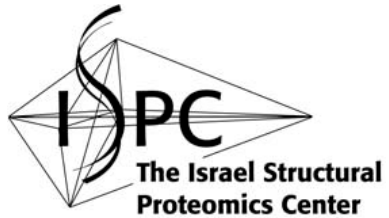
Proteopedia:

A Scientific Wiki Bridging the Gap Between 3D Structure & Function

http://proteopedia.org

Joel L. Sussman
Weizmann Institute of Science
ICTP: Advanced Workshop on Structural Biology
Trieste, Italy

15-19 Dec 2014



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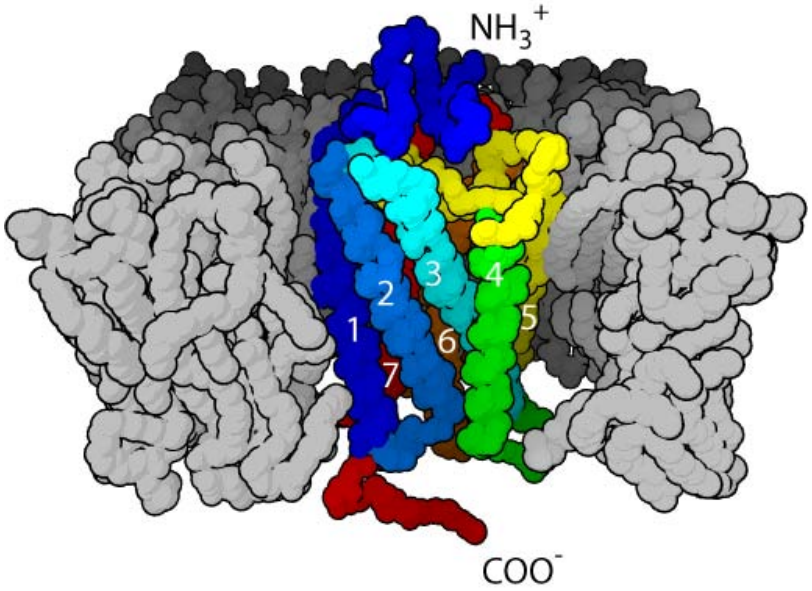
Class of 2025

Snap quiz



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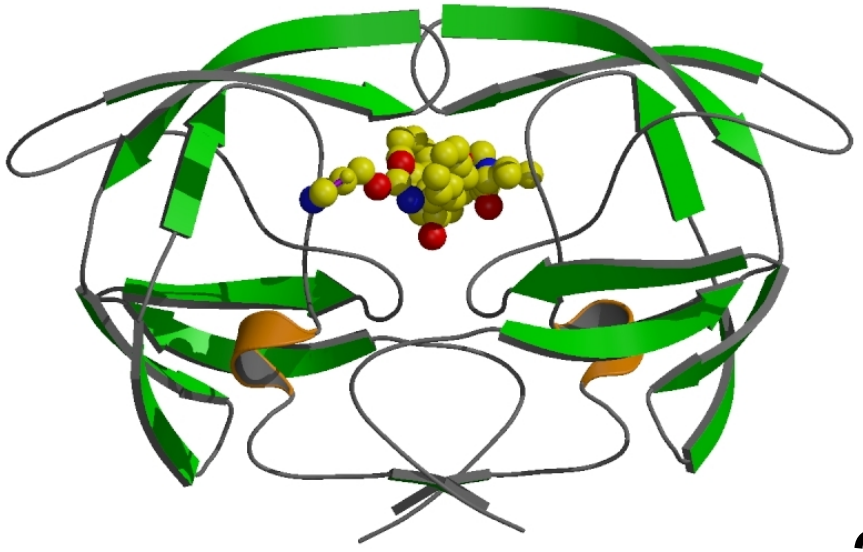

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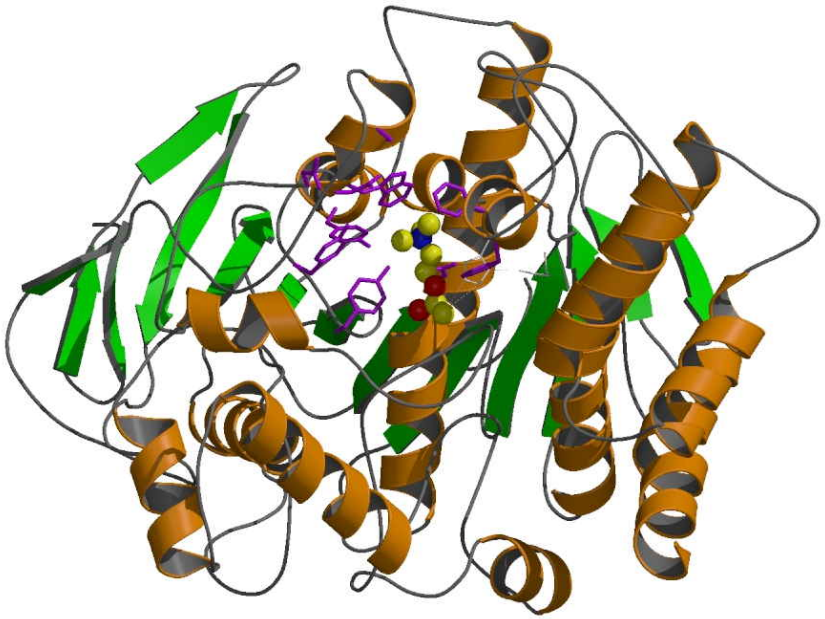

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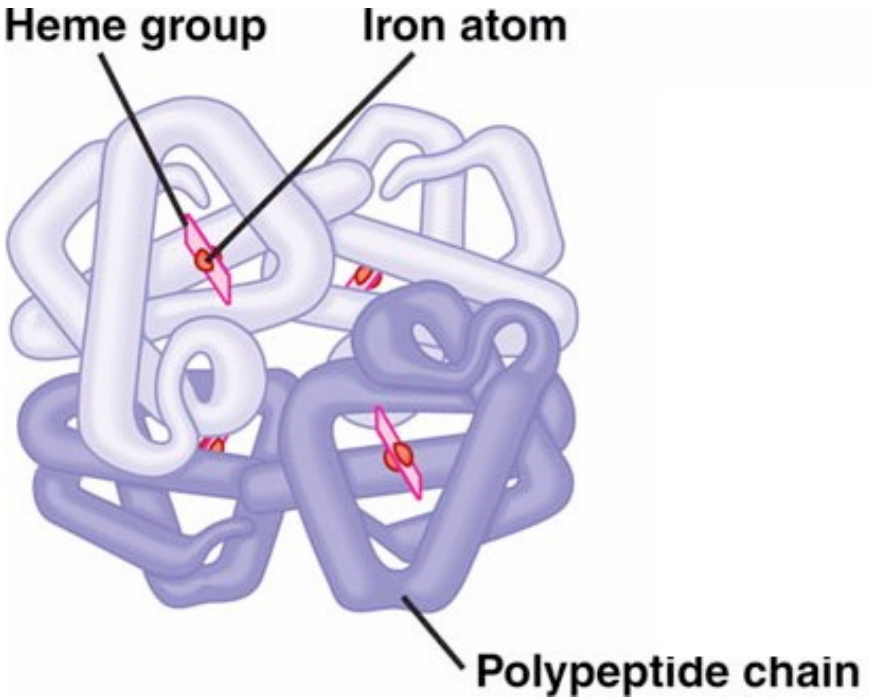


4

It's hard to believe, but…

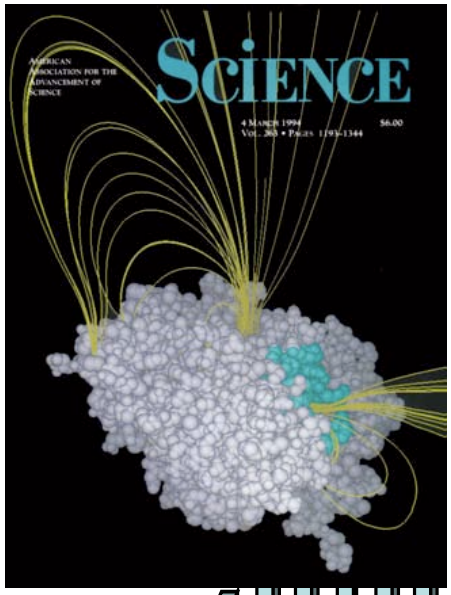
3D structures are often hard to understand:

even for a structural biologist!

