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DivCHED CCCE: Committee on Computers in Chemical Education

## **Proteopedia: A Powerful Tool for Biomolecular Communication and a 3D Web Encyclopedia of Biomolecules**

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### **Abstract:**

*Proteopedia* is an interactive resource that facilitates understanding the role of 3D protein structures have in their biological function <http://proteopedia.org>. *Proteopedia* is widely used in scientific research, in the preparation of papers for publication and teaching from secondary level to post-graduate.

Two main facts explain the popularity of Proteopedia in the teaching community: pages specifically designed for and by educators ([Teaching Scenes, Tutorials, and Educators' Pages](#)) and the exclusive Proteopedia's Scene Authoring Tool that enables the creation of rich Jmol 3D scenes with zero learning effort.

### **Teaching Strategies Using Proteopedia:**

#### *Use Existing Pages*

Of course, you can use existing pages in Proteopedia. Be sure to consider those specifically designed for and by educators, which are listed at [Teaching Scenes, Tutorials, and Educators' Pages](#). Proteopedia pages can be projected during lectures (if you Export them in advance or have an Internet connection in the classroom), and/or assigned to students as homework.

#### *Author Your Own Pages*

If you create your own pages, you will have scenes of the molecules that you are emphasizing in your teaching -- scenes that show exactly the structural features you wish to emphasize. See the [Main Page](#) (Fig. 1) for links to videos that show you how to author pages in Proteopedia. Customizing molecular scenes is amazingly easy with Proteopedia's *Scene Authoring Tool*.

Again, see some examples at [Teaching Scenes, Tutorials, and Educators' Pages](#).

The screenshot shows the Proteopedia main page for HIV-1 protease. The page layout includes a navigation menu on the left, a search box, and a main content area. The main content area features a 3D molecular model of the HIV-1 protease structure, with green hyperlinks overlaid on it. The text describes the structure and function of the enzyme, mentioning its two symmetrically related subunits and the active site. The page also includes a scoreboard table on the right side.

Score	Pages	Changes	Username
31	8	140	Brooke Fenn
24	7	79	Joseph Tiltsky
20	7	52	Ololade Fatunmbi
20	7	47	Abbey Evans
19	4	59	Vesta Nwankwo
18	9	31	Liliya Karasik
18	7	39	Robin Morgan
18	4	52	Natalie Bieł
18	4	50	Alejandro Porto
16	6	31	Karsten Theis

**Fig. 1.** Main Page of Proteopedia showing the **green** hyperlinks that when clicked result in a change in the 3D Jmol figure to reflect what is described in the text.

### Worksheets

A low tech, but quick-to-prepare lesson plan involves distributing worksheets of questions regarding the molecular scenes on a particular Proteopedia page. These worksheets can be on paper, a web page (which could be on a page in Proteopedia), or within your local courseware system. Students in a computer lab can do such worksheets in class, concurrently, perhaps in pairs, which fosters discussion. The questions can be purposefully **vague**, to **encourage discussion** -- in which case completion could be simply "checked off" rather than graded in detail. Such worksheets give **focus** and a finite **completion goal** to each student. In contrast, simply assigning students to read a Proteopedia page may leave them less focused and perhaps uncertain about whether they have absorbed what you intend from the page.

### Quizzes

Proteopedia has a mechanism to include quizzes on pages you prepare for your students. See [Help:Quiz](#).

*Student Authoring of Projects as Permanent Proteopedia Pages*

Upper level undergraduates, e.g. biochemistry majors, or graduate students may be assigned to complete a project in the form of a permanent Proteopedia page. A particularly outstanding example, [Photosystem II](#) (Fig. 2), was authored by [Emily Forschler](#) while she was a senior biochemistry major at Messiah College (Grantham PA US) in a class taught by [Karl Oberholser](#). Professor Oberholser reported "I think that Emily's work on Photosystem II shows that Proteopedia is a system that a Jmol novice can use with good effect. Emily had no experience with using Jmol. The other students in the class ... [made] PowerPoint presentations of their chosen proteins, and after seeing Emily's Proteopedia presentation one student's response was all of us should have used Proteopedia. Thank you for a great product!"

Another strategy for a small, upper level class is to have individuals or small groups author pages that address a particular topic. [Ann Taylor](#) has used this at Wabash College to create pages on [Glycolysis](#) [Enzymes](#), [Citric Acid Cycle](#) and [Proteins involved in cancer](#). Any student planning to author a permanent page should request a personal user account in their own real name, identifying themselves as a student, and their college. See, for example, [Emily Forschler](#). The pages for the project can then be created as subpages of an individual's user page (find out how to do that at [Help:Protected Pages](#)). The use of the protected pages insures that the page will be editable only by the student and not subject to alterations possible for typical sandbox pages. The project could then later always be copied to standard Proteopedia page so others can improve it.

