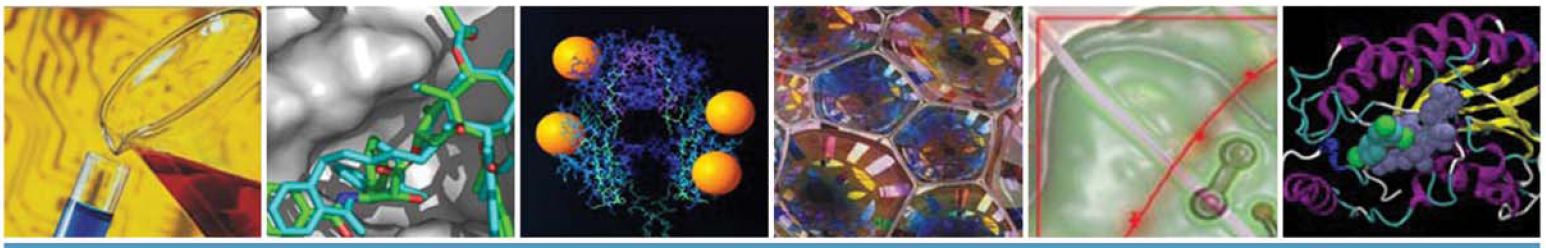
EIGHTEENTH ANNUAL SYMPOSIUM

ICB&DD



Institute of Chemical Biology & Drug Discovery

Frontiers of Neuroscience and Drug Discovery

Thursday, October 10, 2024 ◆ Charles B. Wang Center

Distinguished Speakers

Dr. Anissa Abi-Dargham, *Stony Brook University*
Dr. Cristina Alberini, *New York University*
Dr. Ivet Bahar, *The Laufer Center*
Dr. Michelle James, *Stanford University*
Dr. Scott Laughlin, *Stony Brook University*
Dr. Ivan Montoya, *National Institute on Drug Abuse*
Dr. David Sulzer, *Columbia University*

Poster Sessions ◆ Poster Awards

For more information, please visit
http://ws.cc.stonybrook.edu/icbdd/

Stony Brook University

From the Director

The primary objective of the Institute of Chemical Biology & Drug Discovery (ICB&DD) is to establish and sustain a world-class "Center of Excellence" in chemical biology and drug discovery at Stony Brook University. The rapid and impressive advancements in chemical biology during the last decade have clearly demonstrated that solutions for a vast majority of medical problems rely on the understanding of the molecular basis of diseases, therapeutic targets, drug actions, and drug resistance. ICB&DD promotes highly productive interdisciplinary and collaborative research among chemists, biologists, medicinal chemists, pharmacologists, and physicians to tackle major biomedical problems to find solutions including the discovery of novel therapeutic drugs and innovative diagnostic tools.

—Iwao Ojima, Director, Institute of Chemical Biology & Drug Discovery

Dr. Iwao Ojima received his B.S., M.S., and Ph.D. (1973) degrees from the University of Tokyo, Japan. He joined the Sagami Institute of Chemical Research and held a position of Senior Research Fellow until 1983. He joined the faculty at the Department of Chemistry, State University of New York at Stony Brook first as Associate Professor (1983), was promoted to Professor (1984), Leading Professor (1991), and then to Distinguished Professor (1995). He served as the Department Chair from 1997 to 2003. He has been serving as the founding Director for the Institute of Chemical Biology and Drug Discovery (ICB&DD) from 2003. He has a wide range of research interests in synthetic organic and medicinal chemistry as well as chemical biology, including discovery and development of anticancer agents, antimicrobials, and targeted drug delivery systems. His awards and honors include Arthur C. Cope Scholar Award (1994), E. B. Hershberg Award for Important Discoveries of Medicinally Active Substances (2001), the Medicinal Chemistry Hall of Fame (2006), ACS Award for Creative Work in Fluorine Chemistry (2013), and E. Guenther Award in the Chemistry of Natural Products (2019) from the American Chemical Society; the Chemical Society of Japan Award (1999); Outstanding Inventor Award (2002) from the Research Foundation of the State University of New York; Elected Fellow of J. S. Guggenheim Memorial Foundation, the American Association for the Advancement of Science, the New York Academy of Sciences, the American Chemical Society, the National Academy of Inventors and the European Academy of Sciences.

