Mass Spectrometry	<b>Zahra Moghadam</b> , Jamison Huddleston, Mehdi Shirzadeh and Arthur Laganowsky  Texas A&M University
43	Molecular mechanism underlying the hijacking of host proteins by nonstructural protein 1 of 1918 influenza A virus	<b>Qingliang Shen</b> , Nowlan Savage, Baoyu Zhao, Pingwei Li and Jae-Hyun Cho  Texas A&M University,
44	Transition metal-mediated macromolecular protein conjugation with boronic acids	<b>Michael J. Swierczynski</b> and Zachary T. Ball  Rice University
45	Elucidating Chromatin PTMs via Non-canonical Amino Acids Incorporation	<b>Ge Yu</b> and Wenshe Liu  Texas A&M University
46	An Organometallic Bioconjugation Strategy Using Rhodium(III) and Boronic Acids	<b>Mary Kaitlyn Miller</b> , Jun Ohata and Zachary T. Ball  Rice University
47	Characterize Functional Motions Of Macromolecules By Cryo-EM, Statistical And Computational Modeling	<b>Ran Meng</b> , Huiya Zhou, Yue Cao, Jianhua Huang, Shen Yang and Junjie Zhang  Texas A&M University
48	Identification of flavin-N5-oxide in the bacterial dibenzothiophene, uracil, and hexachlorobenzene catabolic pathway	<b>Sanjoy Adak</b> and Tadhg P. Begley  Texas A&M University
49	A vinylogous one- and two-photon photocleavage strategy allows direct photocaging of amide backbone structure	<b>Alicia E. Mangubat-Medina</b> , Reyner Vargas, S. Cody Martin, Kengo Hanaya and Zachary T. Ball  Rice University
50	Mirror-Image In vitro Selection of Modified L-DNA Aptamer Targeting MicroRNA-155	<b>Sougata Dey</b> and Jonathan T Szczepanski  Texas A&M University
51	Copper(II)-promoted peptide N-terminal arylation with arylboronic acids	<b>Haopei Wang</b> , Mary K. Miller, Olivia Zhang and Zachary T. Ball  Rice University,
52	Towards the Optimization of Dinitrosyl Iron Complexes as Therapeutics for Smooth Muscle Cells	<b>D. Chase Pectol</b> , Sarosh Khan, Rachel B. Chupik, Mahmoud Elsabahy, Karen L. Wooley, Marcetta Y. Darensbourg and Soon-Mi Lim  Texas A&M University

53	Structure and dynamics of the human Fe-S cluster assembly sub-complex: a new morphoein	<b>Seth A. Cory</b> , Cheng-Wei Lin, Steven M. Havens and David P. Barondeau  Texas A&M University
54	Elucidating the Role of Lysine Succinylation on the Function of Isocitrate Lyase 1 from Mycobacterium tuberculosis	<b>Drake Mellott</b> , Zhipeng Wang, Wenshe Liu and Thomas Meek  Texas A&M University
55	Biosynthesis of Azinomycin Epoxide via CYP450 and 2-OOD enzymes	<b>Hyunjin "Jean" Kim</b> , Yohannes Rezenom and Coran M. H. Watanabe  Texas A&M University
56	Thiamin Biosynthesis in Yeast: THI5 - a Remarkable 'Suicide' Enzyme	<b>Anushree Mondal</b> , Nitai Giri, Dmytro Fedoseyenko and Tadhg P. Begley  Texas A&M University
57	Synthesis and incorporation of 1,2-alkanolamine-functionalized lysine as a non-canonical amino acid into GFP	<b>Chesley Marie Rowlett</b> , Jared Morse and Wenshe Liu  Texas A&M University
58	Novel Techniques for Phage Display of Cyclic Peptides	<b>Joshua T. Hampton</b> , <b>Peng-Hsun Chase Chen</b> , Jared S. Morse, Jeffery M. Tharp and Wenshe R. Liu  Texas A&M University