

Back into the Woods

36th Annual Gibbs Conference on Biothermodynamics Touch of Nature • Carbondale, Illinois • October 1-4, 2022

Organized by Aaron L. Lucius & James R. Horn

Sponsors include Beckman Coulter Life Sciences, Bruker, CUNY Institute for Macromolecular Assemblies, Edinburgh Instruments, ISS, Jasco, Lumicks, Malvern, NanoTemper, New England Biolabs, OLIS & Wyatt Technology https://www.gibbssociety.org/annual-conference

Table of Contents

Touch of Nature		
Driving Instructio	ons, Maps & Facilities	2-4
Introduction		
History, Lists of I Gibbs Society G Mission Stateme Gibbs Society By The Gary K. Ack	Past Meetings and Special Lectures overnance – Incorporation, Officers, Committees nt, Confidentiality Statement and Code of Conduct /laws ers Lecture in Biothermodynamics	6-7 8-9 10 11-12 13
Schedule of Eve	ents	
Calendar-Forma	at Schedule	16
Openina Events	5	
Saturday	Saturday Night Thermo – for Trainees Only Reception for All Participants	
Platform Sessio	ons	
Sunday	Platform Session I - Morning	18
	Platform Session II – Late Afternoon	
Monday	Platform Session III - Morning	21
Tuosday	Platform Session V Morning	23 21
Tuesday	Link for Post-Conference Survey	24
Poster Session	S	
General Info	rmation	
Sunday	Poster Session I (M-Z)	27
Monday	Poster Session II (A-L)	32
Abstracts for Al	I Presentations	
Platform Sessior Poster Session I Poster Session I	ns – in chronological order – Sunday I - Monday	37 68 127
Participants		
Listed Individual Listed by Labora	ly tory	
Sponsors		
Special Thanks t	to the Commercial, Academic & Individual Sponsors	

Image Credits

Front outer cover: Watercolor drawing of Little Grassy Lake and bonfire by Angela Retherford. Back outer cover: "E. coli on Elm," a wood burning by Aron Fenton based on a David Goodsell image; Gibbs36 campfire logo by Madeline Shea based on porin (3jty) and nucleosome DNA (6c0w).

In the Schedule of Events, images highlight the research of Liskin Swint-Kruse (Keynote Lecture) and Tobin Sosnick (Gary K. Ackers Lecture in Biothermodynamics).

Southern Illinois University – Carbondale

Touch of Nature (TON) Outdoor Education Center

Driving Directions

https://ton.siu.edu/about-us/

GPS Address: The easiest way to get to Touch of Nature is use this address



in a GPS navigation: 1206 Touch of Nature Road, Makanda, IL 62958

From the north:

Take Interstate 57 South to the Route 13 exit (Carbondale - Exit #54B), turn west (right) onto Route 13 toward Carbondale, go approximately 15 miles. Look for Wal-Mart on your right once you enter Carbondale. Turn left (south) at this light, Giant City Road. Continue 8 miles south on Giant City Road. Touch of Nature Road will be on your left (east). Turn left and continue straight on Touch of Nature Road. Administration building is the first left.

From the south:

Follow I-24 to I-57 North, or stay on I-57, to the Route 148 exit (Exit #45), head northwest on 148 for approximately 2 miles. Turn left on Grassy Road. There is a convenience store on this corner. Follow Grassy Road for about 7 miles. Stay left when you come to a Y. Continue southwest on Grassy Road. Grassy Road will come to a T at Giant City Road. Turn south (left) on Giant City Road. Continue on Giant City Road approximately 1 mile. Touch of Nature Road will be on your left. Turn left and continue straight on Touch of Nature Road. Administration building is the first left.

From the east:

Head west on I-70 or, if you are further south, take I-64 to I-57 South. Continue approximately 50 miles south from I-64 to the Route 13 exit (Marion - Exit #54B), head west on Route 13 toward Carbondale, go approximately 15 miles. Look for Wal-Mart on your right once you enter Carbondale. Turn left (south) at this light, Giant City Road. Continue 8 miles south on Giant City Road. Touch of Nature Road will be on your left (east). Turn left and continue straight on Touch of Nature Road. Administration building is the first left.

From the west:

Head east on I-64 approximately 50 miles from St. Louis. Take the Route 127 (Nashville) exit south. Continue south for approximately 50 miles to Murphysboro. At Murphysboro, go left (east) for approximately 10 miles. You will pass through the town of Carbondale. Watch for the mall on your right. When you see Wal-Mart on your left, this is your light. Turn right (south) at this light, Giant City Road. Continue 8 miles south on Giant City Road. Touch of Nature Road will be on your left (east). Turn left and continue straight on Touch of Nature Road. Administration building is the first left.

History https://ton.siu.edu/about-us/history.php

https://news.siu.edu/2018/03/032718-special-olympics-history.php https://hee-journal.uni-koeln.de/sites/hee-journal/user_upload/Ritzel_2018.pdf

Map of TON Camps 1 & 2 with Carbondale Inset

Going south on Giant City Road, turn left onto Touch of Nature Rd. and proceed to Camp 2.



Camp 2 – Most activities will take place here.



Selected Touch of Nature Facilities

River Radio Retreat Building

Session Breaks and Business Meeting will be held here.



Friends Room in Little Grassy Lodge

Saturday Night Thermo talks/panel and Platform Sessions will be held here.



Lodging ranges from "dormitory-like" to rustic cabins





Introduction History & Governance

The Gibbs Conference on Biothermodynamics

History

Fall, 1986

Discussion of the discipline: Thermodynamics in Biological Systems. The Gill residence in Vail, Colorado. Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee.

February, 1987

Discussion of the discipline: Thermodynamics in Biological Systems. The Gumbo Shop, New Orleans, LA

during the 31st Annual Biophysical Society Meeting. Gary Ackers, Norma Allewell, Wayne Bolen, Ken Breslauer, Ken Dill, Ernesto Freire, Stan Gill, Jim Lee.

A history of the first ten years of the meeting was provided by Gary Ackers and Wayne Bolen in "The Gibbs Conference on Biothermodynamics: Origins and Evolution" published in *Biophysical Chemistry* 64 (1997) 3-5 (doi:10.1016/S0301-4622(96)02246-6).





J. Willard Gibbs

An update was provided by Madeline A. Shea, John J. Correia and Michael D. Brenowitz in "Introduction: Twenty five years of the Gibbs Conference on Biothermodynamics" available in *Biophysical Chemistry* 159 (2011) 1-5 (doi:10.1016/j.bpc.2011.07.002).

Conference Organizers & Keynote Speakers

All in-person meetings have been held at the Touch of Nature Outdoor Education Center (prior to 2022, it was called the Touch of Nature Environmental Center) associated with Southern Illinois University–Carbondale. From 1987 through 1993, all speakers in scientific sessions were students or postdoctoral fellows. In 2020 and 2021, the meeting was held virtually (*via* Zoom) because of the COVID-19 pandemic.

