

**The 9th Telluride Workshop on Coarse-Grained Modeling of Structure and Dynamics of  
Biomacromolecules  
(HYBRID)**

**TIMES LISTED ARE MOUNTAIN TIME  
JULY 28 – AUGUST 1, 2025**

**Location: Our workshop will be held in the Lower Room of the Telluride Innovation Center at  
300 S Townsend St., Telluride, CO 81435.**

Breakfast will be served every morning at the Center. It will be ready by 7:30am. Snacks, coffee, tea, and other beverages are available at the Center throughout the day. We'll use your schedule to make sure there is plenty of coffee during your coffee breaks

**DAY 0**

**Sunday, July 27, 2025**

**5:00pm to 6:30pm                      All-Telluride Science Meet and Greet**

We will host a cash-bar Meet & Greet at our new building, the Telluride Innovation Center, at 300 S Townsend St., Telluride, CO 81435 on Sunday, July 27th from 5:00pm to 6:30pm. A staff member will be on hand to welcome you, distribute badges, and answer any questions. We'll have non-alcoholic beverages and snacks, but this is meant to be a place to meet up with fellow participants before your meeting and possibly head off in small groups for dinner. We will close the building at 6:30pm.

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**DAY 1**

**Monday, July 28, 2025**

**Session 1**

**Chair: Toshiya Senda**

9:00a.m. – 9:10a.m.	<b>Mark Kozak – Telluride Science Research Center</b> Introduction
9:10a.m. – 9:40a.m.	<b>Robert Jernigan – Iowa State University</b> (In-Person) The Explosive AI Protein Renaissance from Large Protein Language Models
9:40a.m. – 10:10a.m.	<b>Jin Wang – Stony Brook University</b> (Virtual) Quantifying specificity for rigid and flexible biomolecular recognition
10:10a.m. – 10:40a.m.	<b>Jeffrey Skolnick – Georgia Institute of Technology</b> (Virtual) Entabolons: How metabolites modify the biochemical function of proteins and cause the correlated behavior of proteins in pathways
10:40a.m. – 11:00a.m.	<b>BREAK</b>
<b>Session 2</b>	
<b>Chair: Robert Jernigan</b>	
11:00a.m. – 11:30a.m.	<b>Toshiya Senda – KEK High Energy Accelerator Research Org</b> (In-Person) A Novel 1C Metabolism Pathway in <i>Sphingobium lignivorans</i> SYK-6
11:30a.m. – 12:00p.m.	<b>Daisuke Kihara - Purdue University</b> (Virtual) Biomolecular Structure modeling beyond Alphafold
12:00p.m. – 12:30p.m.	<b>Miki Senda – KEK High Energy Accelerator Research Org</b> (In-Person) Making X-ray crystallographic refinement accessible for non-structural biologists

Group hike is on Monday (Bear Creek Fall) – this is an excellent opportunity to unwind and get to know each other in a more relaxed setting. Bring comfortable shoes and plenty of water. The altitude at Telluride is ~ 8750 ft so make sure to stay hydrated.

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**DAY 2**

**Tuesday, July 29, 2025**

**Session 3**

**Chair: Wladek Minor**

9:00a.m. – 9:30a.m.	<b>Gaetano T Montelione – Rensselaer Polytechnic Institute (In-Person)</b> Hidden conformational states of proteins revealed by AlphaFold-NMR
9:30a.m. – 10:00a.m.	<b>Shalom Rackovsky – Cornell U. / University of Rochester (In-Person)</b> Extreme Coarse-Graining: Bioinformatics for Protein Dynamics
10:00a.m. – 10:30a.m.	<b>Shi-Jie Chen - University of Missouri-Columbia (Virtual)</b> RNA-Based Therapeutics: From Structure Prediction to Drug Design
10:30a.m. – 10:50a.m.	<b>BREAK</b>

**Session 4**

**Chair: Shalom Rackovsky**

10:50a.m. – 11:20a.m.	<b>Andrzej Joachimiak – The University of Chicago / Argonne (Virtual)</b> Experimental fragment screening and serial crystallography
11:20a.m. – 11:50a.m.	<b>Wladek Minor - University of Virginia (In-Person)</b> AI in Biomedical Sciences - The Good, The Bad and The Ugly
11:50a.m. – 12:20p.m.	<b>Pradeep B K - Iowa State University (Virtual)</b> Identifying New Protein Paralogs by a New Integrated Homolog Detection Method and Functional Clustering
6:30pm – 7:30pm	<b>Telluride Science Town Talk</b> Location: Telluride Conference Center in Mountain Village Cash Bar, Doors Open at 6:00pm Speaker <b>Milan Delor</b>

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**Wednesday, July 30, 2025**