ICB&DD's History and Mission

The ICB&DD was established in 2004 with Stony Brook University's institutional support as well as the NYSTAR Faculty Development Award. One of ICB&DD's strengths is that it was founded by reorganizing existing exceptional talents on campus, and thus the core of the institute is a well proven entity with an excellent history. ICB&DD is open to a wide range of collaborative research programs with pharmaceutical and biotechnology industrial firms. Members of ICB&DD are from the departments of Chemistry, Biochemistry and Cell Biology, Pharmacological Sciences, Microbiology and Immunology, Physiology and Biophysics, Applied Mathematics and Statistics, Medicine, Pathology, Oral Biology and Pathology, Psychiatry and Behavioral Health, Neurobiology and Behavior, Laufer Center for Physical and Quantitative Biology, Cancer Center, and Cold Spring Harbor Laboratory. In addition, ICB&DD has two core laboratories located in the Chemistry Building: Analytical Instrumentation Laboratory and Discovery Chemistry Laboratory.

ICB&DD has three major programs: Structural and Computational Biology Program, Infectious Diseases Research Program, and Cancer Research Program. In addition, ICB&DD has been providing critical support to the Chemical Biology Training Program.

ICB&DD collaborates with the Stony Brook University Cancer Center to develop a Cancer Therapeutics Program. ICB&DD integrates the existing strengths at Stony Brook University in the basic medical sciences as well as medicinal chemistry and brings in complementary expertise from outside to explore drug discovery and development. At present, ICB&DD focuses on drug discovery in therapeutics for cancer, infectious diseases, neurodegenerative diseases, and inflammation.

Through ICB&DD connections, many collaborative research teams have been created, and research proposals have successfully acquired grants from the NIH and other funding agencies. (Total grant funding > 73M). Currently, there are nine ongoing ICB&DD-designated projects (Total funding: $16M).

ICB&DD 18th Annual Symposium

Thursday, October 10, 2024
"Frontiers of Neuroscience and Drug Discovery"

9:15 am to 9:30 am	**Opening Remarks** ***Dr. Alfredo Fontanini***, Professor and Chair, Department of Neurobiology and Behavior, Stony Brook Renaissance School of Medicine. Chair Symposium Organizing Committee ***Dr. Iwao Ojima***, Distinguished Professor and Director, Institute of Chemical Biology and Drug Discovery (ICB&DD), Stony Brook University
9:30 am to 10:15 am	*Moderator:* Markus Riessland **Dr. Anissa Abi-Dargham,** Distinguished Professor and Chair, Department of Psychiatry and Behavioral Health, Stony Brook Renaissance School of Medicine *"Molecular Targets and Associated Functional Domains in Schizophrenia"*
10:15 am to 11:00am	*Moderator:* Markus Riessland **Dr. Cristina Alberini,** Professor of Neural Science, Center for Neural Science, New York University *"From Bench to Bedside: Mechanisms of Long-Term Memory Inform the Development of Novel Treatments for Neurodevelopmental Disorders and Neurodegenerative Diseases"*
11:00 am to 11:45 am	*Moderator:* Markus Riessland **Dr. Michelle James,** Assistant Professor of Radiology, Neurology and Neurological Sciences**,** Stanford University School of Medicine "*Developing a PET Radiotracer Toolbox for Advancing Understanding and Treatment of CNS Diseases"*
11:45 am to 1:00 pm	**Lunch and Poster Session** *(East Hall for faculty and Zodiac Gallery for students)*
1:00 pm to 1:45 pm	*Moderator:* Matthew Parker **Dr. Ivet Bahar**, Louis and Beatrice Laufer Endowed Chair and Director of the Laufer Center for Physical and Quantitative Biology. Professor, Department of Biochemistry and Cell Biology, Renaissance School of Medicine, Stony Brook University *"Signature Dynamics of Neurotransmitter Transporters and Modulation of their Function: Insights from In Silico Studies"*
1:45 pm to 2:30 pm	*Moderator:* Matthew Parker **Dr. David Sulzer**, Professor of Neurobiology in Psychiatry, Neurology and Pharmacology, Columbia University Irving Medical Center *"Autoimmunity in Parkinson's Disease and Potential New Treatments"*
2:30 pm to 3:30 pm	**Coffee Break and Student Poster Session** *(Theatre Lobby)*
3:30 pm to 4:15 pm	*Moderator:* Matthew Parker **Dr. Iván Montoya,** Director, Division of Therapeutics and Medical Consequences at National Institute on Drug Abuse (NIDA) *"Advances in the Development of Therapeutics for Substance Use Disorders"*
4:15 pm to 5:00 pm	*Moderator:* Matthew Parker **Dr. Scott Laughlin**, Associate Professor of Chemistry, Stony Brook University *"Targeting Astrocytes Across the Blood Brain Barrier"*
5:00 pm to **5:05 pm**	**Closing Remarks**: Dr. Anissa Abi-Dargham
5:05 pm to 6:00 pm	**Reception and Poster Session *(three poster awards)***, *(Theatre Lobby)*
6:00 pm to 6:15 pm	**Announcement of Poster Awards:** Dr. Scott Laughlin
6:15 pm	**DINNER,** *East Hall (by invitation only)*