Year	Conference Organizers Keynote Speakers
1987	Jim Lee and Wayne Bolen Philosophical Talks by Gary K. Ackers and Ken Dill
1988	Gary Ackers and Michael Johnson
1989	Susan G. Frasier and Michael Johnson
1990	Michael Johnson and Marty Straume
1991	Gary Ackers and Tim Lohman Ernesto Freire
1992	Jim Lee and Tomasz Heyduk Serge Timasheff and John Schellman
1993	Maurice Eftink and Glen RamsayPeter von Hippel and Julian Sturtevant
1994	Enrico Di Cera and Madeline SheaGary K. Ackers and Kathleen S. Matthews
1995	Kenneth P. Murphy and Michael D. Brenowitz Victor Bloomfield and Mario Amzel
1996	Jonathan B. Chaires and Michael L. DoyleJ. Michael Schurr and Allen Minton
1997	Dorothy Beckett and Jack CorreiaAdrian Parsegian
1998	Andy Robertson David Draper
1999	Bertrand Garcia-Moreno E. and John Shriver Wayne Bolen and Gary Ackers
2000	George Turner and Kim SharpSteve White

Year **Conference Organizers** Keynote Speaker(s) 2001 Margaret A. Daugherty and Luis A. MarkyGeorge Rose 2002 Michael Mossing and George MakhatadzeRodney Biltonen Vince Hilser and Dick SheardyJim Lee 2003 2004 Doug Barrick and Kathleen HallNacho Tinoco 2005 Trevor Creamer and Clay Clark Carl Frieden Karen Fleming and Rohit V. Pappu Madeline A. Shea and Timothy Lohman 2006 2007 Brian M. Baker and Michael T. Henzl Jannette Carey and David Bain Dorothy Beckett and Ken Dill 2008 Nathan Baker and Liskin Swint-KruseLinda Jen-Jacobson 2009 2010 Elisar Barbar and Vince J. LiCata C. Nick Pace 2011 Gibbs Society Board of DirectorsBertrand Garcia-Moreno E. Aaron L. Lucius and Patricia L. Clark Terry G. Oas 2012 James L. Cole and Aron W. Fenton Doug Barrick 2013 2014 Andrew B. Herr and Steven T. Whitten Karen G. Fleming Ernesto J. Fuentes and James R. HornRohit V. Pappu 2015 Sarah Bondos and Nick FitzkeePatricia Clark 2016 Scott Showalter and Ana-Maria Soto Enrique de la Cruz 2017 2018 Chiwook Park and David Draper Kevin Plaxco 2019 Matthew Auton and Carlos Castañeda Cathy Royer 2020 Roberto Galletto and Karen A. Lewis......Kathleen Hall Gibbs Society Board of Directors Brian Baker 2021 Aaron L. Lucius and James R. HornLiskin Swint-Kruse 2022

The Annual Gary K. Ackers Lecture in Biothermodynamics

Since 2009, the Gibbs Society Board of Directors sponsors an annual lecture honoring the scientific contributions of founding organizer Gary K. Ackers (1939-2011) to the field of biothermodynamics.

Lecture	Year	Ackers Lecturer
1	2009	Michael Brenowitz
2	2010	Timothy Lohman
3	2011	Madeline Shea
4	2012	Enrico Di Cera
5	2013	Bertrand Garcia-Moreno E.
6	2014	David E. Draper
7	2015	Walter S. Englander
8	2016	Ken Dill
9	2017	Dorothy Beckett
10	2018	James C. Lee
11	2019	Jack Correia
12	2020	Douglas Barrick
13	2021	David Bain
14	2022	Tobin Sosnick

Gibbs Society Governance

Incorporation

In 2002, the Gibbs Society of Biological Thermodynamics incorporated in the Commonwealth of Virginia, under the guidance of Michael L. Johnson, then Treasurer of the Society. Current bylaws are available online (<u>https://www.gibbssociety.org/</u>) and Articles of Incorporation may be requested from the Treasurer.

Current Officers and Terms

President	Aaron L. Lucius, 2021 – 2022
President-Elect	James R. Horn, 2021 – 2022
Past-President	Liskin Swint-Kruse, 2021 – 2022
Vice President	Aron Fenton, 2022 –
Secretary	Andrew Herr, 2019 – 2025
Treasurer	Aron Fenton, 2017 – 2022
Treasurer-Elect	Karen Lewis, 2022 – 2026

2021 – 22 Board of Directors (alphabetically by last name)

Aron Fenton, Andrew Herr, James R. Horn, Vince J. LiCata, Aaron L. Lucius, Madeline A. Shea, Liskin Swint-Kruse

Former Presidents

2001 – 2002 Gary K. Ackers	201
2002 – 2003 Jack Correia	201
2003 – 2004 D. Wayne Bolen	201
2004 – 2005 Madeline A. Shea	201
2005 – 2006 Dorothy Beckett	201
2006 – 2007 J. Brad Chaires	201
2007 – 2008 Timothy M. Lohman	201
2008 – 2009 Luis A. Marky	201
2009 – 2010 Bertrand Garcia-Moreno E	201
2010 – 2011 Karen G. Fleming	202

2011 – 2012 Douglas Barrick
2012 – 2013 David L. Bain
2013 – 2014 George I. Makhatadze
2014 – 2015 Patricia Clark
2015 – 2016 Vince J. LiCata
2016 – 2017 James Cole
2017 – 2018 Clay Clark
2018 – 2019 Brian Baker
2019 – 2020 Kathleen Hall
2020 – 2021 Liskin Swint-Kruse

Former Treasurers

2001 – 2011 Michael L. Johnson 2011 – 2017 Jack Correia

Former Secretaries

2004 – 2013Margaret A. Daugherty 2013 – 2019Liskin Swint-Kruse

Former Vice President

2010 - 2022 Michael L. Johnson

Committees and Other Contributors To Conference Organization

Ackers Lecturer Selection Committee

Vince J. LiCata (Chair) 2021 – and current members of the Gibbs Society Board of Directors

Fundraising Committee:

Jim Cole (Chair), Ron Koder and Allyn Schoeffler

Local Arrangements Committee

Carlos Castañeda (Chair) and Hui-Ting Lee

Poster Committee

Tonya Zeczycki (Chair) and Steven Whitten

Presentation Logistics Committee

Stephen Fried (chair), Clarissa Durie and Kurt Piepenbrink Trainee members: Edgar Manriquez-Sandoval and Yafan Yu

Program Book Committee

Madeline Shea (Chair) and Justin Miller

Registration – JotForm and PayPal Nicholas C. Fitzkee

Saturday Night Thermo Co-Organizers

Karen Lewis and Vince J. LiCata Trainee members: Shwetha Sreenivasan and Feng Yu

SharePoint Guru

James R. Horn

Speaker Nominating Committee

Michael Brenowitz (Chair), Afua Nyarko and Ernesto Fuentes

Webmasters for Gibbs Society - https://www.gibbssociety.org

Chiwook Park and Sarah E. Bondos (2020 – present)

Mission Statement

The Gibbs Society of Biological Thermodynamics is committed to

- Advancing the development and promoting the use of thermodynamics in biology,
- Fostering the mentoring of and providing development opportunities for students and postdoctoral fellows,
- · Promoting a sense of community in the field of biological thermodynamics, and
- Hosting an Annual Conference that is accessible to as wide a range of participants as possible.

During registration online, all participants have accepted the following policies of the Gibbs Conference on Biothermodynamics.

Confidentiality Statement

Please remember that the content of all presentations (both talks and posters) for this meeting are confidential material and may contain unpublished results. Abstracts will not be posted online.

Please ask permission from the authors before taking photos or screenshots of posters or poster material.

Please do not record or take screenshots of the talks, posters, or any presented material unless a speaker has given you express permission.

Code of Conduct

The Gibbs Society of Biological Thermodynamics is committed to providing a safe and productive environment that fosters open dialogue and the exchange of scientific ideas, promotes equal opportunities and treatment for all participants, and is free of harassment and discrimination.

Harassment includes speech or behavior that is not welcome or is personally offensive, whether it is based on ethnicity, gender, religion, age, body size, disability, veteran status, marital status, sexual orientation, gender identity, or any other reason. It includes stalking, unnecessary touching, and unwelcome attention.

Behavior that is acceptable to one person may not be acceptable to another, so use discretion to be sure that respect is communicated. Harassment intended in a joking manner still constitutes unacceptable behavior. Anyone experiencing conduct that violates this Code should report this conduct to any member of the Gibbs Society Board.

Bylaws to Articles of Incorporation for Gibbs Society of Biological Thermodynamics June 3, 2022

The Gibbs Society of Biological Thermodynamics is committed to:

- Advancing the development and promoting the use of thermodynamics in biology
- Fostering the mentoring of and providing development opportunities for students and postdoctoral fellows
- Promoting a sense of community in the field of biological thermodynamics
- Hosting an Annual Conference that is accessible to as wide a range of participants as possible

Bylaw 1 (established December 11, 2020):

Henceforth, the Board of Directors shall consist of two long term members and up to 5 rotating members. The 5 rotating members shall be the (1) the Past-President, (2) the current President, (3) the President-Elect, (4) Secretary (3-year term), and (5) Treasurer (5-year term). All board members will be listed publicly on the Gibbs Society of Biological Thermodynamics website. The positions of advisory Vice President, Assistant Treasurer, and Webmaster will be appointed by the Board of Directors and publicly posted on the website. Vacancies on the Board of Directors will be filled by a majority vote of the Board of Directors. As needed, other positions may be created and appointed by the Board of Directors must have served as an Organizer of the Gibbs Conference on Biothermodynamics.