**Session 5**

**Chair: Gaetano T Montelione**

9:00a.m. – 9:30a.m.	<b>Domenico Scaramozzino – Karolinska Institutet (Virtual)</b> Breaking the size limit: efficient sampling of large-scale transition pathways and intermediate conformations in large biomacromolecules
9:30a.m. – 10:00a.m.	<b>Xiaoqin Zou - University of Missouri-Columbia (Virtual)</b> In silico screening of protein-binding peptides
10:00a.m. – 10:30a.m.	<b>Ruxandra Dima - University of Cincinnati (In-Person)</b> Modeling microtubule effects on associated proteins
10:30a.m. – 10:50a.m.	<b>BREAK</b>

**Session 6**

**Chair: Ruxandra Dima**

10:50a.m. – 11:20a.m.	<b>Ilya Vakser – University of Kansas (In-Person)</b> Docking-based simulation of the cell
11:20a.m. – 11:50a.m.	<b>George Stan – University of Cincinnati (In-Person)</b> Conformational sampling of functional dynamics of the ClpB disaggregase
11:50a.m. – 12:20p.m.	<b>Discussion</b>
5:30pm - 7:30pm	<b>All Telluride Science Picnic</b>  Free BBQ, Beer, Wine, and Non-Alcoholic Beverages. Friends and Family are invited free of charge.

Location: Tent behind the Intermediate School (which is the location for all workshops - 725 W Colorado Ave)

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**DAY 4**

**Thursday, July 31, 2025**

**Session 7**

**Chair: Ilya Vakser**

- |                       |  |
|-----------------------|--|
| 9:00a.m. – 9:30a.m.   | <b>Adam Liwo – University of Gdansk (Virtual)</b><br>UNICORN package and UNRES server for coarse-grained modeling of structure and dynamics of biological macromolecules |
| 9:30a.m. – 10:00a.m.  | <b>Cristan Micheletti - School of Advanced Sciences Trieste, Italy (Virtual)</b><br>Nanopore translocation of entangled DNA and RNA filaments                            |
| 10:00a.m. – 10:30p.m. | <b>Jeffrey Law – National Renewable Energy Lab (In-Person)</b><br>TBA  |
| 10:30a.m. – 10:50a.m. | <b>BREAK</b>   |

**Session 8**

**Chair: Jeffrey Law**

- |                       |  |
|-----------------------|--|
| 10:50a.m. – 11:20a.m. | <b>Mubasher Hassan - Nationwide Children's Hospital (Virtual)</b><br>TBA   |
| 11:20a.m. – 11:50a.m. | <b>Jarek Meller - University of Cincinnati (Virtual)</b><br>Accelerating drug discovery and repurposing by combining transcriptional signature connectivity with docking |
| 11:50a.m. – 12:20p.m. | <b>Andrzej Kloczkowski – Nationwide Children's Hospital (Virtual)</b><br>TBA   |

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**ZOOM LINK:**

Topic: Coarse-Grained Modeling

<https://us06web.zoom.us/j/89607513215?pwd=IVPj7WerhMI3rDrmGF59buVta3Sjb9.1>

Time: This is a recurring meeting Meet anytime

View meeting insights with Zoom AI Companion

<https://us06web.zoom.us/join/edl?muid=74333a5b-7891-46a2-9e31-5c0e6a190ecb>

Meeting ID: 896 0751 3215

Passcode: 368678

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**ADDITIONAL INFORMATION**

**Local Telluride Science contacts**

Mark Kozak, email: [mark@telluridescience.org](mailto:mark@telluridescience.org), cell: 970-708-4426

Sara Friedberg, email: [sara@telluridescience.org](mailto:sara@telluridescience.org), cell: 970-708-0622

Cindy Fusting, email: [cindy@telluridescience.org](mailto:cindy@telluridescience.org), cell: 970-708-5069

**Code of Conduct**

- Treat your fellow participants and Telluride Science staff with consideration and professionalism, respecting diversity of views and opinions.
- Communicate openly with civility for others, critiquing ideas rather than individuals.
- Be mindful of your surroundings and fellow participants. Anyone requested to stop unacceptable behavior is expected to comply immediately. Telluride Science staff may take any action deemed necessary and appropriate, including immediate removal from the meeting without warning or refund.
- Be kind and considerate of people in the Telluride community. You represent Telluride Science when you are in town.

**Unacceptable Behavior**

Harassment, intimidation, exclusion, or discrimination. Physical or verbal abuse.

**Reporting Unacceptable Behavior**

If you are the target of unacceptable behavior or have witnessed any such behavior, please immediately notify a Telluride Science or the workshop organizer. Alert Telluride Science staff, and 911 if appropriate, if you notice a dangerous situation or someone in distress. Report concerns to [report@telluridescience.org](mailto:report@telluridescience.org). All reports will be treated confidentially and with discretion.

**Values Statement**

Telluride Science values inclusion and is committed to creating a respectful, equitable, and welcoming environment free from discrimination, exclusion, and harassment for all participants. Telluride Science is known for its collegial workshops that spawn new ideas and collaborations. We encourage the open expression and exchange of ideas, and we are dedicated to strengthening our culture of diverse and inclusive workshops, conferences, and schools.

**Most importantly: Have fun! Be inspired! Make new friends!**