Speakers

Dr. Anissa Abi-Dargham, MD. is a Distinguished Professor and Chair of the Department of Psychiatry and Behavioral Health, Lourie endowed Chair in Psychiatry at Stony Brook School of Medicine. Dr Abi-Dargham received her medical degree from Saint Joseph University in Beirut, Lebanon, and her training in Psychiatry at the University of Memphis, TN. She then did two research fellowships, one at NIMH with Dr. Daniel Weinberger and at Yale University with Dr. Robert Innis, learning the fundamentals of molecular imaging and their application to the study of brain disorders. She is currently a leader in the field of Positron Emission Tomography (PET) imaging. She applied PET imaging in combination with multimodal MRI and clinical evaluations to study the neurobiology of severe mental illnesses, including schizophrenia, addiction and their comorbidities. Her work revealed alterations in dopamine transmission in specific areas of the brain in patients with schizophrenia and addiction and led to the generation of preclinical animal models aimed at understanding the mechanisms and consequences of these alterations, creating a truly translational program from men to mice and back. More recently her team has focused on understanding the disconnection between striatal and extra-striatal dopamine and the modulation of dopamine by other neurotransmitter systems such as the cholinergic system and the Kappa Opioid receptor system. Her work has been recognized with many awards including the Lieber Award for Outstanding Schizophrenia Research from the Brain and Behavior Foundation in 2018 and her election to the National Academy of Medicine in 2016. She served as President of the American College of Neuropsychopharmacology (ACNP) in 2017 and received the Paul Hoch Distinguished Service Award from ACNP in 2023. She is Associate Editor for Biological Psychiatry, and she serves on the Council for the Society of Biological Psychiatry and BBRF.

"Molecular Targets and Associated Functional Domains in Schizophrenia"

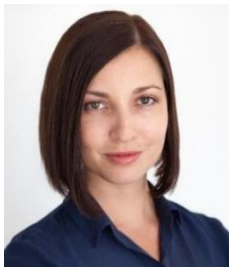
Patients with schizophrenia have positive symptoms, such as hallucinations and delusions, negative symptoms, such as anhedonia, and cognitive deficits. In addition, patients exhibit mood disturbances and motor symptoms, suggesting that the multiple circuits in the brain that subserve these functions are affected. The cortico-basal ganglia-thalamo-cortical loops have been central to the search for clues. Using multimodal imaging, we have gained insights into the molecular and functional targets in these loops that are associated with behavioral and cognitive alterations. We uncovered that dopaminergic excess stimulation of D2 receptors in the associative striatum is associated with psychosis, altered connectivity of the associative striatum, and altered perceptual inference, a basic mechanism contributing to auditory hallucinations. We also found lower levels of dopaminergic transmission in extra-striatal and cortical regions of the brain in schizophrenia, associated with cognitive deficits and negative symptoms. More recently we found that cholinergic alterations as well and the kappa opioid system may contribute to certain symptom domains, possibly via dopaminergic modulation. While more must be done to uncover the mechanisms of multilayered symptomatology in schizophrenia, these findings provide rationale for future investigations and possible leads into better therapies.