The "Kluge" 1965, MIT

Dec 17, 2014

Growth in PDB
105,097 structures



But hard to explain 3D structures in 2D

JBIC Journal of Biological Inorganic Chemistry

A publicatio
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Structure of Anticancer Ruthenium Half-Sandwich Complex Bound to Glycogen Synthase Kinase 3ß

G. Atilla-Gocumen, L. Di Costanzo, E. Meggers [1]

A crystal structure of an organometallic half-sandwich ruthenium complex bound to the protein kinase glycogen synthase kinase 3ß (GSK-3ß) has been determined and reveals that the inhibitor binds to the ATP binding site via an induced fit mechanism utlizing several hydrogen bonds and hydrophobic interactions. Importantly, the metal is not involved in any direct interaction with the protein kinase but fulfills a purely structural role. The unique, bulky molecular structure of the half-sandwich complex with the CO-ligand oriented perpendicular to the pyridocarbazole heterocycle allows the complex to stretch the whole distance sandwiched between the faces of the N- and C-terminal lobes and to interact tightly with the flexible glycine-rich loop. Although this complex is a conventional ATP-competitive binder, the unique shape of the complex allows novel interactions with the glycine-rich loop which are crucial for binding potency and selectivity. It can be hypothesized that coordination spheres which present other ligands towards the glycine-rich loop might display completely different protein kinase selectivities.

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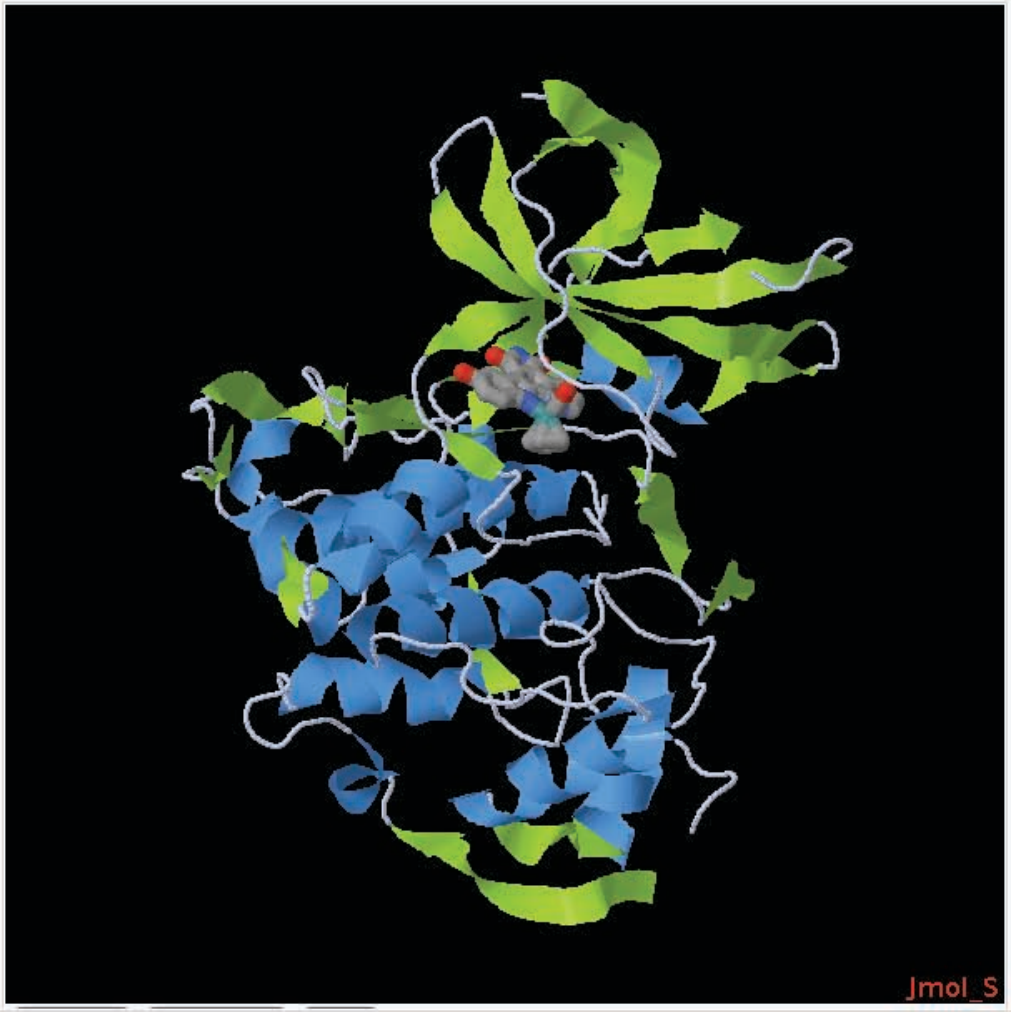

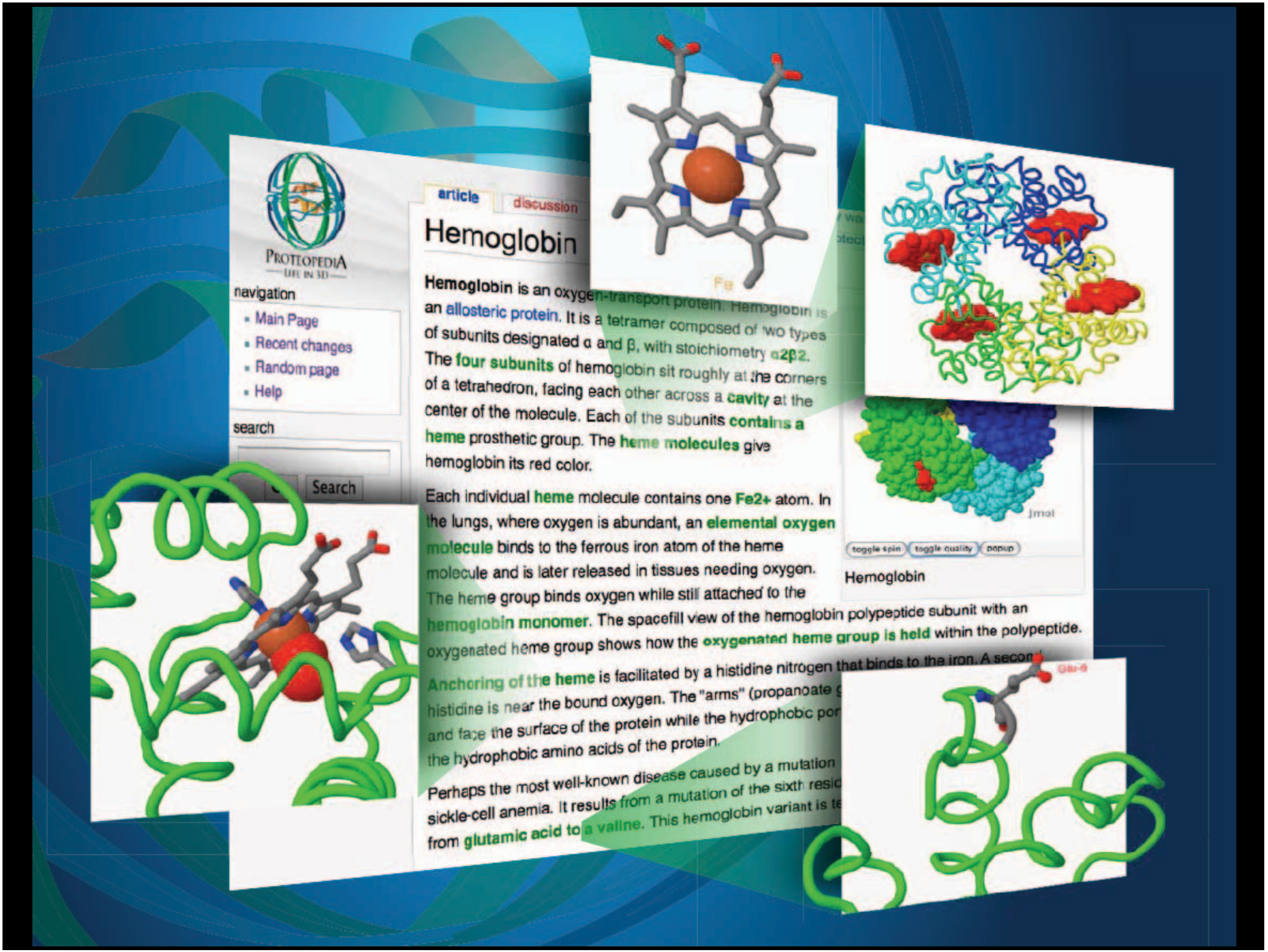
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Hemoglobin
Hemoglobin is an oxygen-transport protein. Hemoglobin is an allosteric protein. It is a tetramer composed of two types of subunits designated α and β, with stoichiometry α2β2. The four subunits of hemoglobin sit roughly at the corners of a tetrahedron, facing each other across a cavity at the center of the molecule. Each of the subunits contains a heme prosthetic group. The heme molecules give hemoglobin its red color.
Each individual heme molecule contains one Fe2+ atom. In the lungs, where oxygen is abundant, an elemental oxygen molecule binds to the ferrous iron atom of the heme molecule and is later released in tissues needing oxygen. The heme group binds oxygen while still attached to the hemoglobin monomer. The spacefill view of the hemoglobin polypeptide subunit with an oxygenated heme group shows how the oxygenated heme group is held within the polypeptide.
Anchoring of the heme is facilitated by a histidine nitrogen that binds to the iron. A second histidine is near the bound oxygen. The "arms" (propanoate g
and face the surface of the protein while the hydrophobic por
the hydrophobic amino acids of the protein.
Perhaps the most well-known disease caused by a mutation
sickle-cell anemia. It results from a mutation of the sixth resic
from glutamic acid to a valine. This hemoglobin variant is te
Fe
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Hemoglobin
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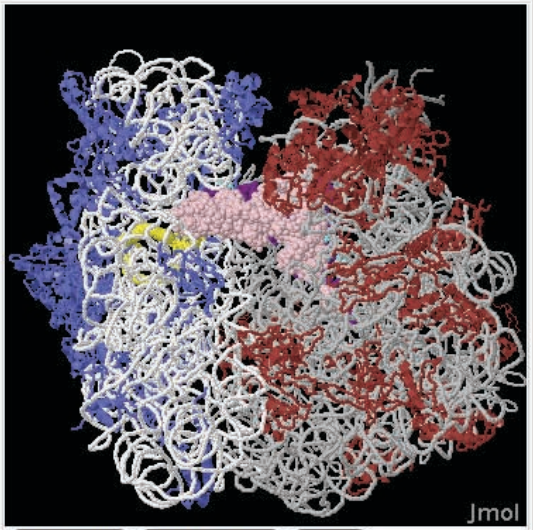

