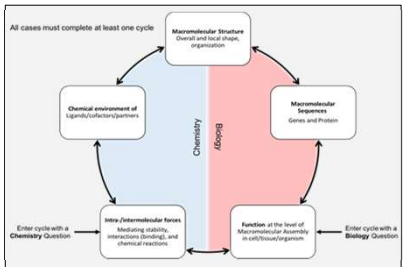
The Molecular CaseNet Pipeline for Authoring, Piloting, and Evaluating Molecular Case Studies

Alexandra Pettit (Carleton University) Elizabeth Pollock (Stockton University) Kristen Procko (University of Texas at Austin) Kasandra J. Riley (Rollins) Didem Vardar-Ulu (Boston University) Shuchismita Dutta (Rutgers)

Molecular CaseNet - a community of educators and scholars

- developing & using Molecular Case Studies (MCS),
- promoting exploration of the molecular basis of biological phenomena,
- understanding real world problems, and
- developing solutions at the interface of biology & chemistry.



What is a Molecular Case Study?

They are case studies that provide opportunities for telling molecular stories to engage students in exploring biomolecular structure and function. Each molecular case study (MCS) completes at least one MCS cycle (shown above) and includes

- **a hook** (such as a video, narrative, image, or report), to engage and present the case context
- guidance to **identify key molecular players** in the story and find relevant 3D structures to study
- guidance for **molecular visualization and analysis** of case theme related 3D structures
- opportunities to **integrate information** from the literature, bioinformatics resources, and connect with biomolecular structure and function to synthesize new knowledge or perspectives.

Where can you find MCSs?

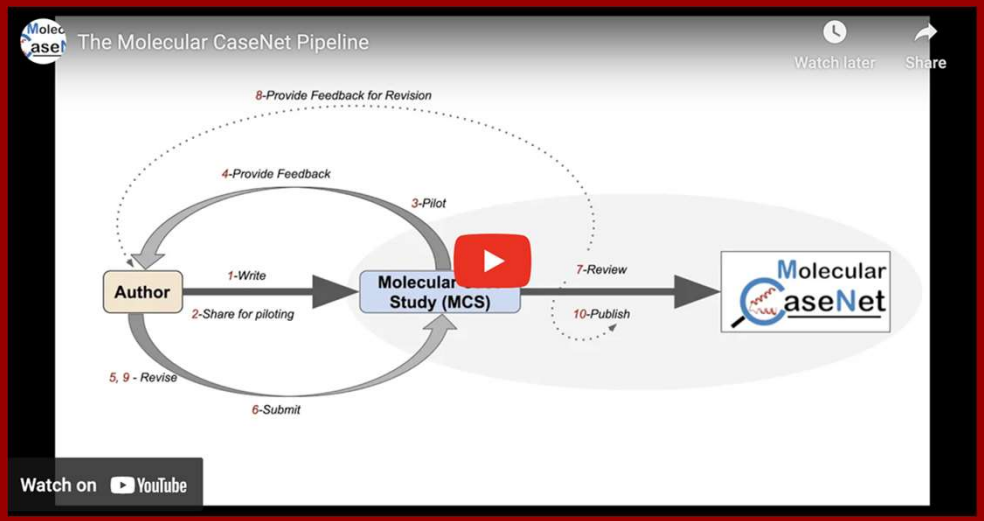
- Browse molecular case studies at Molecular CaseNet (molecular-casenet.rcsb.org).
- Educators can request for a free account and password to access answer keys and teaching notes.
- Adopt and adapt case studies to meet your curricular needs.
- Adaptations of MCSs are available for use at https://qubeshub.org/community/groups/molcasenet

Funding

- Supported by the National Science Foundation awards NSF DBI-1827011 and 2018884.
- MCSs are published as open education resources using the QUBES hub

NSF QUBES A BioQUEST Project

Molecular CaseNet Pipeline now has detailed guidelines for Authoring, Piloting, Evaluating, and Publishing Molecular Case Studies



https://youtu.be/UfsqZ1vpFDY

Have Questions? Write to Shuchi (sdutta@rcsb.rutgers.edu)

Why consider using MCSs?

They provide opportunities to practice:

- query, navigation, and integration of information from various public bioinformatics resources,
- visualization and analysis of biomolecular structures, and
- exploring biomolecular structures for in-depth understanding of intra- and inter-molecular forces in proteins, nucleic acids and their complexes facilitating their functions.

They are:

- modular, flexible, and adaptable,
- active learning opportunities,
- accompanied by answer keys and teaching notes, and
- opportunities to apply multidisciplinary concepts learned in class to authentic societal issues.

The MCN Pipeline

- Collaboratively developed by experienced members of the MCN community
- Provides detailed guidelines and instructions for free
- Includes detailed guidelines for reviewers of MCS

Molecular CaseNet invites you to

- **Explore** published Molecular Case Studies and use ones that meets your course objectives and curricular goals.
- **Adapt** published MCSs to meet your specific curricular needs and share these adaptations.
- **Author** a Molecular Case Study independently or collaboratively about a topic of your choice. A new cohort starts in September 2023.
- **Engage your students** in authoring molecular case studies as a partial Course based Undergraduate Research Experience (CURE)
- **Pilot** 'Molecular Case Studies for Field Testing' and provide feedback to the authors
- **Join** the Molecular CaseNet Review Committee to help review Molecular Case Studies

References:

- Goodsell D.S., Dutta S., Voigt M., Zardecki C. (2021) Molecular storytelling for online structural biology outreach and education. Struct Dyn. 8(2):020401. doi: 10.1063/4.0000077.
- Riley, K.J., Vardar-Ulu, D., Pollock, E., Dutta, S. (2021) Students authoring molecular case studies as a partial course-based undergraduate research experience (CURE) for lab instruction, BAMBEd 49: 853-855, doi: 10.1002/bmb.21578
- Dutta S. (2020) The Molecular Case Study Cycle. CCCE: Committee on Computers in Chemical Education Newsletter
- Dutta S., Dries D.R. (2019) Virtual Exploration of Biomolecular Structure and Function. Biochemistry Education: From Theory to Practice, Chapter 2pp 21-41, ACS Symposium Series Vol. 1337, doi: 10.1021/bk-2019-1337.ch002