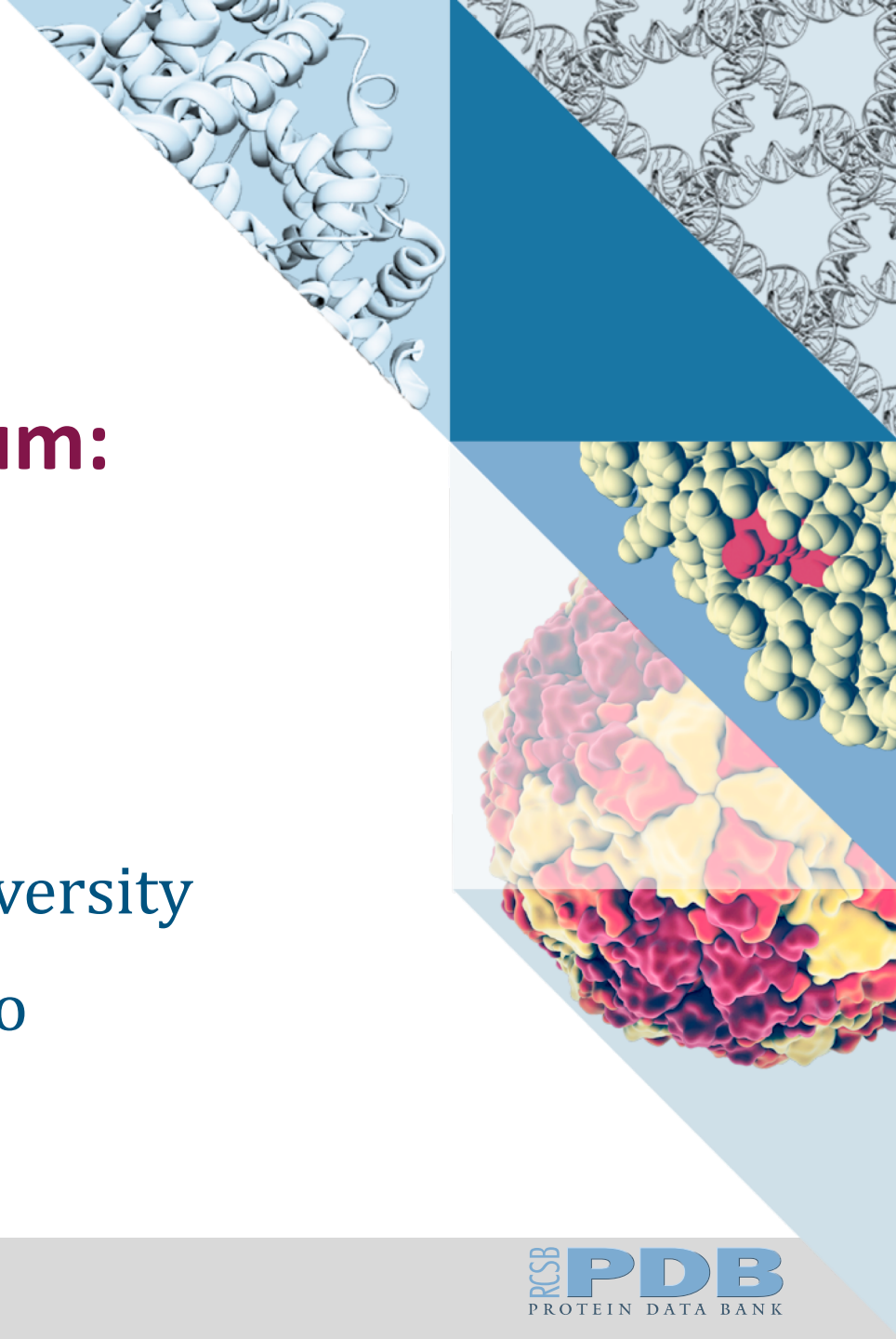

New Online Curriculum: The PDB Pipeline & Data Archiving

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NIH Big Data to Knowledge (BD2K)

BD2K Call for Proposals

- Develop open educational resources for sharing, annotating and curating "Biomedical Big Data"
- Target audience: librarians/instructors, for training biomedicine students and researchers

Enabling Data Science in Structural Biology (eDSB) Project

- Unique opportunity to document RCSB's development and management practices

Project Goals are Consistent with RCSB's Educational Mission

- Promote understanding of biomolecules and PDB
- Provide a structural view of biology and medicine