The Ribosome

by Wayne Decatur

On October 7th, 2009 the Nobel Committee announced three structural biologists would share the 2009 Nobel Prize in Chemistry for studies of the The Ribosome. The ribosome is the machine in your cells that accurately and efficiently decodes the genetic information stored in your genome and synthesizes the corresponding polypeptide chain one amino acid at a time in the process of translation. Venkatraman Ramakrishnan of the M.R.C. Laboratory of Molecular Biology in Cambridge, England;

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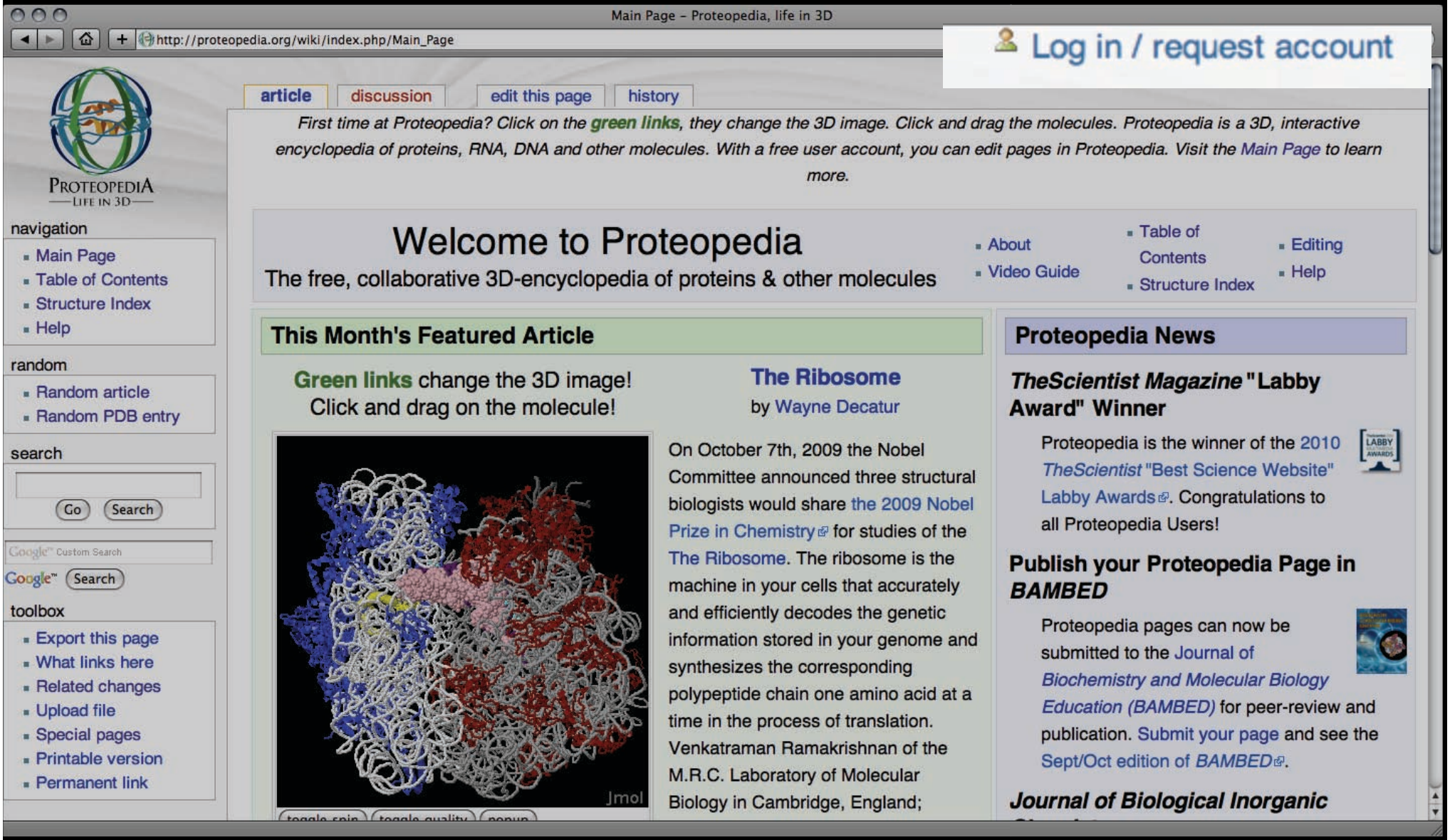
Journal of Biological Inorganic

Proteopedia – Joel L. Sussman – December 2014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Main Page – Proteopedia, life in 3D

http://proteopedia.org/wiki/index.php/Main_Page

clearly the major contributions to decoding and peptide bond synthesis come from RNA and not protein, as well as for the sheer size of the structures determined. These structures represent tour-de-force efforts in understanding fundamental processes in every organism on earth and will have direct impacts on how we fight pathogenic bacteria in the immediate future. Shown **here (restore initial scene)** are both subunits of the ribosome, as well as **mRNA and tRNA** that bind in the complex during the process of translation. (**more...**)

Recently featured: Neuraminidase – Poly(A) Polymerase
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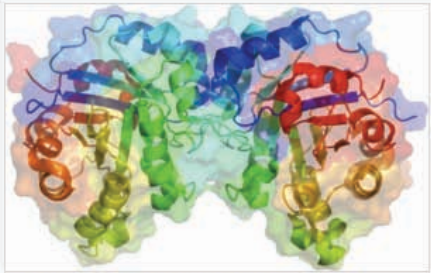

Triose Phosphate Isomerase

The Scoreboard

Last 30 Days (Top 10)

Score	Pages	Changes	Username
19	4	64	Gregg Snider
18	3	62	Adithya Sagar
16	6	33	Bryant Chen
16	2	52	Alexandra Clement
16	5	33	Yuping Zhou
12	4	22	Amy Kerzmann
12	8	13	Sarah Wilson
12	4	20	Allison Granberry
11	6	12	Angel Herraez
10	2	20	Tilman Schirmer

Score based on pages-edited and number-of-edits
All scores...

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and **green links** are fun & easy to make!

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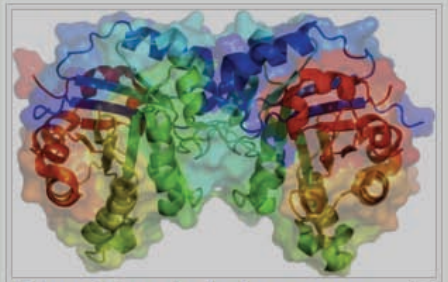

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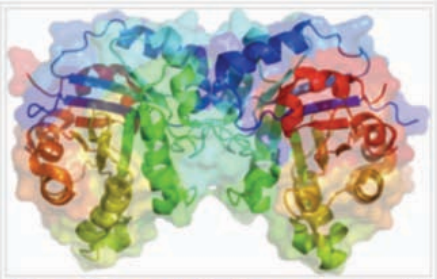