Bylaw 2 (established February 22, 2017; edited May 13, 2022):

Officers of the Gibbs Society of Biological Thermodynamics shall be elected at the annual meeting of the Board of Directors during the annual conference. A President-Elect shall be chosen at each annual meeting. At the close of the annual meeting, the President-Elect will become the current President and the current President will become the Past-President. The Secretary and Treasurer shall serve renewable 3-5-year terms. The Treasurer is authorized to invest society funds in checking accounts and interest-bearing accounts such as money market accounts, savings accounts and/or certificates of deposit. The Treasurer will inform the Board of Directors prior to transfers of Society funds. The Treasurer shall provide the Board of Directors and 2) after all expenses and income from the meeting have been resolved. Two members of the Board of Directors in addition to the Treasurer will be authorized to have access to the bank account.

Bylaw 3 (established February 22, 2017; edited May 16, 2022):

The Board of Directors shall provide oversight and serve as advisors to the current organizers of the Gibbs Conference on Biothermodynamics. It is the responsibility of the Board of Directors to provide documentation on how to organize a Gibbs Conference to the conference organizers. This includes a summary of financial reports from the treasurer; a list of email addresses from the secretary; and a check list of organizational tasks that will be revised in consultation with the organizers of the immediate past meeting.

Bylaw 4 (established May 13, 2022):

All donations to the Gibbs Society of Biological Thermodynamics, regardless of source, will be unrestricted, will be deposited in the general fund, and will be used at the discretion of the Board of Directors to support and improve the conference and other activities of the Gibbs Society of Biological Thermodynamics. All donors will be informed of this before their gifts are accepted, and donations will be acknowledged in the program book and on the website for the conference.

These Bylaws were discussed by email exchanges and approved by vote during a zoom meeting of the Board of Directors:

Madeline Shea, Long-Term Board Member Vince LiCata, Long-Term Board Member Aaron Lucius, President Jim Horn, President-Elect Liskin Swint-Kruse, Past-President Andrew Herr, Secretary Aron Fenton, Treasurer

These bylaws replace those established Dec 11, 2020.

14th Annual Gary K. Ackers Lecture in Biothermodynamics 2022 Lecturer – Tobin Sosnick, University of Chicago

This lecture honors the scientific contributions of Gary K. Ackers (1939-2011) to the field of Biological Thermodynamics. He served on the faculty at the University of Virginia, Johns Hopkins University and Washington University in St. Louis School of Medicine. He was a Fellow of the Biophysical Society and was one of the founding organizers of the Gibbs Conference.

Gary demonstrated a lifelong commitment to the growth and development of an intellectual community of scholars devoted to furthering the field of biothermodynamics. Gary was an active member of the Biophysical Society throughout his career and served as President of the Society, as well as Organizer of the annual meeting. While on the faculty of the University of Virginia, he was a leader in the graduate biophysics training program. When on the faculty in the Department of Biology at the Johns Hopkins University, he conceived and organized the Institute for Biophysical Studies of Macromolecular Assemblies, a university-wide training program in molecular biophysics that has continued for decades. While at Johns Hopkins, he also played a leading role in the establishment of the Gibbs Conference on Biothermodynamics, an annual meeting organized to promote innovative development of biophysical principles applied to current problems in biology and to train the next generation of molecular biophysicsts to tackle hard problems rigorously. After moving to St. Louis to chair the Department of Biochemistry and Molecular Biophysics at Washington University, he spearheaded a new graduate program in biophysics and hired many faculty who have joined the community of regular contributors to the Gibbs Conference.

Gary was a pioneer in the development of methods and application of principles of equilibrium thermodynamics to the study of linkage in complex macromolecular assemblies. Studies from his laboratory on the energetics of self-association and ligand binding in human hemoglobin proved unequivocally that the classic and elegant MWC model of intersubunit allostery was insufficient to explain cooperative oxygen binding: the position, as well as the number, of ligands matters. His contributions in this area greatly enhanced our understanding of the relationship between structure, energy and function in hemoglobin, and in multimeric allosteric systems in general. By probing ever more deeply into the molecular mechanism of cooperativity, he demonstrated a beautiful, useful, and general strategy for dissecting functional energetics in macromolecular assemblies.

His quantitative study of the interactions between proteins and nucleic acids in the bacteriophage lambda system included the development of quantitative DNase footprinting methods for measuring free energies of repressor-operator interactions. The footprinting assay remains an effective tool for measuring the extremely tight binding constants that are often encountered in site-specific interactions between proteins and nucleic acids. Those studies paved the way for similar methods to study protein-nucleic acid interactions in more complex systems, including time-resolved studies of the kinetics of RNA folding. Based on his experimental studies of phage lambda, his group developed statistical thermodynamic models to simulate the lysogenic-to-lytic growth switch: the series of macromolecular events that determine the fate of bacteriophage lambda during infection of E. coli. This work demonstrated how a complex biological function could be predicted quantitatively, strictly from the kinetics of transcription and translation, and the Gibbs free energy of interactions between the key macromolecular components in the genetic switch.

During Gary's early career, he developed methods to measure association constants in selfassociating systems based on analytical gel permeation chromatography. Those methods have since become standard tools in the field. His group was also responsible for modifications of the cryo-gel electrophoresis methods, moving from applying them to hemoglobin to protein-DNA interactions. These contributions focused on developing the capacity to quantify intermediate states that are only transiently populated during the course of a biochemical process. His more than 200 articles and chapters changed our view of the molecular mechanisms that govern complex biochemical reactions.



Schedule of Events October 1-4, 2022





Time listed in leftmost column indicates approximate starting time for event in that block.

		Saturday + October 1, 2022
4:0	00 – 10:00 pm	Check-in at Little Grassy Lodge for payment for lodging, and pick- up of name badge and program book.
7:	30 – 10:00 pm	Opening Reception in Freeberg & Burke & Surrounding Tents Light refreshments, beer, wine, and soft drinks will be served. Participants are expected to make dinner arrangements independently.
Satı	ırday Night	Thermo – Event for trainees only
Co	o-Organizers Karen Lew	is , Texas State University & Vince J. LiCata , Louisiana State University
М	oderators	
	Shwetha S Feng Yu, S	r eenivasan , Swint-Kruse Lab, University of Kansas Medical Center Sukenik Lab, University of California, Merced
5:3	30 pm	Little Grassy Lodge "Friends Room" Dinner for trainees who registered in advance
6:0	00 – 7:00 pm	Flash Talks in Little Grassy Lodge "Friends Room" Open to trainees only. No registration required.
Sp	beakers - please	e work with Moderators to connect and test your laptop in advance.
1.	Inter-domain f Naiduwadura Poster M20	Texibility of human SRSF1 allows flexibility in RNA binding Ivon De Silva, Zhang Lab, University of Alabama at Birmingham –
2.	Conformation Mithun Nag Ka	al Landscape of Initiator Caspases aradi Giridhar, C. Clark Lab, University of Texas at Arlington - Poster S17
3.	lf you think yo Sahiti Kuppa,	ou know RPA-ssDNA filaments, think again! Antony Lab, Saint Louis University – <i>Poster M51</i>
4.	Protein Charg in the Nanopa	e Distribution Alters Thermodynamics rticle Protein Corona
	Cnatnuri Kariyawasam, Fitzkee Lab, Mississippi State University - Poster M44	
5.	Thermodynam from model pe Uroš Zavrtanil	nics of α-helix formation: eptides to intrinsically disordered proteins k, Lah Lab, University of Ljubljana - <i>Poster S56</i>
6.	Allosteric con Stephen Doka	trol in cAMP receptor protein from Mycobacterium tuberculosis s, Maillard Lab, Georgetown University – Poster M24
7:0	00 – 7:15 pm	Refreshment Break
7:′	15 – 8:15 pm	Career Panel in Little Grassy Lodge "Friends Room" Session open to all trainees Sponsored by the Serge N. Timasheff Scholarship

8:15 pm Adjourn to join ongoing reception for all participants.