Dr. Cristina Alberini, Ph.D is the Julius Silver, Roslyn S. Silver and Enid Silver Winslow Professor of the Center for Neural Science, New York University. Dr. Alberini received her PhD in Immunological Sciences from the University of Genoa (Italy), and then trained in neurobiology as a post-doctoral fellow at Columbia University. From 1997-2000 she was an Assistant Professor in the Department of Neuroscience at Brown University and then Associate and Full Professor at Mount Sinai School of Medicine in New York from 2001 to 2011. In 2011 she joined the Center for Neural Science at New York University where she is currently a Professor in Neuroscience. Dr. Alberini's research focuses on understanding the molecular and cellular mechanisms underlying long-term memory formation and strengthening, and the role of these mechanisms in cognitive impairments, neurodevelopmental disorders, and neurodegenerative diseases. Her studies target different ages of lifespan and different brain cell types. The results of her studies provided information for improving brain functions and developing potential therapeutics against cognitive impairments and psychopathologies. As a result of her research, Alberini founded a biotech startup company, Ritrova Therapeutics Inc., for which she is the current CEO. Dr. Alberini underwent psychoanalytic training from 2002 to 2012 at the National Psychological Association for Psychoanalysis (NPAP) in New York and received a NY State license in 2013. Dr. Alberini received several awards including the Hirschl-Weill Career Scientist Award, NARSAD Independent Investigator Award, Golgi Medal, Athena Award, NIH-MERIT Award, the 2018 Jacob K. Javits NYU Award, and the NYU Julius Silver, Roslyn S. Silver & Enid Silver Winslow professorship. Dr. Alberini is an elected member of the American Academy of Arts and Sciences.

"From bench to bedside: mechanisms of long-term memory inform the development of novel treatments for neurodevelopmental disorders and neurodegenerative diseases"

Insulin-like growth factor 2 (IGF2) has emerged as a critical mechanism of synaptic plasticity and learning and memory. IGF2 is expressed at the highest levels in brain pericytes, mural cells of the microvessels that regulate blood flow, vessel formation, and blood-brain barrier functions. Pericytic IGF2 levels increase upon learning or neuronal activity, and this increase is required for long-term memory formation. Deficits in IGF2 in the brain, serum, or cerebrospinal fluid (CSF) are associated with aging, neurodegenerative brain diseases, and neurodevelopmental disorders. A common problem of these diseases is an impaired protein metabolism along with protein overaccumulation in the brain. Administration of IGF2 enhances memory in healthy rodents and reverses cognitive impairment in aged rats as well as core symptoms in models of neurodegenerative diseases and neurodevelopmental disorders. These effects occur via the IGF2 receptor (IGF2R) - a receptor that is highly expressed in neurons and regulates protein trafficking, synthesis, and degradation. We will discuss the efficacy of novel synthetic small molecules targeting IGF2R that are effective memory enhancers in healthy rodents and reverse core deficits of Angelman syndrome in a mouse model. These or similar small molecules may represent potential novel treatments for several neuropsychiatric disorders characterized by neuronal protein metabolism impairment and protein depositions in the brain.

Speakers



Dr. Michelle James, Ph.D. is an Assistant Professor in the Departments of Radiology and Neurology, within the Molecular Imaging Program at Stanford University (MIPS). She received her BS in pharmacology and organic chemistry at the University of Sydney, where she also earned her PhD in pharmacology and was awarded the University Medal. She served as the co-chair of the World Molecular Imaging Congress in 2021 and has received numerous awards for her research, teaching, and mentoring, including the Suffrage Science Award from the Medical Research Council in the UK, and the Exceptional Mentor Award from the American Medical Women's Association, and the Roger Tsien Award for significant contributions to the field of molecular imaging in the area of chemical biology. Her research is focused on developing new PET tracers for detecting immune cells in the context of neurological diseases. As part of her work, Dr. James has translated multiple tracers to the clinic, many of which are patented and being used in clinical neuroimaging research studies at Stanford University and around the world. She also co-founded a company called Willow Neuroscience which is focused on developing immune-targeted therapeutics and PET tracers for neurodegenerative diseases.

"Developing a PET Radiotracer Toolbox for Advancing Understanding and Treatment of CNS Diseases

Inflammation is a multifaceted, dynamic, and biologically necessary response to injury or infection. Transient inflammation can be beneficial, leading to the clearance of damaged cells, tissue repair, toxin neutralization, and mitigation of pathogens. However, insufficient resolution of inflammation can lead to progressive tissue damage via unrestrained production of pro-inflammatory cytokines and chemokines, inflammasome activation, and generation of reactive oxygen species. Such harmful immune responses are a common hallmark of many chronic diseases, including neurodegenerative diseases like Alzheimer's disease and Multiple Sclerosis. Likewise, harmful inflammatory reactions can significantly worsen outcomes in acute conditions like sepsis or stroke. Real-time non-invasive monitoring of immune responses is critical to improve understanding, staging, and treatment of these diseases; however, current methods for detecting specific immune cells and their functional phenotypes in vivo are very limited. In this talk I will summarize the current state-of-the-art for imaging immune responses in CNS diseases using positron emission tomography (PET), and in doing so will highlight key advances from my lab, including the development of new radiotracers targeting the pro-inflammatory innate immune receptor GPR84 in addition to progress being made with other new and available tracers for illuminating innate and adaptive immune responses in the preclinical and clinical research settings.