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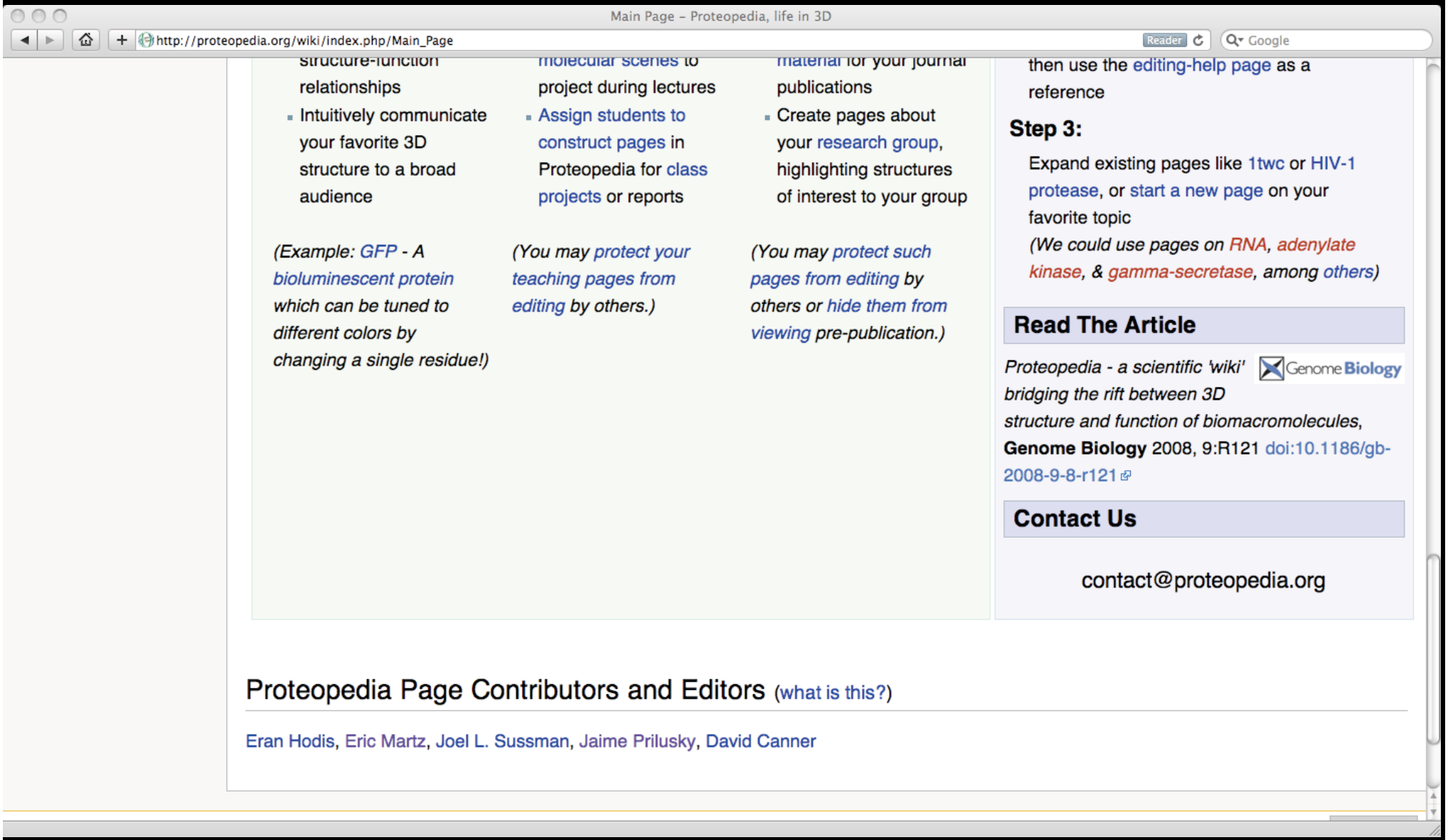
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Create pages about your research group, highlighting structures of interest to your group
(Example: GFP - A bioluminescent protein which can be tuned to different colors by changing a single residue!)
(You may protect your teaching pages from editing by others.)
(You may protect such pages from editing by others or hide them from viewing pre-publication.)
then use the editing-help page as a reference
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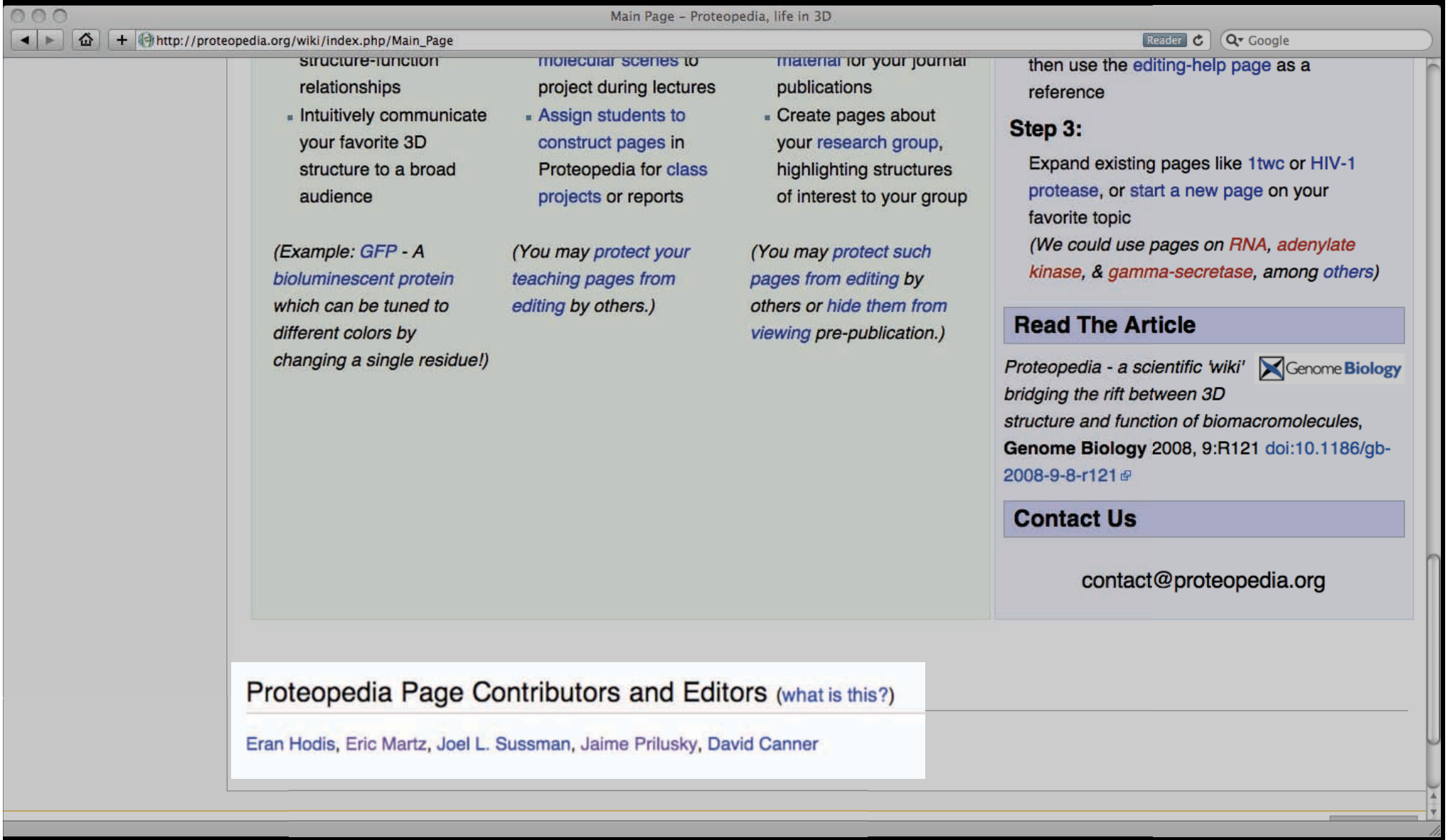
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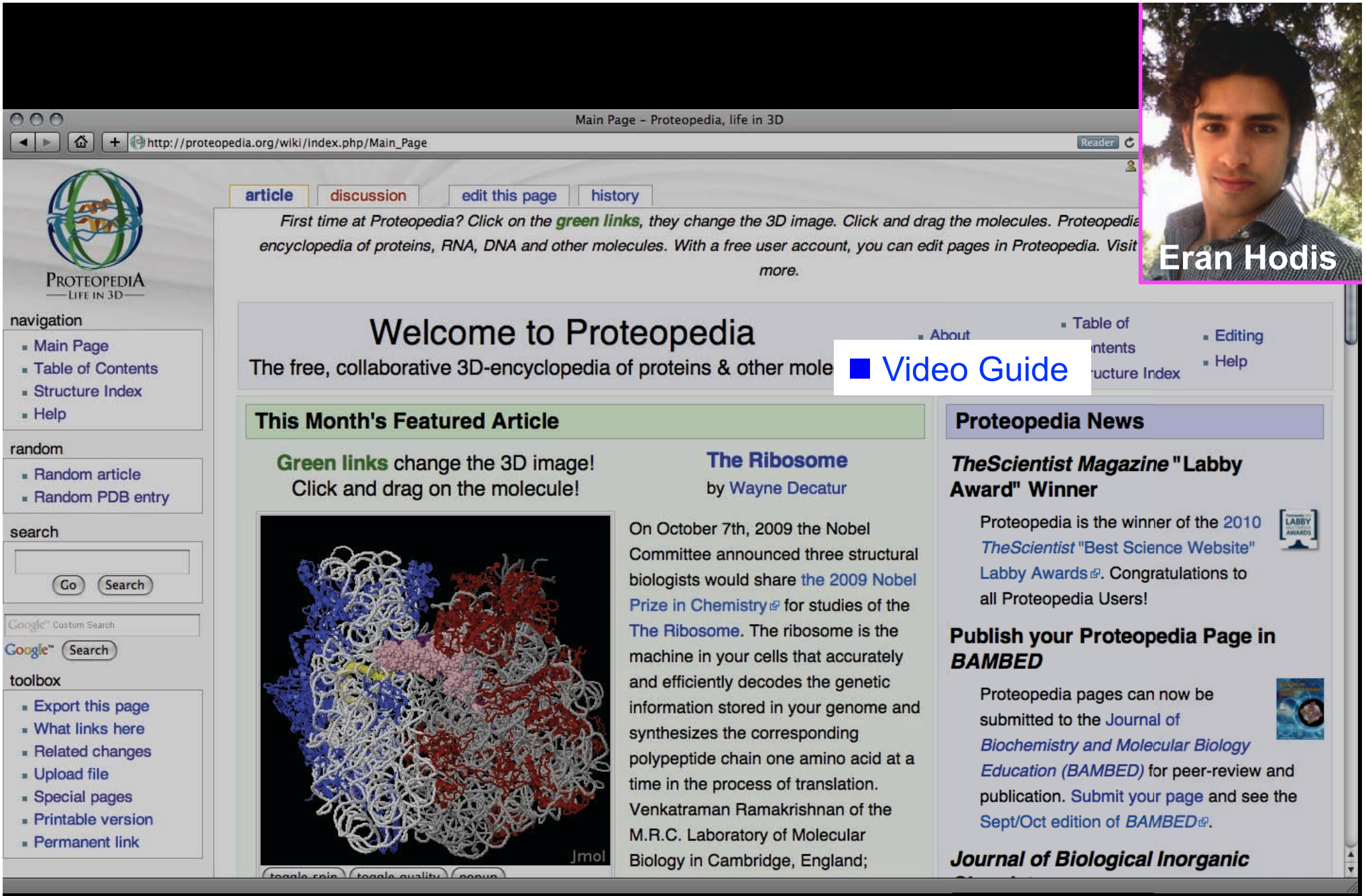