Sunday Morning + October 2, 2022

• Posters in Poster Session I may be mounted on Sunday morning. Use assigned number.

7:00 – 8:20 am Breakfast in Freeberg & Burke & Surrounding Tents

Platform Session I

8:15 am	Speakers - Please connect your laptop in advance of the session. AV support provided by Yafan Yu , Piepenbrink Lab, Univ. of Nebraska
8:30 – 8:40 am	President's Welcome Aaron L. Lucius, University of Alabama at Birmingham
8:40 – 8:50 am	Organizers' Remarks James R. Horn, Northern Illinois University
Moderator	Elizabeth Duran, Walter Lab, University of Michigan
36 th Annual G	bibbs Conference Keynote Lecture
8:50 – 9:00 am	Speaker Introduction Sarah Bondos, Texas A&M University
9:00 – 9:50 am	Rheostats, Toggles, and Neutrals, Oh My! Liskin Swint-Kruse, University of Kansas Medical Center
9.50 - 10.00 am	Questions for Keynote Speaker



Platform Session I - continued

10:00 – 10:30 am	Break – Refreshments in River Radio Retreat	
10:30 – 10:45 am	Mechanism of Peptide Register Shift in a Class I MHC Protein Tatiana J. Rosales, Baker Lab, University of Notre Dame	
10:45 – 10:50 am	Questions for speaker	
10:50 – 11:15 am	Single-molecule Fluorescence Spectroscopy of Apolipoprotein E Andrea Soranno, Washington University in St. Louis	
11:15 – 11:20 am	Questions for speaker	
11:20 – 11:35 am	Negative Cooperativity and Allostery in Rad52 Regulates Pre-Synaptic Events in Homologous Recombination Jaigeeth Deveryshetty, Antony Lab, Saint Louis University	
11:35 – 11:40 am	Questions for speaker	
11:40 – 11:50 am	General Discussion for Session	
12:00 pm	Conference Photo near Freeberg Hall Photographer Brian Baker Gather on hill near the parking lot by Freeberg Hall	
12:15 pm	/ I \	
1:00 – 2:45 pm	Free Time until Afternoon Session Information about local parks and attractions is available near the entrance to	

Little Grassy Lodge. See easel near counter for possible organized events.

Sunday Afternoon + October 2, 2022

Platform Session II

2:45 pm	Speakers - Please connect your laptop in advance of the session. AV support provided by Edgar Manriquez-Sandoval , Fried Lab, Johns Hopkins University
Moderator	Michael Baxa, Sosnick Lab, University of Chicago
3:00 – 3:25 pm	Deciphering the Dynamic Language of Histones Emma Morrison, Medical College of Wisconsin
3:25 – 3:30 pm	Questions for speaker
3:30 – 3:45 pm	Periplasmic Chaperone FkpA Utilizes an Extensive Binding Interface to Enable Its Intermediate Chaperone Function Taylor Devlin, Fleming Lab, Johns Hopkins University
3:45 – 3:50 pm	Questions for speaker
3:50 – 4:05 pm	The Metabolome Weakens RNA Helix Stability and Increases RNA Chemical Stability Jacob Sieg, Bevilacqua Lab, Penn State University
4:05 – 4:10 pm	Questions for speaker
4:10 – 4:40 pm	Break – Refreshments in River Radio Retreat
4:40 – 5:05 pm	Clues to Understanding the Structural Origins of Electro-Chemical Linkage in a Novel Membrane Transporter Sandipan Chowdhury, University of Iowa
5:05 – 5:10 pm	Questions for speaker
5:10 – 5:25 pm	Energetics of Nanoparticle-Protein Binding: Influence of Surface Curvature on Protein Stability Radha Somarathne, Fitzkee Lab, Mississippi State University
5:25 – 5:30 pm	Questions for speaker
5:30 – 5:55 pm	Telomere G-quadruplexes: What Does "Stability" Mean? Hui-Ting Lee, University of Alabama at Birmingham
5:55 – 6:00 pm	Questions for speaker
6:00 – 6:10 pm	General Discussion
6:30 pm	Dinner in Freeberg & Burke & Surrounding Tents

Sunday Evening + October 2, 2022

Poster Session I (M-Z)

8:00 – 10:00 pm	Posters on display in Freeberg Hall and Burke Lounge	
	Instructions & assigned numbers are listed after the schedule of talks.	

Sponsor's Displays in Freeberg Hall (upper level) Please set up displays near beer, wine, and soft drinks

Monday Morning + October 3, 2022

• Posters in Poster Session II may be mounted on Monday morning. Use assigned number.

♦ A white board will be available in Little Grassy Lodge, near the check-in window. <u>If you can offer someone a ride to the St. Louis airport</u>, please write your name, the time when you are leaving Touch of Nature, and number of people you can accommodate.

7:00 – 8:20 am Breakfast in Freeberg & Burke & Surrounding Tents

Platform Session III

8:15 am	Speakers - Please connect your laptop in advance of the session. AV support provided by Yafan Yu, Piepenbrink Lab, Univ. of Nebraska	
Moderator	Emery Usher, Holehouse Lab, Washington University in St. Louis	
8:30 – 8:40 am	Announcements – Aaron L. Lucius & James R. Horn, Organizers	
14 th Annual Gary K. Ackers Lecture in Biothermodynamics		
8:40 – 8:50 am	Speaker Introduction Patricia Clark, Notre Dame University	
8:50 – 9:40 am	Biothermodynamics (and Kinetics) Still Amazes Me Tobin Sosnick, University of Chicago	
9:40 – 9:50 am	Questions for Ackers Lecturer	



Platform Session III - continued

9:50 – 10:20 am	Break – Refreshments in River Radio Retreat
10:20 – 10:35 am	Effects of pH on the Stability of Monomeric Caspases Isha Joglekar, C. Clark Lab, University of Texas at Arlington
10:35 – 10:40 am	Questions for speaker
10:40 – 11:05 am	Proton Coupling in Transport Katherine Henzler-Wildman, University of Wisconsin Madison
11:05 – 11:10 am	Questions for speaker
11:10 – 11:25 am	Investigating Natural Variation in SAM-I Riboswitch Ligand Binding and Transcription Termination Ian Hall, Keane Lab, The University of Michigan
11:25 – 11:30 am	Questions for speaker
11:30 – 11:40 pm	General Discussion
11:40 – 12:00 pm	Introduction of Attending Commercial Sponsors Reminder of Meeting of Conference Volunteers & Past Organizers Aaron L. Lucius & James R. Horn, Organizers
12:00 pm	Lunch in Freeberg & Burke & Surrounding Tents
1:00 – 2:45 pm	Free Time until Afternoon Session Information about local parks and attractions is available near the entrance to Little Grassy Lodge. See easel near counter for possible organized events.
1:15 – 2:15 pm	Business Meeting of Conference Volunteers and Past Organizers
	River Radio Retreat Building

Area will be unavailable to other meeting attendees during this time.