Dr. Ivet Bahar, Ph.D. is the Louis and Beatrice Laufer Endowed Chair and Director of the Laufer Center for Physical and Quantitative Biology, and a professor in the Department of Biochemistry and Cell Biology at the Renaissance School of Medicine, Stony Brook University. Dr. Bahar's major areas of research are structural computational, and systems biology, with applications to computer-aided drug discovery. Before joining Stony Brook University, she served as a distinguished professor, and JK Vries Chair, in the Computational and Systems Biology Department that she founded and led between 2004 and 2022 at the University of Pittsburgh. She also co-founded the joint PhD program in Computational Biology between the University of Pittsburgh and Carnegie Mellon University in 2005. The Bahar laboratory is known for pioneering novel models and methods in structural, computational, and molecular biophysics and systems biology and pharmacology, including the widely used Elastic Network Models for protein dynamics. Dr. Bahar's lab is supported by several national and international grants on a broad range of topics. At the Laufer Center, using a combination of structure-based modeling and machine learning methods, she conducts integrative research across multiple disciplines, from basic modeling of biomolecular dynamics and interactions, to identifying disease-causing mutations and developing drug candidates and therapeutic strategies for complex diseases, including cancer and neurological disorders. Understanding the mechanism of neurotransmitter transport by transporters and developing modulators of transporter function has been a major research area in her lab, supported by several NIH projects/centers that she has led. Dr. Bahar is a member of the National Academy of Sciences, and elected member of the European Molecular Biology Organization (EMBO). She has more than 340 publications.

Signature Dynamics of Neurotransmitter Transporters and Modulation of Their Function: Insights from In Silico Studies

Significant progress has been made in recent years in resolving the structures of several neurotransmitter transporters, in alternative conformations, outward-facing, inward-facing, or occluded, and bound/unbound to neurotransmitters, ions and/or small molecule modulators (SMM) of function. The progress in structure determination has been accompanied by those in developing new models and methods in silico, which now permit us to have a deeper understanding of the major determinants of transporters function at the molecular level. Our lab has focused on two groups of transporters in particular, dopamine transporters, and excitatory amino acid transporters, toward gaining their evolutionarily conserved structural and dynamic features and developing specific and potent modulators of their activity. Recent progress in this field, including the characterization of the signature dynamics of these transporters, as well as the discovery of new allosteric modulators will be presented. Notably, family members share conserved mechanisms of motions robustly allowing for alternating access of the substrate, while also possessing distinct mechanisms that differentiate family members and underlie substrate specificity and multimerization. The impact of structural dynamics on the function of specific members is illustrated, with focus on the function of the two classes of transporters, and relation to experimental observations.

Speakers

Iván D. Montoya, M.D., M.P.H. is the Director of the Division of Therapeutics and Medical Consequences (DTMC) of the National Institute on Drug Abuse (NIDA), which is one the institutes of the National Institutes of Health (NIH). He has a Medical and Psychiatrist degrees from the University of Antioquia in Colombia, and a master's in public health from Johns Hopkins University. He was a Fulbright-Humphrey Fellow at Johns Hopkins and Visiting Fellow at the Intramural Research Program of NIDA. He joined NIDA's extramural program in 1999 as Medical Officer of the Clinical Trials Network, became the Deputy Director of DTMC in 2008 and the Director of DTMC in 2024. He has published extensively about treatments (pharmacological and non-pharmacological), and medical consequences of substance use disorders (SUDs). He has received multiple awards including the NIH Director's Award and the Michael Morrison Award from CPDD. He is also Honorary Professor of the University of Valencia (Spain).