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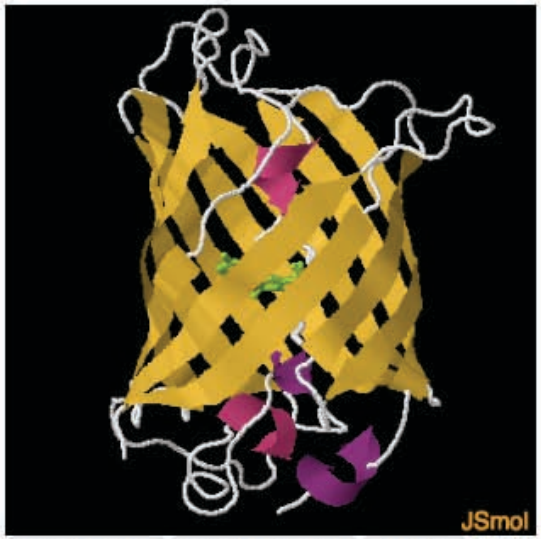
Green Fluorescent Protein
by Eran Hodis



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Green fluorescent protein (GFP) is a bioluminescent polypeptide consisting of 238 residues isolated from the body of Aequorea victoria jellyfish.[1] GFP converts the blue chemiluminescent of aequorin in the jellyfish into green fluorescent light.[2] It remains unclear why these jellyfish use fluorescence, why green is better than blue, or why they produce a separate protein for green fluorescence as opposed to simply mutating the present aequorin to shift its wavelength,[3] but in the laboratory, GFP can be incorporated into a variety of biological systems in order to function as a marker protein. Since its discovery in 1962, GFP has become a significant contributor to the research of monitoring gene expression, localization, mobility, traffic, interactions between various membrane and cytoplasmic proteins, as well as many others. (**more...**)

Previously featured articles...

Proteopedia News

- Talking about Proteopedia on 12/04/14-12/06/14, a live online talk organised by DivCHED CCCE: Committee on Computers in Chemical Education
- Course in Spanish/English on Proteopedia and its uses to study, display and teach macromolecules.
- How to create fast loading pages in Proteopedia.
- How to be as safe as possible with Java (a *Must read* for Proteopedia users)
- Proteopedia on iPads!
- What version of Jmol is running?
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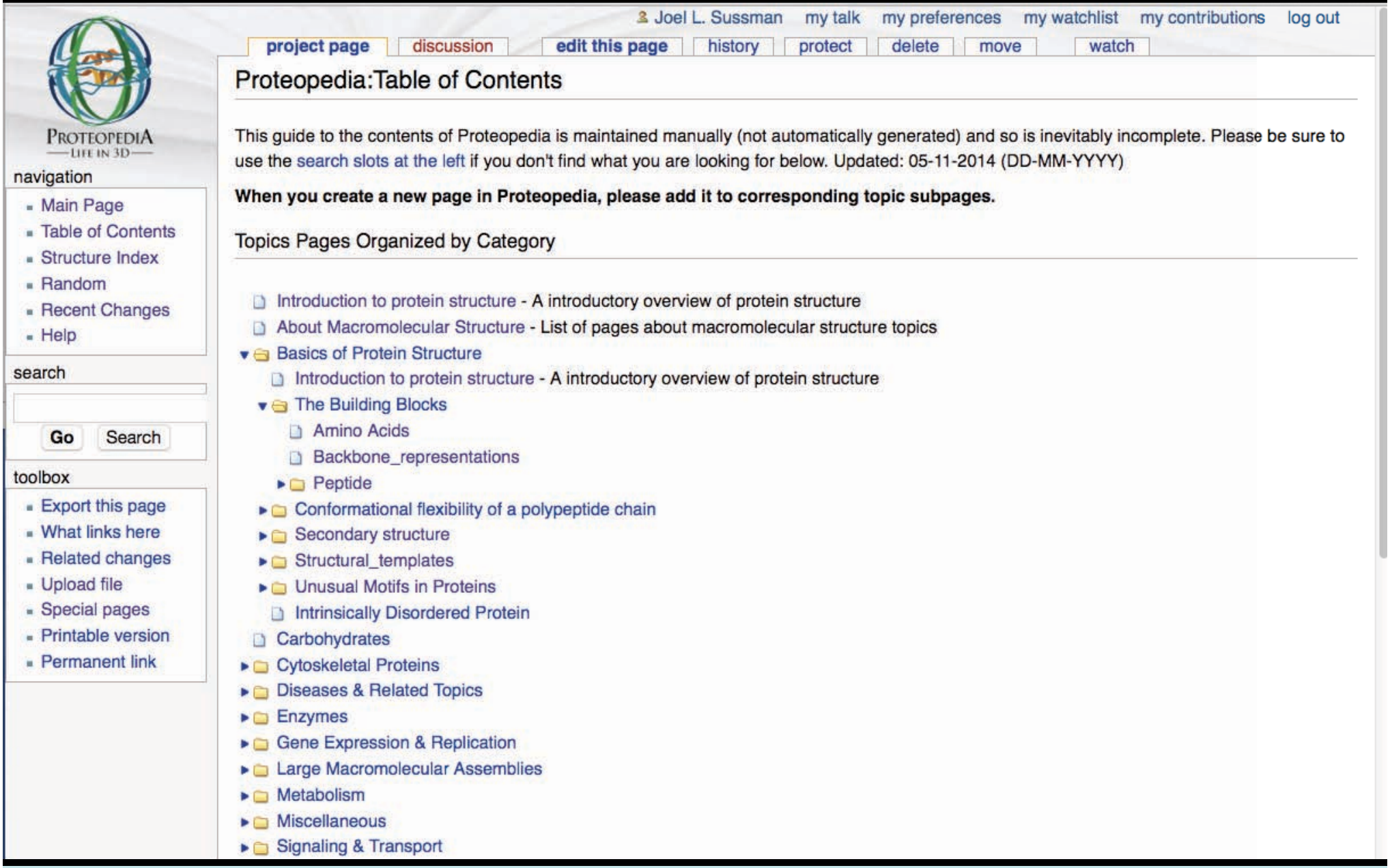

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When you create a new page in Proteopedia, please add it to corresponding topic subpages.

Topics Pages Organized by Category

- Introduction to protein structure - A introductory overview of protein structure
- About Macromolecular Structure - List of pages about macromolecular structure topics
- Basics of Protein Structure
  - Introduction to protein structure - A introductory overview of protein structure
  - The Building Blocks
    - Amino Acids
    - Backbone_representations
    - Peptide
  - Conformational flexibility of a polypeptide chain
  - Secondary structure
  - Structural_templates
  - Unusual Motifs in Proteins
  - Intrinsically Disordered Protein
- Carbohydrates
- Cytoskeletal Proteins
- Diseases & Related Topics
- Enzymes
- Gene Expression & Replication
- Large Macromolecular Assemblies
- Metabolism
- Miscellaneous
- Signaling & Transport

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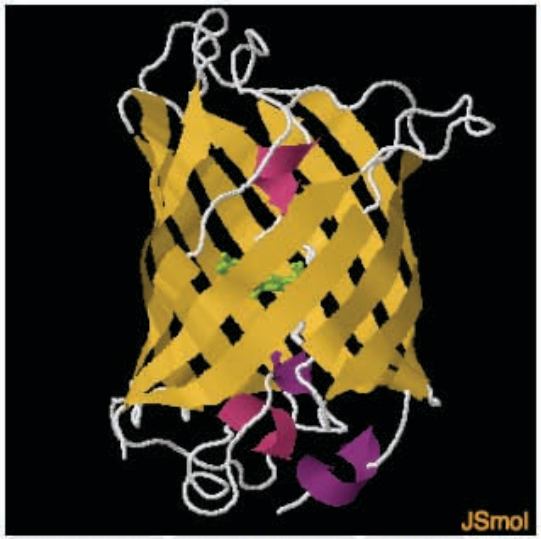

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Green fluorescent protein (GFP) is a bioluminescent polypeptide consisting of 238 residues isolated from the body of Aequorea victoria jellyfish.[1] GFP converts the blue chemiluminescent of aequorin in the jellyfish into green fluorescent light.[2] It remains unclear why these jellyfish use fluorescence, why green is better than blue, or why they produce a separate protein for green fluorescence as opposed to simply mutating the present aequorin to shift its wavelength,[3] but in the laboratory, GFP can be incorporated into a variety of biological systems in order to function as a marker protein. Since its discovery in 1962, GFP has become a significant contributor to the research of monitoring gene expression, localization, mobility, traffic, interactions between various membrane and cytoplasmic proteins, as well as many others. (**more...**)

Previously featured articles...