Monday Afternoon + October 3, 2022

Platform Session IV

2:45 pm	Speakers - Please connect your laptop in advance of the session. AV support provided by Edgar Manriquez-Sandoval , Fried Lab, Johns Hopkins University
Moderator	Dagan Marx , Eliezer & Levitz Labs, Weill Medical College of Cornell University
3:00 – 3:25 pm	The Role of Folded-State Dynamics in Protein-DNA Selectivity Gregory Poon, Georgia State University
3:25 – 3:30 pm	Questions for speaker
3:30 – 3:45 pm	Solute Probes of Large Conformational Changes in the Steps of Transcription Initiation Max Rector, Record Lab, University of Wisconsin-Madison
3:45 – 3:50 pm	Questions for speaker
3:50 – 4:05 pm	Modulating Multivalent Ligand Binding Accessibility and Affinity to Tune Heterotypic Phase Separation of UBQLN2 Sarasi Galagedera, Castañeda Lab, Syracuse University
4:05 – 4:10 pm	Questions for speaker
4:10 – 4:40 pm	Break – Refreshments in River Radio Retreat
4:40 – 5:05 pm	Deciphering How Allosteric Redox Switches Regulate Transglutaminase 2's Conformations Tonya Zeczycki, Brody School of Medicine at East Carolina University
5:05 – 5:10 pm	Questions for speaker
5:10 – 5:25 pm	The Thermodynamics of Assembly of the Bivalent Notch Ternary Complex Cyril Cook, Barrick Lab, Johns Hopkins University
5:25 – 5:30 pm	Questions for speaker
5:30 – 5:55 pm	Protein Evolution and Conformational Ensembles Mike Harms, University of Oregon
5:55 – 6:00 pm	Questions for speaker
6:00 – 6:10 pm	General Discussion
6:10 pm	Announcements - New Officers 2022-23 & Organizers for Gibbs37 Aaron L. Lucius, President
6:30 pm	Dinner in Freeberg & Burke & Surrounding Tents

Monday Evening + October 3, 2022

Poster Session II (A-L)

8:00 – 10:00 pm **Posters on display in Freeberg Hall and Burke Lounge** Instructions & assigned numbers are listed after the schedule of talks.

> **Sponsor's Displays in Freeberg Hall (upper level)** Please set up displays near beer, wine, and soft drinks

Tuesday Morning + October 4, 2022



When you leave Touch of Nature, please leave your room key at the counter in Little Grassy Lodge.



7:00 – 8:20 am Breakfast in Freeberg & Burke & Surrounding Tents

Platform Session V

8:25 am	Speakers - Please connect your laptop in advance of the session. AV support provided by Yafan Yu , Piepenbrink Lab, Univ. of Nebraska
8:40 – 8:45 am	Announcements – Aaron L. Lucius & James R. Horn, Organizers
Moderator	Liana Islam, Lucius Lab, University of Alabama at Birmingham
8:45 – 9:10 am	Nuclear Receptor Function Made Crystal Clear with NMR Spectroscopy Doug Koietin, UF Scripps Biomedical Research
9:10 – 9:15 am	Questions for speaker
9:15 – 9:30 am	Extremophilic Proteome Refoldability Studies Reveal Distinct Biophysical Strategies to Protect Protein Structure In Vivo Haley Moran, Fried Lab, Johns Hopkins University
9.30 - 9.35 and 9.35	Questions for speaker
9:35 – 9:50 am	SARS-CoV-2 Variants
9:50 – 9:55 am	Vaibhav Upadhyay, Mallela Lab, University of Colorado Questions for speaker
9:55 – 10:10 am	Break – Refreshments in River Radio Retreat
10:10 – 10:35 am	Identification and Prediction of Fold-Switching Proteins Lauren Porter, NIH
10:35 – 10:40 am	Questions for speaker
10:40 – 10:55 am	Clostridioides difficile biofilm formation via DNA binding by Type IV Pili Leslie Ronish, Piepenbrink Lab, University of Nebraska-Lincoln
10:55 – 11:00 am	Questions for speaker
11:00 – 11:15 am	A Quantitative Model of Structure and Disorder: Agreement Between Single Molecule FRET Experiments and Simulations Justin Miller, Bowman Lab, University of Pennsylvania
11:15 – 11:20 am	Questions for speaker
11:20 – 11:25 am	Closing Remarks by Incoming President James R. Horn
11:30 am	Lunch-to-Go - Pickup in Freeberg Hall



On your way home, please complete the post-conference survey. You may reach it using the QR code or the <u>link</u> below. <u>https://forms.gle/SmLUJps5wsERWx2f8</u>





Poster Information & Assigned Boards

Poster Sessions - General Information

Dates and Locations

Posters will be presented during evening sessions on Sunday and Monday in both Burke Lounge and Freeberg Dining Hall. Each poster session will start at 8:00 pm.

Session I - Sunday evening

Posters whose abstracts have first authors with last names M-Z.

Session II - Monday evening

Posters whose abstracts have first authors with last names A-L.

Poster Numbers

Boards are numbered according to the last name of the first author, regardless of who is presenting the poster.

Presenters are asked to place their poster on the board that corresponds to the numeral in their poster listing for Sunday (S1, S2, etc.) or Monday (M1, M2, etc.). That listing follows these instructions.

Poster Sizes & Boards

The poster boards are come from a variety of sources. They are variable in size and made of materials ranging from foamcore boards to repurposed cubicle dividers.

Width: Making posters no more than 48 inches wide is recommended.

Mounting: Pushpins will be provided, but some boards are very dense. You may wish to bring your own Velcro (hook and loop) buttons for mounting your poster.

Times

Posters may be mounted in the morning for viewing during the day,

Posters should be taken down by midnight.

Confidentiality – No photos without permission

Please remember that the content of all presentations (both talks and posters) for this meeting are confidential material and may contain unpublished results. Abstracts will not be posted online.

Please **ask permission** from the authors before taking photos or screenshots of posters or poster material.

Please do not record or take screenshots of the talks, posters, or any presented material unless a speaker has given you express permission.

Poster Session I + Sunday, October 2, 2022

Posters numbered alphabetically by first author's last name (M-Z) (Posters S1-S58)

- **S1** Specific T cell recognition of a public neoantigen derived from the driver oncogene *PIK3CA*. Jiaqi Ma, Smita S. Chandran, Christopher A. Klebanoff, Brian M. Baker, University of Notre Dame
- S2 How does sequence affect the dynamics of a cryptic allosteric site in ebolavirus VP35? Upasana L. Mallimadugula, Matthew A. Cruz, Maxwell I. Zimmerman, Gregory R. Bowman, Washington University
- **S3 Role of lipids in modifying mGluR2/3 function through interactions with the CTD.** Chiara Mancinelli, Dagan Marx, Joshua Levitz, David Eliezer, Weill Cornell Medicine
- **S4 DomainMapper: Accurate domain structure annotation.** <u>Edgar Manriquez-Sandoval</u>, Stephen D. Fried, Johns Hopkins University
- S5 Roles of electrostricted and structural hydration in modified DNA duplex stability. Luis A. Marky, University of Nebraska Medical Center
- S6 Linkage Analysis of PahZ1 binding of poly(aspartic acid) and ssDNA. <u>Justin D.</u> <u>Marsee</u> and Justin M. Miller, Middle Tennessee State University
- **S7 Molecular determinants of mGluR-β-arrestin interactions.** <u>Dagan Marx</u>, Alexa Strauss, David Eliezer, Josh Levitz, Weill Cornell Medicine
- **S8** Maximizing signal enhancement and binding affinity in supercharged phasechanging sensor proteins. <u>Jim J. McCann</u>, Eduard Augustine, Gehan Ranepura, Marilyn R. Gunner, Ronald L. Koder, The City College of New York
- **S9 "Helicase" activity promoted through dynamic interactions between a ssDNA translocase and a diffusing SSB protein.** <u>Kacey Mersch</u>, Joshua E. Sokoloski, Binh Nguyen, Roberto Galletto, Timothy M. Lohman, Washington University in Saint Louis
- S10 Biophysical differences between immunoglobulin light chain (AL) full length proteins expressed in human and bacteria cells. <u>Pinaki Misra</u>, Alexander Tischer, Christopher J. Dick, Valeria Pierluissi-Ruiz, Benoit Bragantini, Matthew Auton, Marina Ramirez-Alvarado, Mayo Clinic
- S11 Role of secondary structure conformation on the allosteric regulation of cAMP receptor protein (CRP) from *Mycobacterium tuberculosis*. <u>Sanuja Mohanaraj</u>, Stephen Dokas, Miray Samuel, Rodrigo Maillard, Georgetown University
- S12 Uncovering the mechanism of potassium channel folding: Hydrogen- deuterium exchange mass spectrometry and tryptophan fluorescence identify pore helix and selectivity filter folding events. <u>Andrew V. Molina</u>, Kevin C. Song, Michael Baxa, Isabelle Gagnon, Benoît Roux, Tobin R. Sosnick, University of Chicago