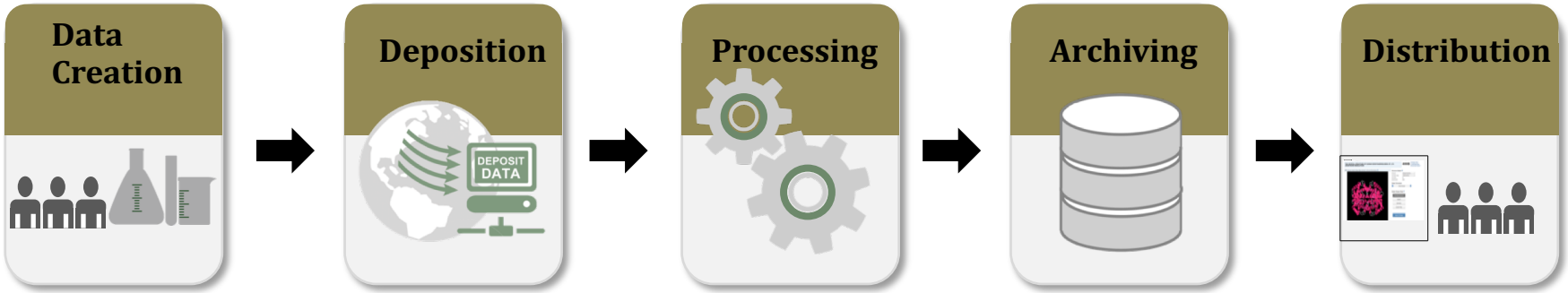
Project can Support Expanding Experimental Data Archives in Structural Biology

- Trained scientists are needed to develop federated data archives supporting new methods/model types (e.g. FRET, Mass Spectrometry …)

Hybrid Methods Task Force EMBL-EBI, Hinxton 2014

Eight Curriculum Modules Follow the Data Pipeline

1 *Enabling Data Science in Biology: Overview*



3 *Designing a Data Structure*

5 *Curating Deposited Data*

7 *Creating & Maintaining a Data Archive*

2 *Creating Archive Requirements*

4 *Assembling Data Sets*

6 *Ensuring Data Consistency*

8 *Sharing Data with End Users*

Modules

1. Overview	5. Curating the Data
2. Creating Archive Requirements	6. Ensuring Data Consistency
3. Designing the Infrastructure	7. Creating and Maintaining an Archive
4. Data Deposition	8. Data Distribution