Proteopedia News

- Talking about Proteopedia on 12/04/14-12/06/14, a live online talk organised by DivCHED CCCE: Committee on Computers in Chemical Education
- Course in Spanish/English on Proteopedia and its uses to study, display and teach macromolecules.
- How to create fast loading pages in Proteopedia.
- How to be as safe as possible with Java (a *Must read* for Proteopedia users)
- Proteopedia on iPads!
- What version of Jmol is running?
- Proteopedia status
- Awards

The Scoreboard

Last 30 Days (Top 10)

Score	Pages	Changes	Username
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3 Key Elements

- Presents **3D information** in an **intuitive manner**
- A **web browser** is **all you need**
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- And it is ***free(!)***

Proteopedia pages contain *Jmol* scenes

Jmol

www.jmol.org

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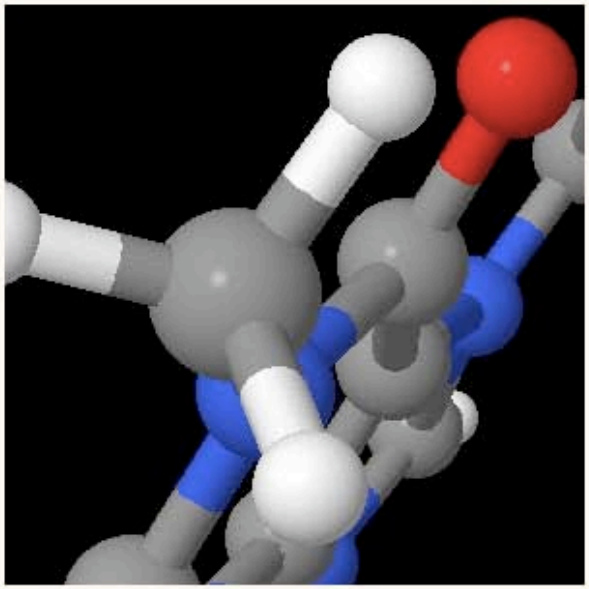
Documentation | Wiki | History | FAQs
Browser check | Download | Project pages

Jmol: an open-source Java viewer for chemical structures in 3D

with features for chemicals, crystals, materials and biomolecules



Jmol is an interactive web browser applet.

This is a still image, but you can get an animated display of Jmol abilities by clicking here.

(The applet may take some seconds to load. Please, wait and do not reload the page in the meantime.)

Robert Hanson

JSmol now runs without Java on iPads, iPhones & Androids

Chemistry

The Nobel Prize in Chemistry 2009

"for studies of the structure and function of the ribosome"

Photo: MRC Laboratory of Molecular Biology

Venkatraman Ramakrishnan

1/3 of the prize

United [illegible]

MRC [illegible] Molec[illegible] Camb[illegible]ge, United Kingdom

Credits: Michael Marsland/Yale University

Thomas A. Steitz

1/3 of the [illegible] prize

[illegible] Haven, CT, USA; Howard Hughes Medical Institute

Credits: Micheline Pelletier/Corbis

Ada E. Yonath

[illegible] prize

Weizmann Institute of Science Rehovot, Israel

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Sat 9:56 PM (Charged)

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Wayne Decatur

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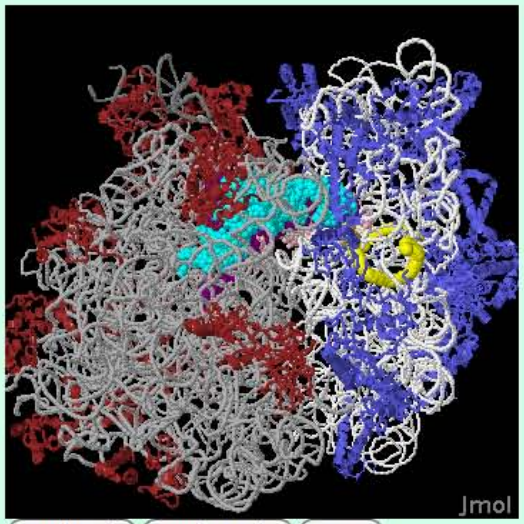

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·· large subunit on/off ·· small subunit on/off ··
·· tRNAs on/off ·· mRNA on/off ·· rRNA on/off ·· proteins on/off ··
·· Aminoacyl(A)-site tRNA on/off ·· Peptidyl(P)-site tRNA on/off ·· Exit(E)-site tRNA on/off ··

Green links change the 3D image! Click and drag on the molecule!

The Ribosome

by Wayne Decatur

On October 7th, 2009 the Nobel Committee announced three structural biologists would share the 2009 Nobel Prize in Chemistry for studies of the The Ribosome. The ribosome is the machine in your cells that accurately and efficiently decodes the genetic information stored in your genome and synthesizes the corresponding polypeptide chain one amino acid at a time in the process of translation. Venkatraman Ramakrishnan of the M.R.C. Laboratory of Molecular Biology in Cambridge, England; Thomas A. Steitz of Yale University; and Ada E. Yonath of the Weizmann Institute of Science in Rehovot, Israel share the prize for the first atomic-resolution structures of the two subunits that come together to form an active ribosome. These structures are considered landmarks for the fact they showed clearly the major contributions to decoding and peptide bond synthesis come from RNA and not protein, as well as for the sheer size of the structures determined. These structures represent tour-de-force efforts in understanding fundamental processes in every organism on earth and will have direct impacts on how we fight pathogenic bacteria in the immediate future. Shown **here (restore initial scene)** are both subunits of the ribosome, as well as **mRNA and tRNA** that bind in the complex during the process of translation. Read more....

H1N1 Flu, Tamiflu & Neuraminidase were featured here earlier. See all previously featured articles...

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What's new?

How people are using it?

- Student assignments to create pages
- Professors create pages to **aid in teaching**, *e.g.* showing conformational changes
- **There are 2 kinds of pages**
  - ***Seeded* pages**: Based on PDB entry
  - **Topic pages**: Structural Biology topics

Dr. Jaime Prilusky

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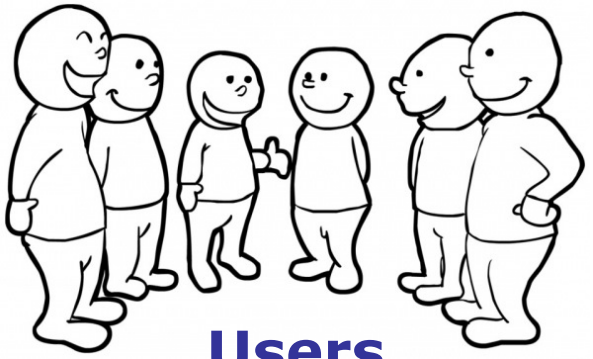

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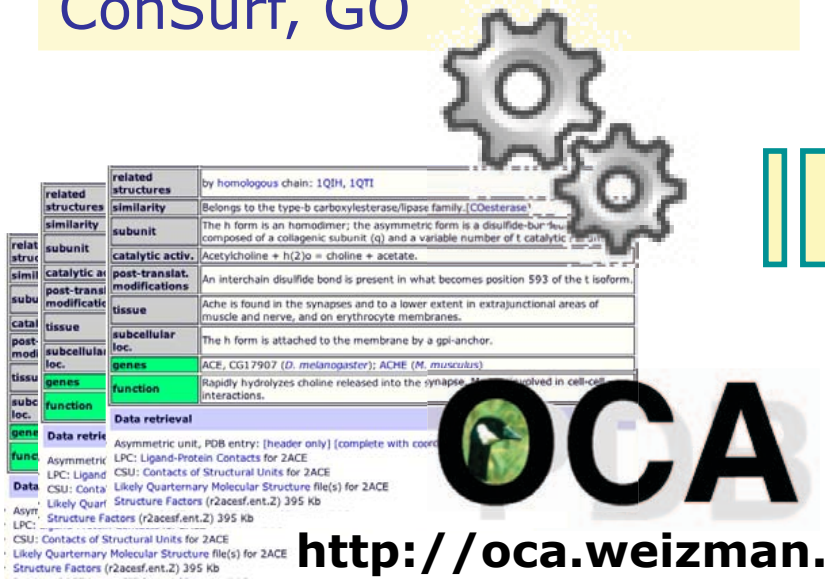