- S13 Structure and dynamics of a duplex-embedded G-quadruplex system resolved to 7.4 Å resolution by cryo-EM and SAXS. Robert C. Monsen, Jonathan B. Chaires, John O. Trent, University of Louisville
- **S14** Identifying substrate requirements for the DDX1 protein's catalytic activity. Anthony F.T. Moore and Eda Koculi, University of Texas at El Paso
- S15 Testing "Co-Post" versus other assembly mechanisms for homomeric protein assembly in vivo. McKenze Moss and Patricia L. Clark, University of Notre Dame
- S16 Investigating autotransporter sequence features that facilitate translocation across the bacterial outer membrane. <u>Cedrick Mukinay</u> and Patricia L. Clark, University of Notre Dame
- **S17** Conformational dynamics of initiator caspases. <u>Mithun Nag</u> and A. Clay Clark, University of Texas at Arlington
- **S18** Gain of SF1 helicase function by hetero-dimerization. <u>Binh Nguyen</u>, John Hsieh, Elizabeth Weiland, Timothy M Lohman, Washington University School of Medicine
- **S19** Symmetry-breaking mechanisms of the SARS-CoV-2 main protease. <u>Hong-Ha</u> <u>Nguyen</u>, James Tufts, David D. L. Minh, Illinois Institute of Technology
- **S20** Evaluating folding dynamics and ligand binding of a Cbl-riboswitch through single molecule optical tweezers. <u>Therese Oertel</u>, Amy Chau, Rodrigo Maillard, Esther Braselmann, Georgetown University
- S21 Zymomonas mobilis Pyruvate Kinase: Rise of the unstable zombies. <u>Pierce T.</u> <u>O'Neil,</u> Katheryn Vela, Braelyn M. Page, Jeffrey S. McFarlane, Collette L. Wright, Kathleen M. Meneely, Aron Fenton, Audrey L. Lamb, Liskin Swint-Kruse, University of Kansas Medical Center
- **S22** Non-Equilibrium statistical physics beyond the ideal heat bath approximation. Jonathan Asher Pachter and Ken A. Dill, Stony Brook University
- S23 Z. mobilis pyruvate kinase, the pyruvate kinase isozyme that lacks conservation of positional contributions to function. <u>Braelyn Page</u>, Qingling Tang, Tyler Martin, Liskin Swint-Kruse, Aron W. Fenton, University of Kansas Medical Center
- S24 Characterization of CENP-A tail and DNA interactions in centromeric nucleosome organization. <u>Emeleeta Paintsil</u> and Emma Morrison, Medical College of Wisconsin
- S25 Biophysical characterization of VHH domains as protein stabilization modules. <u>Niyati Patel</u>, Nourhan Mustafa, Kyle T. Mondron, James L. Gorman, James R. Horn, Northern Illinois University
- **S26** Characterization of the early stages of spliceosomal assembly through interaction between U1-70K and SRSF1. <u>Trent Paul</u>, Jamal Shariq, Ethan Ekpenyong, Talia Fargason, Zihan Zhang, Jun Zhang, University Alabama at Birmingham

- **S27** Early events of immunoglobulin light chain aggregation: Role of the C-terminus disulfide bond. <u>Valeria Pierluissi-Ruiz</u>, Pinaki Misra, Alexander Tischer, Christopher J. Dick, Marina Ramirez-Alvarado, Mayo Clinic
- S28 Calorimetric and stability study of tryptophan and PrnA from Burkholderia ambifaria. <u>KD Power</u>, M Akter, JP Emerson, Mississippi State University
- **S29** Identifying the mechanism of protein translocation by DotB. <u>Ciairra J. Riley</u>, Wing-Cheung Lai, Clarissa Durie, University of Missouri-Columbia
- **S30** Free-Energy shifts and epistasis from mutations to an allosteric transcription factor. David Ross, Drew Tack, Peter Tonner, Olga Vasilyeva, National Institute of Standards and Technology
- **S31 FLIM-Riboglow, a novel fluorescence lifetime-based platform for tracking RNAs in live mammalian cells.** Nadia Sarfraz and Esther Braselmann, Georgetown University
- S32 Using HDX-MS to probe the dynamics and denatured state of GlpG, a helical membrane protein. <u>Abigail L. Schroeter</u>, Saba Kanwal, Heedeok Hong, Tobin R. Sosnick, University of Chicago
- **S33** In situ tracking of serum albumin binding to gold nanoparticles in the presence of serum and serum proteins. <u>Tanveer Shaikh</u> and Nicholas Fitzkee, Mississippi State University
- **S34 Proteome-wide stochastic orthogonal recoding of translation with an MScleavable photo-xlinker to probe quinary interactions** *in vivo.* <u>Piyoosh Sharma,</u> Anneliese M. Faustino, Divya Yadav, Stephen D. Fried, Johns Hopkins University
- **S35** Intermediate states of β-barrel membrane protein insertion. <u>Zhongtian Shen</u> and Karen Fleming, Johns Hopkins University
- **S36** Conformational dynamics determine recognition of bacterial enzyme-I by a substrate homologue. <u>Aayushi Singh</u>, Daniel Burns, Sergey L. Sedinkin, Brett VanVeller, Davit Potoyan, Vincenzo Venditti, Iowa State University
- **S37** Recapitulating the vectorial appearance of polypeptide chains enhances folding to the native structure *in vitro*. <u>Iker F. Soto-Santarriaga</u> and Patricia L. Clark, University of Notre Dame
- S38 Multi-Valent binding and inherent properties of intrinsically disordered transcription factors influence the functional outcomes of single substitutions. <u>Shwetha Sreenivasan</u>, Paul Heffren, Nilusha Kariyawasam, Mykola V. Rodnin, Edina Kosa, Aron W. Fenton, Alexey S. Ladokhin, Paul Smith, Joseph Fontes, Liskin Swint-Kruse, University of Kansas Medical Center
- S39 Conservation and co-evolution in protein design: residue couplings are destabilizing but specify protein function. Matt Sternke, <u>Katherine W. Tripp</u>, Doug Barrick, Johns Hopkins University

- **S40 Configurational entropy dictates activity of estrogen receptor ligands.** <u>Sivanujan</u> <u>Suthaharan</u>, Bing Xie, David Minh, Illinois Institute of Technology
- S41 Hox transcription factors adopt multiple conformations, allowing intrinsically disordered regions to regulate DNA binding. <u>Sydney Tippelt</u>, Kelly Churion, Madelyn Terrell, Sarah Bondos, Texas A&M University
- S42 Thermodynamic properties of the von Willebrand Factor A2 domain assessed by a ternary urea-temperature-calcium phase diagram. <u>Alexander Tischer</u> and Matthew Auton, Mayo Clinic
- **S43** *Staphylococcus aureus* **SrrB** Is a heme-binding sensor histidine kinase. Nitija Tiwari, Lici A. Schurig-Briccio, <u>Nicholas A. Hammons</u>, Young Joo Sun, Lokesh Gakhar, Patrick M. Schlievert, Robert B. Gennis and Ernesto J. Fuentes, University of Iowa
- **S44** Impacts of phosphorylation on the properties of intrinsically disordered proteins. <u>Emery T. Usher</u> and Scott A. Showalter, The Pennsylvania State University
- S45 Effects of domain deletions and mutations on phase separation of UBQLN2. Bridget M. Varner, Thuy P. Dao, Carlos A. Castañeda, Syracuse University
- **S46 Probing the interfacial hydration of PU.1/DNA complexes.** <u>Tyler N. Vernon</u>, J. Ross Terrell, Amanda V. Albrecht, W. David Wilson, Gregory M. K. Poon, Georgia State University
- **S47** How disulfide bonds shape energy landscapes and impact the detection of highenergy intermediates in class A β-lactamases. Miranda Villanueva, Lauren Vostal, Drew Cohen, Sasha Driver, Elise Kuwaye, <u>Kathryn Hart</u>, Williams College
- **S48 pH responsive proteins in cellular stress.** Allison Whited, Jeffre Allen, Emma L. Seidler, Génesis M. Ferrer Imbert, Loren E. Hough, University of Colorado
- S49 ParSe Version 2: A second-generation predictor of protein phase separation based upon intrinsic sequence-based properties. <u>Colorado Wilson</u>, Ayyam Y. Ibrahim, John J. Correia, Nicholas C. Fitzkee, Karen A. Lewis, Loren E. Hough, Steven T. Whitten, Texas State University
- **S50 Coarse-grained simulations of RNAs Allowing for conformational transitions of the sugar pucker.** <u>Yiheng Wu</u>, Riccardo Alessandri, Aria Coraor, Xiangda Peng, Tobin Sosnick, Juan de Pablo, University of Chicago
- **S51** Systematic identification of co-translational folding of *E.coli* proteome. <u>Divya</u> <u>Yadav</u> and Stephen D. Fried, Johns Hopkins University
- **S52** Structural analysis of antagonistic interactions in hormone resistant breast cancer advances antiestrogen development. <u>Kristen Young</u>, Govinda Hancock, Sean W. Fanning, Loyola University of Chicago
- **S53** The entropic force exerted by disordered proteins is determined by their structural biases. <u>Feng Yu</u> and Shahar Sukenik, University of California at Merced