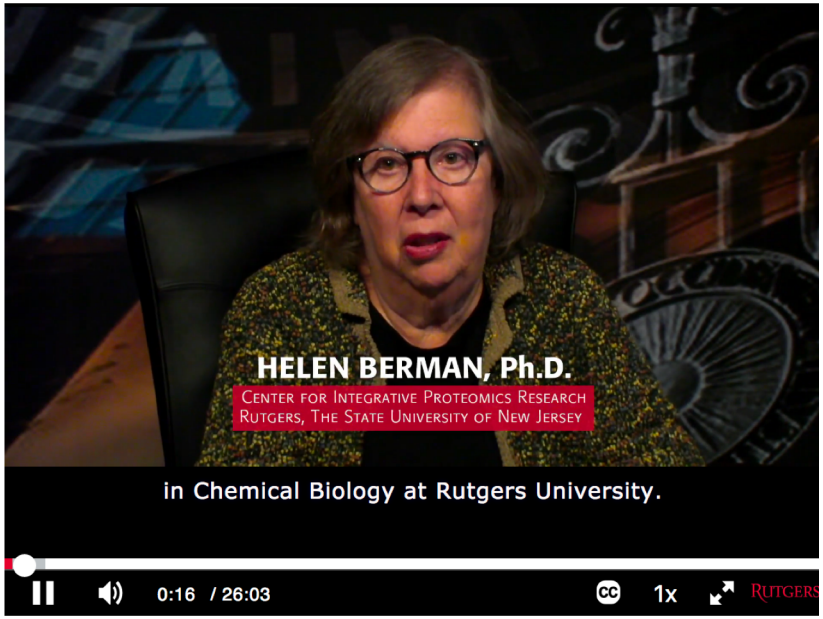
Learning Objectives/Skills

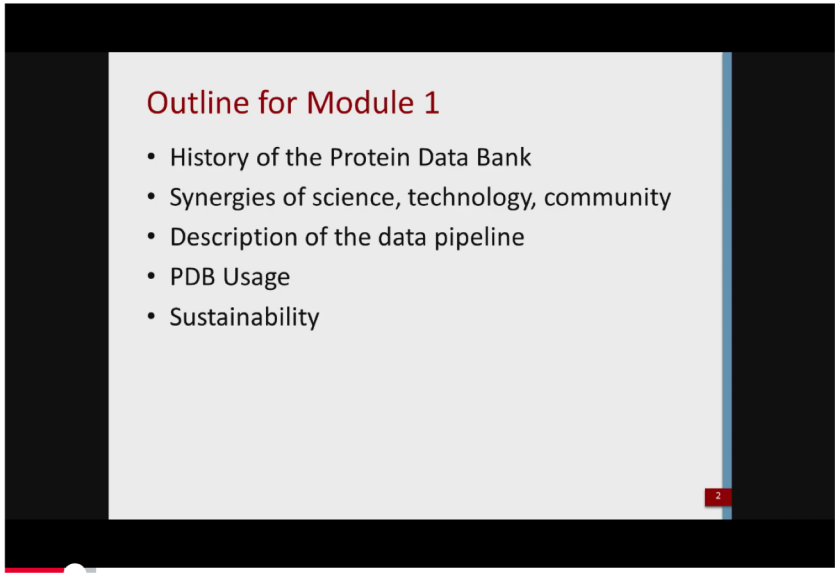
- Recognize what is involved in designing and maintaining an archive for shared data
- Identify key stakeholders
- Develop requirements for what data to include
- Understand how to develop a data dictionary with the appropriate level of granularity
- Construct a deposition and annotation workflow based on a data dictionary

Lectures

- Lectures were developed and delivered by RCSB PDB group members according to their expertise
- 3-5 video segments per Module
- Transcripts were carefully curated to support closed-captioning

Module 1: Introduction





Exercises/Homework

- Students are guided step-by-step to design, create, and query a database on a topic of their own interest
- Exercises introduce tools needed to complete assignments
- Worked example included in all assignments

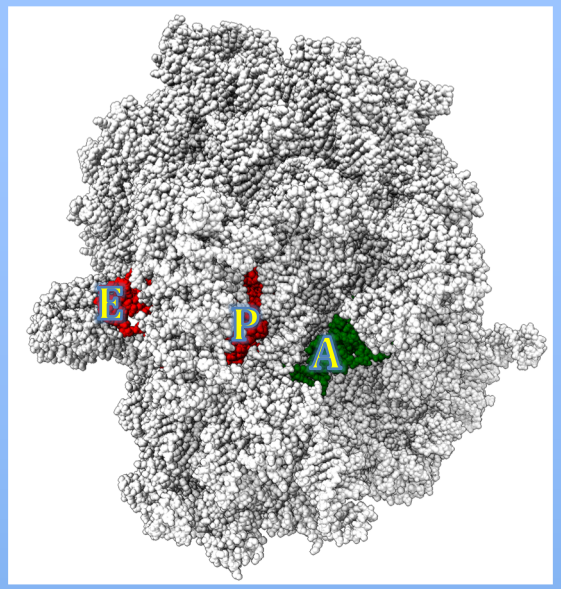
Homework Flow

Module	Goal
1	Select set of PDB entries on topic of interest (50-100)
2	Create PDB data reports, get primary citations
3	Define questions about your topic, create new data terms
4	Create a deposition form for your new terms and fill it in
5	Review validation reports for your PDB entries
6	Check filled data for errors
7	Create a database combining PDB data and your new data
8	Perform queries to answer the questions about your topic

Tools used:
RCSB PDB website search/browse/reports, simple text editor, Excel or equivalent, Google Forms, MySQL Server and MySQL Workbench

Worked Example

- Recent E. coli ribosome cryoEM structures (61)
- Example Questions:
  - How many structures have both ribosomal subunits?
  - Which structures include messenger RNA?
  - What type of tRNA is bound in the P (peptidyl) site?
  - Do ribosome structures with bound antibiotics have good model quality?