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A Seeded Page

2cdn – Proteopedia, life in 3D

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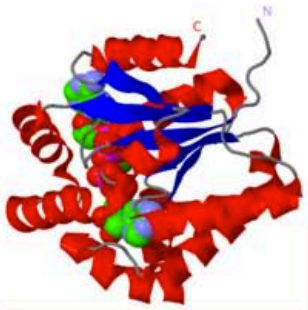


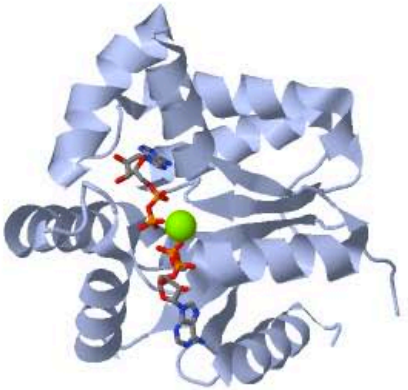
CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS ADENYLATE KINASE COMPLEXED WITH TWO MOLECULES OF ADP AND MG [edit]

Publication Abstract from PubMed

The crystal structure of Mycobacterium tuberculosis adenylate kinase (MtAK) in complex with two ADP molecules and Mg2+ has been determined at 1.9 A resolution. Comparison with the solution structure of the enzyme, obtained in the absence of substrates, shows significant conformational changes of the LID and NMP-binding domains upon substrate binding. The ternary complex represents the state of the enzyme at the start of the backward reaction (ATP synthesis). The structure is consistent with a direct nucleophilic attack of a terminal oxygen from the acceptor ADP molecule on the beta-phosphate from the donor substrate, and both the geometry and the distribution of positive charge in the active site support the hypothesis of an associative mechanism for phosphoryl transfer.

The crystal structure of Mycobacterium tuberculosis adenylate kinase in complex with two molecules of ADP and Mg2+ supports an associative mechanism for phosphoryl transfer., Bellinzoni M, Haouz A, Grana M, Munier-Lehmann H, Shepard W, Alzari PM, Protein Sci. 2006 Jun;15(6):1489-93. Epub 2006 May 2. PMID:16672241

From MEDLINE®/PubMed®, a database of the U.S. National Library of Medicine.



Jmol

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2cdn, resolution 1.90Å (default scene)

Sites:	AC1
Ligands:	ADP, MG
Activity:	Adenylate kinase, with EC number 2.7.4.3
Domains:	ADK, Adk
Structural annotation:	[show]
Functional annotation:	[show]
Evolutionary conservation:	[show]
Resources:	FirstGlance, OCA, PDBsum, RCSB
Coordinates:	save as pdb, mmCIF, xml

About this Structure [edit]

2CDN is a 1 chain structure of sequence from Mycobacterium tuberculosis. Full crystallographic information is available from OCA.

Reference [edit]

- Bellinzoni M, Haouz A, Grana M, Munier-Lehmann H, Shepard W, Alzari PM. The crystal structure of Mycobacterium tuberculosis adenylate kinase in complex with two molecules of ADP and Mg2+ supports an associative mechanism for phosphoryl transfer. Protein Sci. 2006 Jun;15(6):1489-93. Epub 2006 May 2. PMID:16672241 doi:10.1110/ps.062163406

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James Holton

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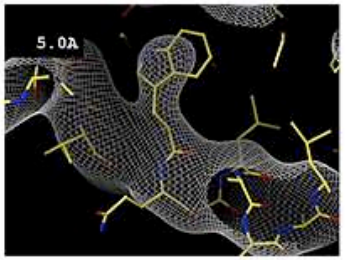
Resolution

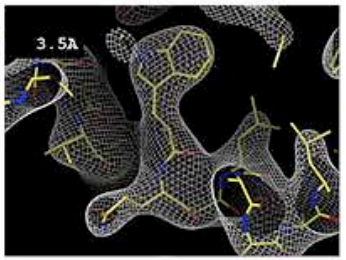
Resolution is an average value for the uncertainty of atomic positions in a crystallographic model. High values for resolution (e.g. 5.0 Å) mean high uncertainty, and low values (e.g. 1.0 Å) mean much less uncertainty. **2.05 Å** is the **median** resolution for X-ray crystallographic results in the Protein Data Bank (43,066 on May 2, 2008).

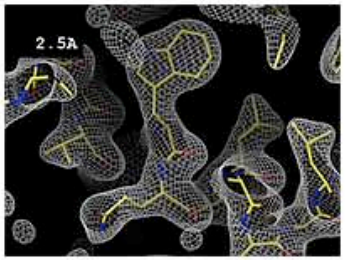
The uncertainty for each atom is quantitated in its temperature value.

The **images at right** show how the electron density map[1] becomes more accurate and detailed as the uncertainty (resolution value) decreases from 5.0 Å to 0.5 Å.

The images at right were taken from a movie[2] in which the atomic model and electron density map rock back and forth while the resolution value (uncertainty) increases from 0.5 to 5.0 Å.



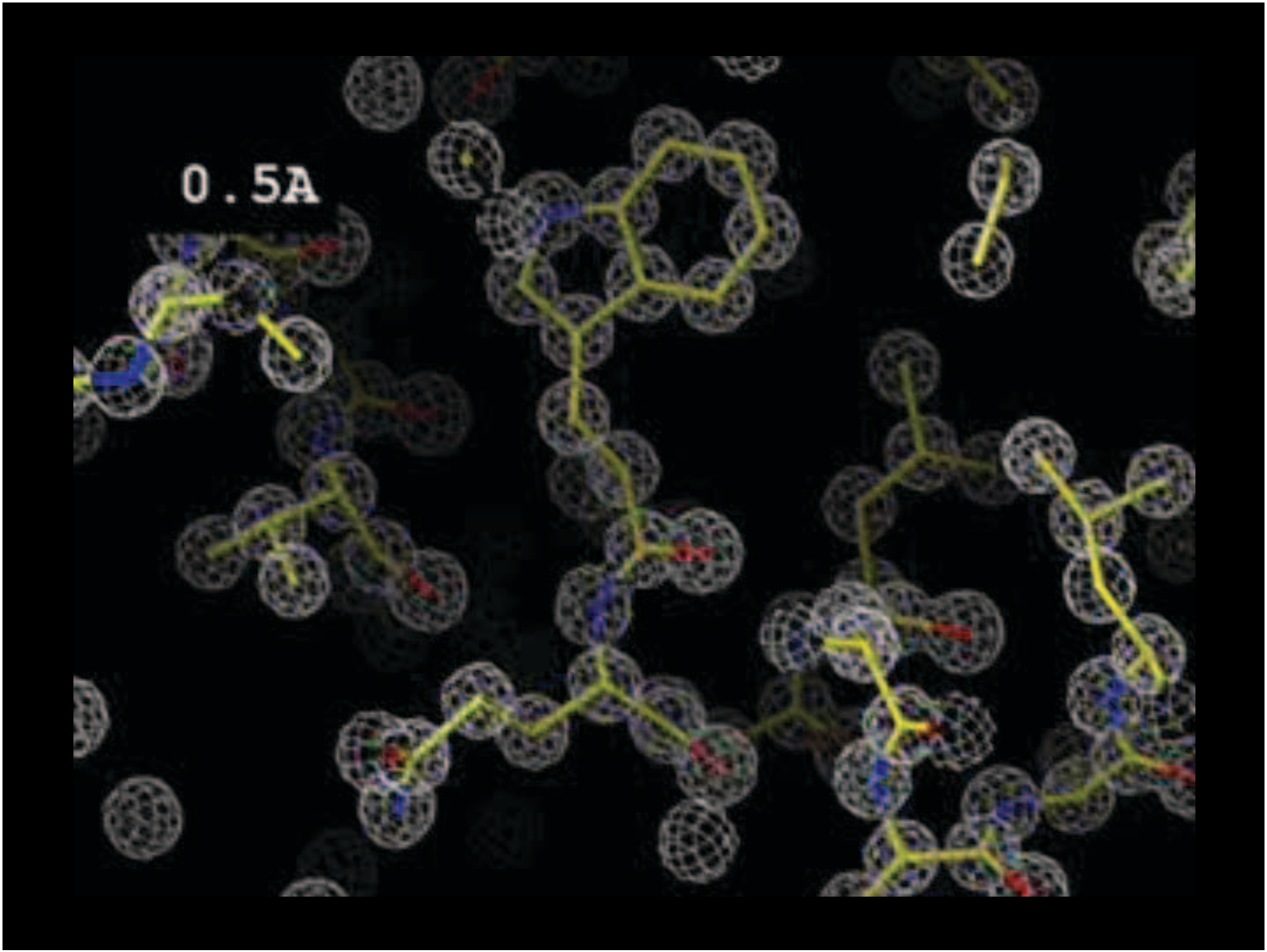




PLAY MOVIE

At 0.5 Å in the movie, every atom[1] of the tryptophan sidechain in the top center of the frame is clearly represented by a sphere of electron density. At 2.5 Å (a bit worse than the median in the PDB), the overall shape and position of the Trp sidechain is still clear, as is the alpha helical conformation of the main chain. However, at 5.0 Å, only an