- **S54** The structural basis for DNA-uptake by *Acinetobacter*. <u>Yafan Yu</u> and Kurt Piepenbrink, University of Nebraska-Lincoln
- **S55** Electronegative clusters modulate folding status and rna binding of unstructured RNA-binding proteins. <u>Steve Zaharias</u>, Talia Fargason, Rory Greer, Yuhua Song, Jun Zhang, The University of Alabama at Birmingham
- **S56** Thermodynamics of α-helix formation: From model peptides to intrinsically disordered proteins. Uroš Zavrtanik, San Hadži, Jurij Lah, University of Ljubljana
- **S57** Mechanistic insights into the type IV secretion system of *Legionella pneumophila*. <u>Mishghan Zehra</u>, Wing-Cheung Lai, Clarissa Durie, University of Missouri
- **S58 Probing the molecular interactions that stabilize FUS-RNA granules.** <u>Tongyin</u> Zheng and Nicolas L. Fawzi, Brown University

Poster Session II + Monday, October 3, 2022

Posters numbered alphabetically by first author's last name (A to L) (Posters M1- M57)

- M1 Understanding SARS CoV-2 genome packaging with simulations and singlemolecule fluorescence spectroscopy. Jhullian Alston, Jasmine Cubuk, J. Jeremías Incicco, Melissa Stuchel-Brereton, Kathleen Hall, Alex S. Holehouse, Andrea Soranno, Washington University in St. Louis School of Medicine
- M2 Using protein engineering to improve thermal response in anti-biofilm gold nanoparticles. <u>Dhanush L. Amarasekara</u>, Chathuri S. Kariyawasam, Madison A. Hejny, Nicholas C. Fitzkee, Mississippi State University
- M3 Kinetic mechanism of protein unfolding and translocation catalyzed by *E. coli* clpb. <u>Jaskamaljot Kaur Banwait</u> and Aaron L. Lucius, University of Alabama at Birmingham
- M4 Which thermodynamic properties induce collapse in idps? <u>Michael Baxa</u>, Xiaoxuan Lin, Cedrick Mukinay, Srinivas Chakravarthy, Joseph Sachleben, Joshua Riback, Isabelle Gagnon, Patricia Clark Tobin Sosnick, The University of Chicago
- M5 Determine the contribution of charged amino acid sidechains to protein-protein interfacial stability. <u>Soumya P. Behera</u>, Mark Petersen, Ananya Majumdar, Doug Barrick, T.C. Jenkins, Johns Hopkins University
- M6 Conformational Entropy in Protein Structure, Stability and Function. Anthony C. Bishop, Hayley Boswell, José A. Caro, Taylor Cole, Karen G. Fleming, Brian Fuglestad, Jeffrey Granja, Kushol Gupta, Kyle W. Harpole, Vignesh Kasinath, Mauricio Lasagna, Henry J. Lessen, Jackwee Lim, Danny W. Lin, Bryan S. Marques, Evan S. O'Brien, Kim A. Sharp, Matthew A. Stetz, Weimin Tan, Kathleen G. Valentine, Xiang Ye, <u>A. Joshua Wand</u>, Texas A&M University and University of Pennsylvania
- M7 Transglutaminase 2 conformations are differentially regulated by sulfate and phosphate. <u>Whitney G. Bond</u> and Tonya N. Zeczycki, Brody School of Medicine at East Carolina University
- M8 Applications of ligand-binding theory for understanding cooperativity. <u>Jannette</u> <u>Carey</u>, Princeton University
- M9 Identification of thermodynamic parameters for protein unfolding processes using linearly polarized resonance synchronous spectroscopy: a comparison of results to established methods. <u>Kyle R. Carter</u>, Sean L. Stokes, Dongmao Zhang, Joseph P. Emerson, Mississippi State University
- M10 Van't hoff analysis of clc-ec1 dimerization in *Escherichia coli* lipid membranes. Rahul Chadda, Taeho Lee, Priyanka Sandal, Robyn Mahoney-Kruszka, Janice L. Robertson, Washington University in St. Louis

- M11 Rnp formation and retrotransposition mechanism of restriction like endonuclease long interspersed elements (RLE LINEs). Joydeep Chatterjee and Shawn M. Christensen, University of Texas at Arlington
- M12 Conformational stability of G4 DNA has differential effect on ssDNA-RNA G4 hybrid and R-loop formation. <u>Tanvir Ahmed Chowdhury</u> and Hui-Ting Lee, University of Alabama at Birmingham
- M13 Evaluating T-Cell allospecificity in acute cellular recognition. <u>P. Chukwunalu</u> <u>Chukwuma</u>, George Gray, Sara Foote, Tiffany Shi, Ashley Burg, David Hildeman, Brian M. Baker, University of Notre Dame
- M14 PahZ1 binding of ssDNA. <u>Joshua R. Couch</u> and Justin M. Miller, Middle Tennessee State University
- M15 Single-molecule fluorescence spectroscopy of the SARS-COV-2 nucleocapsid protein. Jasmine Cubuk, Juan J. Incicco, Jhullian J. Alston, Melissa D. Stuchell-Brereton, Kathleen B. Hall, Alex S. Holehouse, Andrea Soranno, Washington University in St. Louis
- M16 Neoantigen effects on peptide-MHC complexes: structure, modeling and enhanced accuracy for H2-Dd and H2-Kd prediction. Jean Custodio, Cory Ayres, Brian Baker, University of Notre Dame
- M17 Thermodynamically characterized conformational changes of zinc dependent AdcR by structurally inspired inhibitors. <u>Alexander J. Cutright</u>, Erin L. Matthews, James M. Aulds, Justin A. Thornton, Sean L. Stokes, Joseph P. Emerson, Mississippi State University
- **M18** Solution dynamics of human guanylate kinase. <u>Mark Vincent C. dela Cerna</u> and T. Michael Sabo, University of Louisville
- M19 Protein-ligand binding free energy estimation by learned mappings. <u>Joseph</u> <u>DePaolo-Boisvert</u>, Soohaeng Yoo Willow, David D. L. Minh, Illinois Institute of Technology
- M20 Inter-domain flexibility of human SRSF1 allows flexibility in RNA binding. <u>N. Ivon</u> <u>De Silva</u>, Talia Fargason, Zihan Zhang, Jun Zhang, University of Alabama at Birmingham
- M21 Characterizing the ancestor of apoptotic caspases. <u>David Diaz</u>, Melissa Fee, A. Clay Clark, University of Texas at Arlington
- M22 Thermodynamic analysis of GASright dimerization supports a model in which stability is modulated by weak hydrogen bonding and van der Waals packing. <u>Gladys Díaz Vázquez</u>, Qiang Cui, Alessandro Senes, University of Wisconsin-Madison
- M23 Quantifying what we can't see: Protein degradation in the cell. <u>Jacob Diehl</u> and Patricia Clark, University of Notre Dame