Distribution of tRNA types in the peptidyl site of recent *E. coli* ribosome structures:

COUNT(pdb_id)	p_site_trna_aa_type
1	Glycine
2	Aspartate
3	Proline
4	Unknown
17	none
34	Initiator Methionine

Initial Implementation

- The curriculum was pilot-tested at Rutgers in Spring 2016, and then again in Spring 2018
- Students included:
  - Rutgers Graduate Students (Chemistry, Mol Bio)
  - Information Specialists from Rutgers Libraries
  - International Scientists interested in developing data archives

Use in a Flipped Classroom

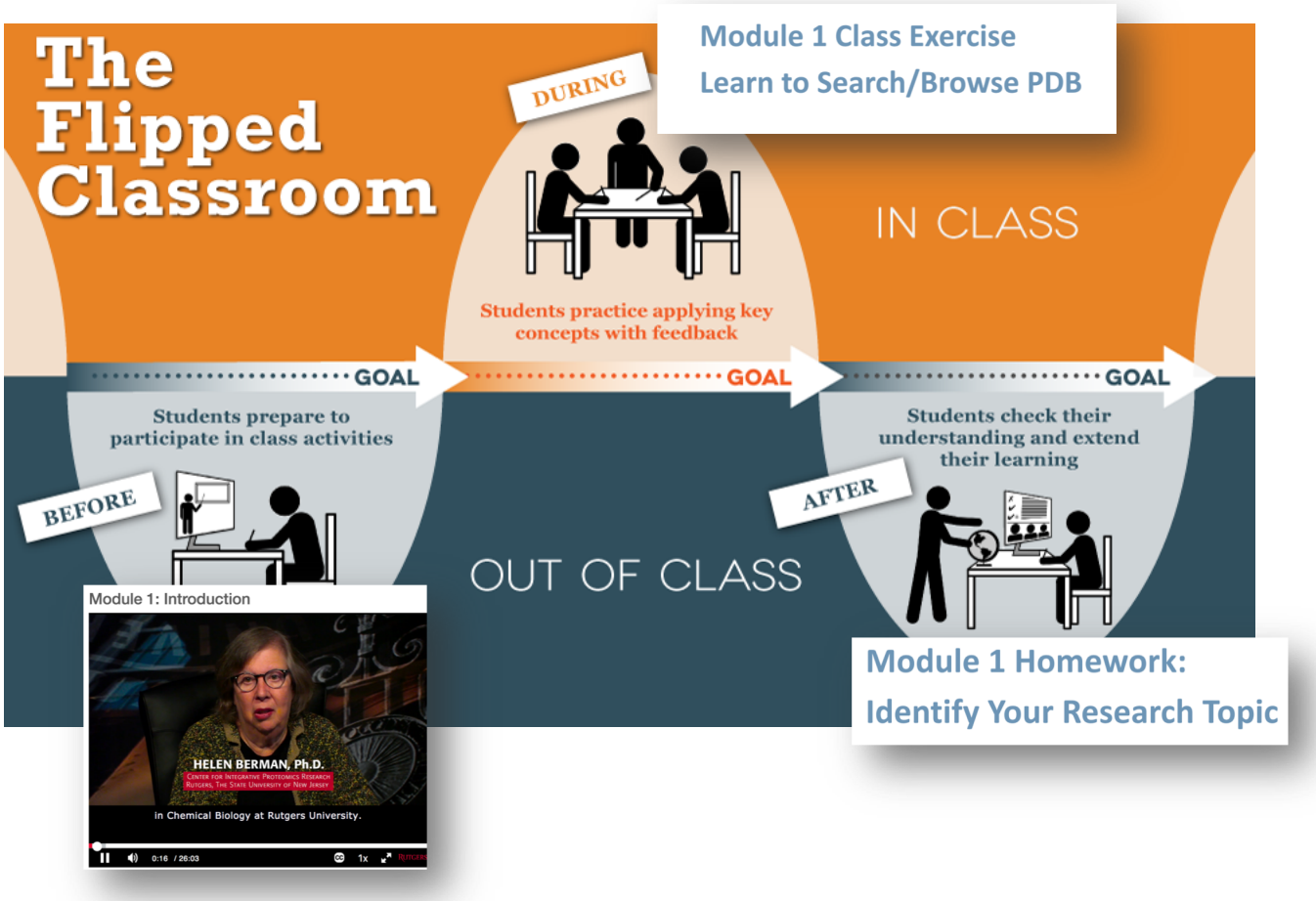


Image Source: U. Texas at Austin Faculty Innovation Center

Dissemination

- All materials will be accessible via PDB-101 and http://edsb.rcsb.org
  - Lectures: Slides, Transcripts, Videos
  - Exercise, Homework Slides
  - Links to Additional Resources
  - Licensing: Attribution-NonCommercial-ShareAlike 4.0 International

- Coursera MOOC: to be developed

Project Personnel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Jasmine Young


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Brian P. Hudson


Ezra Peisach


Peter Rose


Jose Duarte


Stephen K. Burley


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CCDC

Interested in using this curriculum? Let us know: edsb@rcsb.org

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