The screenshot shows the Proteopedia article for Photosystem II. The page layout includes a navigation sidebar on the left, a main content area with a table of contents and a background section, and a 3D molecular model on the right. The background section contains the following text:

This structure of **Photosystem II** was crystallized from the cyanobacteria, *Thermosynechococcus elongatus*, at 3.0Å [1] and at 3.50 Å [2]. PDB codes are 2axt and 1s5l, respectively. Cyanobacteria and plants both contain Photosystem II while photosynthetic bacteria contain the bacterial reaction center. This photosynthetic protein complex is associated with a variety of functional ligands. It is a **dimer** composed mainly of alpha-helices. Nineteen **subunits** are in each monomer, with multiple extrinsic subunits associated with the oxygen evolving complex missing from this crystallization. Photosystem II is a membrane bound protein complex that in plants is associated with the thylakoid membrane of chloroplasts. **Polar and hydrophobic** regions correlate with membrane associated nature of the protein. Hydrophobic helices make up the transmembranal portion, while **polar** residues are concentrated externally on either side of the membrane.

**Fig. 2.** Photosystem II page of Proteopedia was authored by [Emily Forschler](#) while she was a senior biochemistry major at Messiah College (Grantham PA US) in a class taught by [Karl Oberholser](#). *Student Authoring of Temporary Proteopedia Pages: Sandboxes*  
Some educators have assigned their students to try out authoring a Proteopedia molecular scene or two, just to learn the process, without making permanent pages in Proteopedia. Proteopedia has Sandbox pages where you or your students are invited to try authoring. The contents of these pages are not permanent, and will be erased or replaced at a later time.

#### *Molecular Structure: FirstGlance in Jmol*

Every page in Proteopedia that is titled with a 4-character [PDB code](#) has a link to [FirstGlance in Jmol](#). *FirstGlance* makes it easy to explore the molecular structure in more detail (and, like Proteopedia, it can use [Java](#) but also works without Java). *FirstGlance* reports the number of chains of protein, DNA, RNA, and lists all ligands and non-standard residues with their full names. You can click on any of these to find them. Sequences can be displayed and short sequences can be found. With one click each you can see secondary structure, amino and carboxyl termini, hydrophobic cores (two clicks, one to slice through the center with "Slab"), positive and negative charges, and much more. Tools locate disulfide bonds, salt bridges, cation-pi interactions, and non covalent bonds to any moiety you specify. Help and color keys appear automatically.

When students are given a worksheet or a list of suitable questions, *FirstGlance* provides an easy way to see answers. [Here are 20 questions](#) assigned to students in a [workshop](#). These questions apply to any protein; each student chose a different protein to investigate. Jaswal, O'Hara, Williamson and Springer (2013)<sup>[1]</sup> describe in detail how they use *Proteopedia*, *FirstGlance in Jmol* and student-authored presentations about their structure-function analysis projects in a one-semester biochemistry course at Amherst College (Amherst, Massachusetts, USA).

#### **Who's using Proteopedia?:**

##### High School:

- as live support for lectures
- as live support for student's self-paced learning

##### Universities:

- as live support for lectures

- as live support for student's self-paced learning
- as media for Final Projects/Thesis
- as driving topic for Student's Clubs

Researchers:

- as a source of information
- as a shared secure shared collaboration site

Journals:

- as an Interactive 3D Complement

**Current modes for pages in Proteopedia:**

Community domain:

Open read access, registered users write access  
/Ribosomal\_protein\_S13

User domain:

Open read access, owner write access  
/User:Eric\_Martz/Resolution

User workbench:

Selected users read access, owner write access  
/User:Eric\_Martz/Workbench/Movements

Sandbox:

Scratch testing open pages  
/Sandbox\_prueba

**Special Areas in Proteopedia:**

Group domain:

Open read and write access  
/Group:MUZIC:Interactome  
/Group:SMART:Teams

Journal domain:

*before paper publication:* Restricted read and write access  
*after publication:* Open read access, restricted write access  
/Journal:PLoS\_ONE:2

Studio domain:

Selected users read and write access

/Studio:G1SecL01

**Proteopedia off-line:**

Exported pages:

Off-line, self-contained, active Proteopedia pages

**References:**

1. Jaswal SS, O'Hara PB, Williamson PL, Springer AL. Teaching structure: student use of software tools for understanding macromolecular structure in an undergraduate biochemistry course. *Biochem Mol Biol Educ*. 2013 Sep-Oct;**41**(5):351-9. doi: 10.1002/bmb.20718. Epub, 2013 Sep 10. PMID:[24019219](#) doi:<http://dx.doi.org/10.1002/bmb.20718>