- M24 Allosteric control in cAMP receptor protein from *Mycobacterium tuberculosis*. <u>Stephen Dokas</u>, Sanuja Mohanaraj, D. Kyle Taylor, Lydia Good, Wilfredo Evangelista Falcón, Mark White, Rodrigo Maillard, Georgetown University
- M25 Single molecule study of the DEAH-box Helicase Prp22. Elizabeth C. Duran, Sujay Ray, Nils G. Walter, University of Michigan
- M26 A single-molecule method for measuring fluorophore labeling yields for the study of membrane protein oligomerization. <u>Melanie Ernst</u>, Tugba N. Ozturk, Janice L. Robertson, Washington University School of Medicine
- M27 Repetitive peptides increase the critical point for phase separation of the protein SRSF1 and reveal a reliance on cation-pi interactions. <u>Talia Fargason</u>, Erin King, Ivon Upekala De Silva, Trenton Paul, Zihan Zhang, Jamal Shariq, Steve Zaharias, Jun Zhang, University of Alabama at Birmingham
- M28 Transcription activation domain structure correlates with gene expression levels. Eduardo Flores, Max V. Staller, Shahar Sukenik, University of California-Merced
- M29 Determining the mechanistic role of the A12.2 subunit in the kinetics of multinucleotide addition catalyzed by RNA Polymerase I. <u>Kaila Fuller</u>, Ruth Jacobs, David Schneider, Aaron Lucius, University of Alabama at Birmingham
- M30 A comprehensive analysis tool for thermal shift assay data and a database for intrinsic thermodynamic parameters of protein-ligand interaction. <u>M. Gedgaudas</u>, D. Lingė, A. Merkys, A. Vaitkus, A. Grybauskas, A. Zubrienė, V. Paketurytė-Latvė, E. Urniežius, A. Zakšauskas1, A. Mickevičiūtė, J. Smirnovienė, L. Baranauskienė, E. Čapkauskaitė, V. Dudutienė, D. Baronas, E. Kazlauskas, W.Y. Chen, J.E. Ladbury, S. Gražulis, D. Matulis, and V. Petrauskas, Vilnius University
- M31 Proton-driven alternating access and broad-specificity in spns lipid transporters. <u>Samantha Gies</u>, Reza Dastvan, Ali Rasouli, Sepehr Dehghani-Ghahnaviyeh, Emad Tajkhorshid, University of Illinois at Urbana-Champaign
- M32 Binding to highly curved membranes induces distinct structural change in the Cterminal domain of mouse Complexin-1. <u>Emily M. Grasso</u>, Mayu S. Terakawa, Alex L. Lai, Ying Xue Xie, Trudy F. Ramlall, Jack H. Freed, David Eliezer, Weill Cornell Medicine
- M33 Characterizing and quantifying TCR cross-reactivity. <u>George Gray</u>, Sara Foote, Brian Baker, University of Notre Dame
- M34 Engineering a pH-dependent anti-caffeine VHH antibody via aspartic acid ionization triggers within a homodimer interface. <u>Peter Gungel</u>, Tosha Laughlin, Hyeyoung Eom, Aaron Manz, Kevin Beck, Kylie Zawisza, Moly Eilbes, James R. Horn, Northern Illinois University
- M35 Effects of salt conditions on the reaction between the porphyrin TMPyP4 and the G-quadruplex. <u>Alan Gunter</u> and Hui-Ting Lee, University of Alabama at Birmingham

- M36 Unconventional estrogen receptor antagonists reveal cryptic therapeutic antibreast cancer transcriptional pathways. <u>Govinda Hancock</u>, Kristen Young, Sean W Fanning, Loyola University of Chicago
- M37 Dysfunctional target recognition by pathogenic mutants of the essential calcium sensor calmodulin. <u>Emily R. Herum</u>, Cade Rahlf, Madeline A. Shea, University of Iowa
- M38 Insight into EmrE's proton coupled transport through NMR-based structure studies. <u>Ashley B. Hiett</u>, Nathan E. Thomas, Katherine A. Henzler-Wildman, University of Wisconsin-Madison
- M39 Thermodynamic stability as a molecular determinant of the pK_a values of buried ionizable residues in proteins. <u>Miranda Hurst</u>, Ananya Majumdar, Bertrand García-Moreno, Johns Hopkins University
- M40 Membrane phospholipids induce positive cooperativity in closed pacemaker channels. Vinay K. Idikuda, <u>Susovan Roy Chowdhury</u>, Randall H. Goldsmith, Baron Chanda, Washington University in St. Louis
- M41 Unfoldase and translocase activity of ClpA on folded protein substrates. Liana Islam and Aaron L. Lucius, University of Alabama at Birmingham
- M42 Binding analysis of ubiquitin ligase SPOP with intrinsically disordered proteins. Nolan P. Jacob, Emery T. Usher, Scott A. Showalter, The Pennsylvania State University
- M43 Arginine residues determine the mobility of the H3 tail in the nucleosome core particle. <u>Christine Jennings</u>, Casey Zoss, Erin Hammonds, Sarah Meidl Zahorodny, Emma Morrison, The Medical College of Wisconsin
- M44 Protein charge distribution alters thermodynamics in the nanoparticle protein corona. <u>Chathuri S. Kariyawasam</u>, Radha P. Somarathne, Railey S. Mayatt, Rebecca A. Conner, Nicholas C. Fitzkee, Mississippi State University
- M45 Wandering around in circles: A mechanism to pinch of ssDNA from ScRad52 during homologous recombination, Simrithaa Karunakaran, Jaigeeth Deveryshetty, Rahul Chadda, Edwin Antony, Saint Louis University School of Medicine
- M46 Watching RPA flirt with ssDNA: Non canonical amino acid based fluorescent RPA to track dynamics on ssDNA. <u>Vikas Kaushik</u> and Edwin Antony, Saint Louis U
- M47 Elucidating the structure of the HU-Junction complex. <u>Qura-Tul-Ain Khan</u>, Rich Olson, Ishita Mukerji, Wesleyan University
- M48 Biophysical mechanisms driving graded hormone response in steroid receptors. Sabab Hasan Khan, Sean M Braet, Stephen John Koehler, Elizabeth Elacqua, Ganesh S Anand, C. Denise Okafor, Pennsylvania State University

- M49 CsgA's native conformational ensemble shows α-helical characteristics. Jude <u>Kinkead</u>, Whitney G. Bond, Tonya N. Zeczycki, Brody School of Medicine at East Carolina University
- M50 Thermodynamic and kinetic properties of amyloidogenic protein Wil and new insight in the role of the C-terminus disulfide bond. <u>Nikita Kormshchikov</u>, Alexander Tischer, Matthew Auton, Marina Ramirez- Alvarado, Mayo Clinic
- **M51** If you think you know RPA-ssDNA filaments, think again! <u>Sahiti Kuppa</u> and Edwin Antony, Saint Louis University School of Medicine
- M52 Including control data in fits to concentration-response curves improves estimates of half-maximal concentrations. <u>Van N. T. La</u>, Stanley Nicholson, Amna Haneef, Lulu Kang, David D. L. Minh, Illinois Institute of Technology
- M53 Beyond the end replication problem: Using smFRET to investigate the formation and dynamics between G-Quadruplexes and T-loops in human telomeres. <u>Arianna</u> <u>Lacen</u> and Hui-Ting Lee, University of Alabama at Birmingham
- M54 Engineering sensitive pH switches using combinatorial histidine scanning libraries and a fab antibody fragment model system. <u>Tosha Laughlin</u> and James R. Horn, Northern Illinois University
- M55 Comprehensive conformational and colloidal stability of biopolymers. <u>Camille</u> <u>Lawrence</u>, Andreas Langer, Jonathan Derix, Nanotemper Technologies
- M56 Quantitative visualization of proteins and RNA in live mammalian cells using fluorescence lifetime imaging microscopy (FLIM) through cell mixing. <u>Harrison Lee</u>, Nadia Sarfraz, Esther Braselmann, Georgetown University
- M57 Development of *in vivo* HDX-MS with applications to a TonB-dependent transporter and other proteins. <u>Xiaoxuan Lin</u>, Adam M. Zmyslowski, Isabelle A. Gagnon, Robert K. Nakamoto, Tobin R. Sosnick, The University of Chicago