"Advances in the Development of Therapeutics for Substance Use Disorders"

Substance use disorders (SUD) and drug overdose deaths are significant public health burdens. There are safe and effective pharmacotherapies for opioid use disorders and to prevent/reverse overdose, but their efficacy can be improved. There are no FDA-approved medications to treat psychostimulant (cocaine and methamphetamine) use and cannabis use disorders or overdose. Therefore, there is an urgent need to develop safe and effective medications to prevent and treat SUDs and overdose. Advances in the understanding of the effects of those drugs on the brain are providing new opportunities to improve their treatment outcome. Some of the advances include the new findings of receptors, neurotransmitters, neuromodulators, and brain circuits associated with SUDs. Furthermore, advances in the development of biologics can offer an opportunity to investigate vaccines and monoclonal antibodies for the prevention or treatment of SUDs and overdose. In addition, new digital and neuromoduladory devices are offering new therapeutic opportunities alone or in combination with medications. The purpose of this presentation is to provide an overview of the advances in the development of therapeutics for SUDs at NIDA. It includes a presentation of the pipeline of medications, devices and digital tools that are being investigated to treat opioid, stimulant, cannabis and tobacco use disorders. The goal is to inform the participants about the potential therapeutics that may be available in the future armamentarium of treatments for SUDs.

David Sulzer, Ph.D. is Professor of Psychiatry, Neurology and Pharmacology, at the School of the Arts at Columbia University and New York State Psychiatric Institute. He received a PhD in biology from Columbia University. Dr. Sulzer's research laboratory has published over 250 studies on synaptic function, particularly of the basal ganglia and dopamine systems, and neuroimmunology, in normal and diseased states that are cited over 76,000 times (h-index 106). He is the founder of the Dopamine Society, the Gordon Conference on Parkinson's Disease, and the journal Nature Parkinson's Disease. Dr. Sulzer has received awards from the McKnight, Simons, Helmsley, NARSAD, Huntington's, and Aaron Diamond Foundations and the Universities of Jerusalem, Minnesota, University College London, national science foundations of Israel, Austria, Portugal, and given named lectureships at the National Institutes of Health, Harvard, Yale, UCSF, Emory, UC Irvine, and the Vatican. He has trained 23 graduate students and 34 postdocs of which 11 are current, and his students and postdocs have received Fulbright, Marshall, and Regeneron awards for their work in his research laboratory. Furthermore, past trainees are current professors at Columbia, Rutgers, Cornell, Yale, Lund, Pittsburgh, Georgia, Tufts, Emory, Karolinska, École Normale Supérieure (Paris France), and NYU, while others run pharmaceutical and biotech companies, and one is the science editor at the Wall Street Journal.

"Autoimmunity in Parkinson's Disease and Potential New Treatments"

We will discuss evidence that Parkinson's disease may have autoimmune features that are initiated in the gut, with specific T cells that are transported to the CNS, including cells reactive to antigens derived from the Parkinson's-related genes, alpha-synuclein and PINK1. We will also discuss evidence supporting treatment by axonal reinnervation of surviving dopamine neurons into depleted regions by pharmacological and other methods that may provide clinical approaches even for later stage patients

Speakers

Dr. Scott Laughlin, Ph.D. is an Associate Professor in the Department of Chemistry at Stony Brook University and a member of the Institute for Chemical Biology and Drug Discovery. Dr. Laughlin graduated from the University of Michigan, Ann Arbor, with a B.S. in Biochemistry and Philosophy. He received his PhD from the University of California, Berkeley, working with Professor Carolyn Bertozzi on the development of bioorthogonal chemistry. After his PhD, Dr. Laughlin completed postdoctoral training in neuroscience at the Helen Wells Neuroscience Institute of UC Berkeley, under the direction of Professor John Ngai and working towards understanding neural circuits underlying zebrafish behaviors. In the fall of 2013, Dr. Laughlin began his independent laboratory at Stony Brook University. Dr. Laughlin's research is focused on the development of chemical methods for understanding the brain. Projects in Dr. Laughlin's group focus on the synthesis and evaluation of probes for astrocytes broadly and astrocytes with functional connections to neurons, on the design, synthesis, and analysis of activatable bioorthogonal reactions with application in the imaging of neural circuit connectivity, and on the development of engineered enzymes for long term recording of neuron and astrocyte activity.

"Targeting Astrocytes Across the Blood Brain Barrier"

The brains of even simple organisms can do amazing things, but the brain's complexity makes understanding exactly how it works incredibly challenging. The research group of Dr. Laughlin focuses on using chemistry to understand the architecture of the brain's functional units called neural circuits. In one such project, the Laughlin group has identified a chemical scaffold that enables visualization of astrocytes and neuron-interacting astrocytes in the brains of both mammals and zebrafish. Dr. Laughlin will present on the discovery of this new class of chemical astrocyte label and on recent findings of these molecule's ability to cross the blood brain barrier, which enables new applications for these compounds in the fields of drug delivery and human brain imaging.

NOTES

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