Movie by James Holton, ALS, UC Berkeley, who kindly gave permission for its use in ***Proteopedia***. Original source is http://ucxray.berkeley.edu/~jamesh/movies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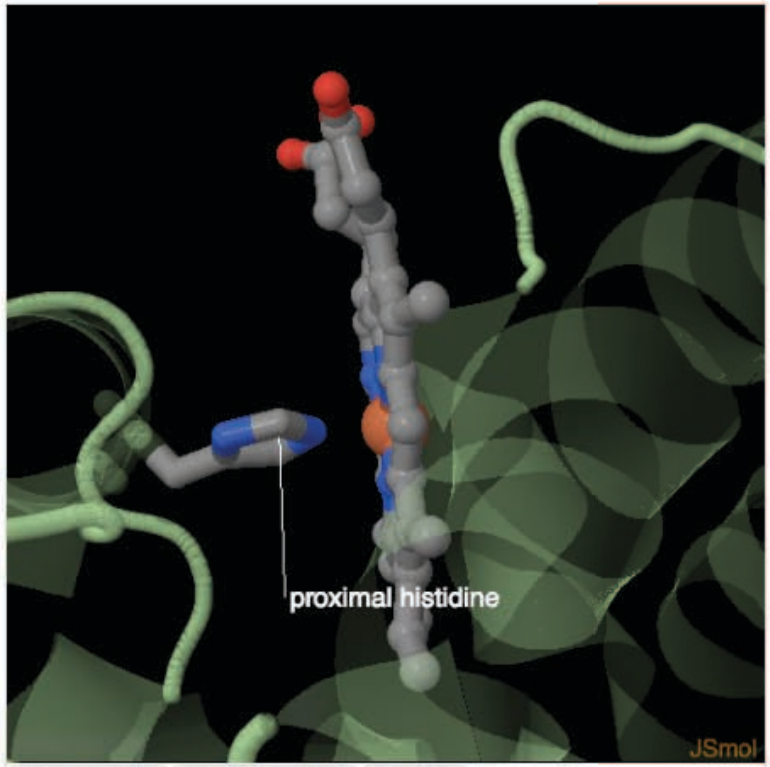
Tutorial:How do we get the oxygen we breathe

oxygen binds to hemoglobin, which we will soon observe. Do the colors of the spheres represent the true colors of the heme group? No, they do not. Remember that we are looking at a representation of the real structure, and in this case we have artificially colored each atom in the heme according to a common color scheme called the Corey-Pauling-Koltun scheme (C H O N S Fe). Remember too that although we cannot change the positions of the atoms in our experimentally determined protein structure, we can freely choose different ways to show, color, and connect these atoms in order to best comprehend and convey the niceties of the complex 3D structure. We have previously represented the atoms of the heme group as individual spheres in what is called a **spacefilling representation**, but we could just as easily represent the atoms as very small spheres with thick lines connecting the bonded atoms in what is called a **ball and stick representation**. Notice that the positions and identities of the atoms do not change. (*THINK*: Earlier we learned that the α- and β-monomers have so far been shown in cartoon representation. Why can't we show the heme groups in cartoon representation?)



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Capturing oxygen

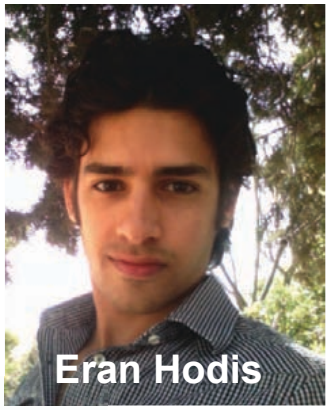
Hemoglobin captures oxygen and transports it through the bloodstream by binding oxygen to each of its **four heme groups**. These **heme**

See Also

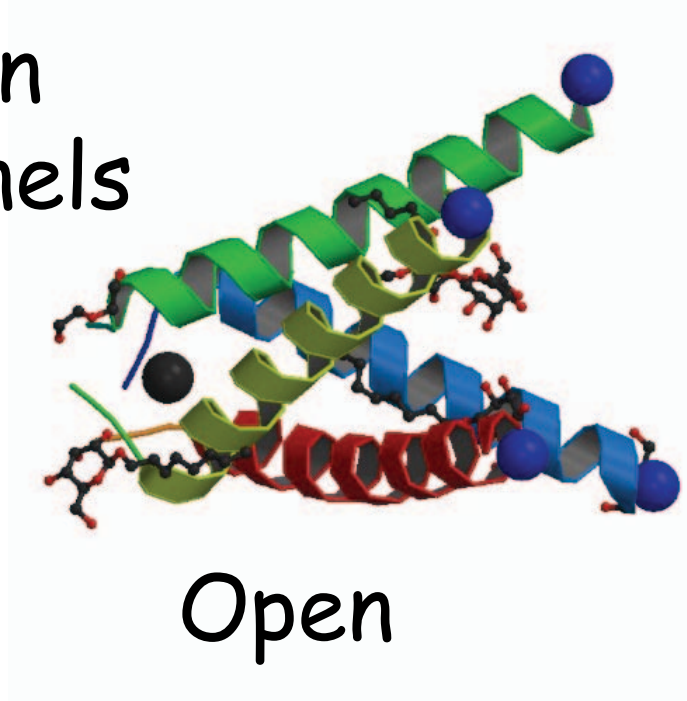
- Hemoglobi
- PDB entry 1hho (oxygenated, 2.1 Å)
- PDB entry 1hga (deoxygenated, 2.1 Å)
- PDB entry 1hbs (deoxygenated, sickle cell mutant, 3.0 Å)

DOI: http://dx.doi.org/10.14576/431679.1869588

Conformation Changes



Proton Channels



Open

closed

Schnell & Chou (2008) “Structure and mechanism of the M2 proton channel of influenza A virus” *Nature* **451**, 591-5.

Stouffer et al & DeGrado (2008) “Structural basis for the function and inhibition of an influenza virus proton channel” *Nature* **451**, 596-9.

Proton Channels

The M2 protein of influenza A virus is a proton channel. Its function is essential for productive infection by the virus.

See Category:Proton_channel for a list of all proton channel structures.

In January, 2008, crystallographic and NMR structures were published side by side in *Nature* for the transmembrane domains of the M2 protein: 3bkd to 2rlf. The former appeared to be in an open conformation blocked by amantadine, while the latter appeared to be in a closed conformation stabilized by rimantadine. (Neither drug is shown in the morph at right.)

At right is a linear-interpolation morph between 3BKD and 2RLF, showing the proposed opening and closing of this channel.

In addition to watching the animation as alpha-helical ribbons, it is useful to watch it **spacefilled**. **Be sure to rotate the molecule with your mouse to watch the animation from different perspectives!**

His37 and Trp41 are believed to be crucial for pH-dependent gating. (The apparent collapse and re-expansion of their sidechains is an artifact due to the linear interpolation method of morphing.) Here are His and Trp **spacefilled**.

To be explained in a later revision, along with new scenes: Morph from Yale

Linear interpolation morph from 3bkd to model 1 of 2rlf.

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Eran Hodis, Eric Martz

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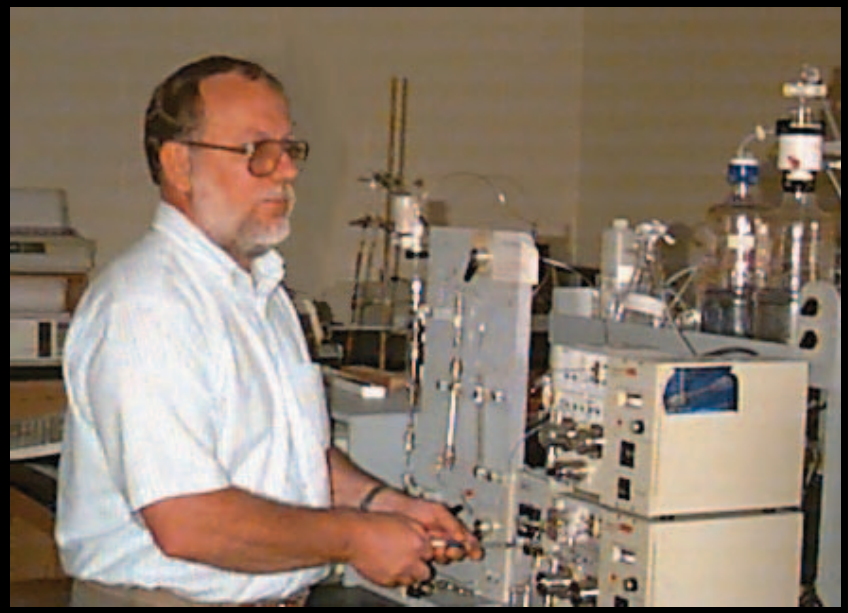
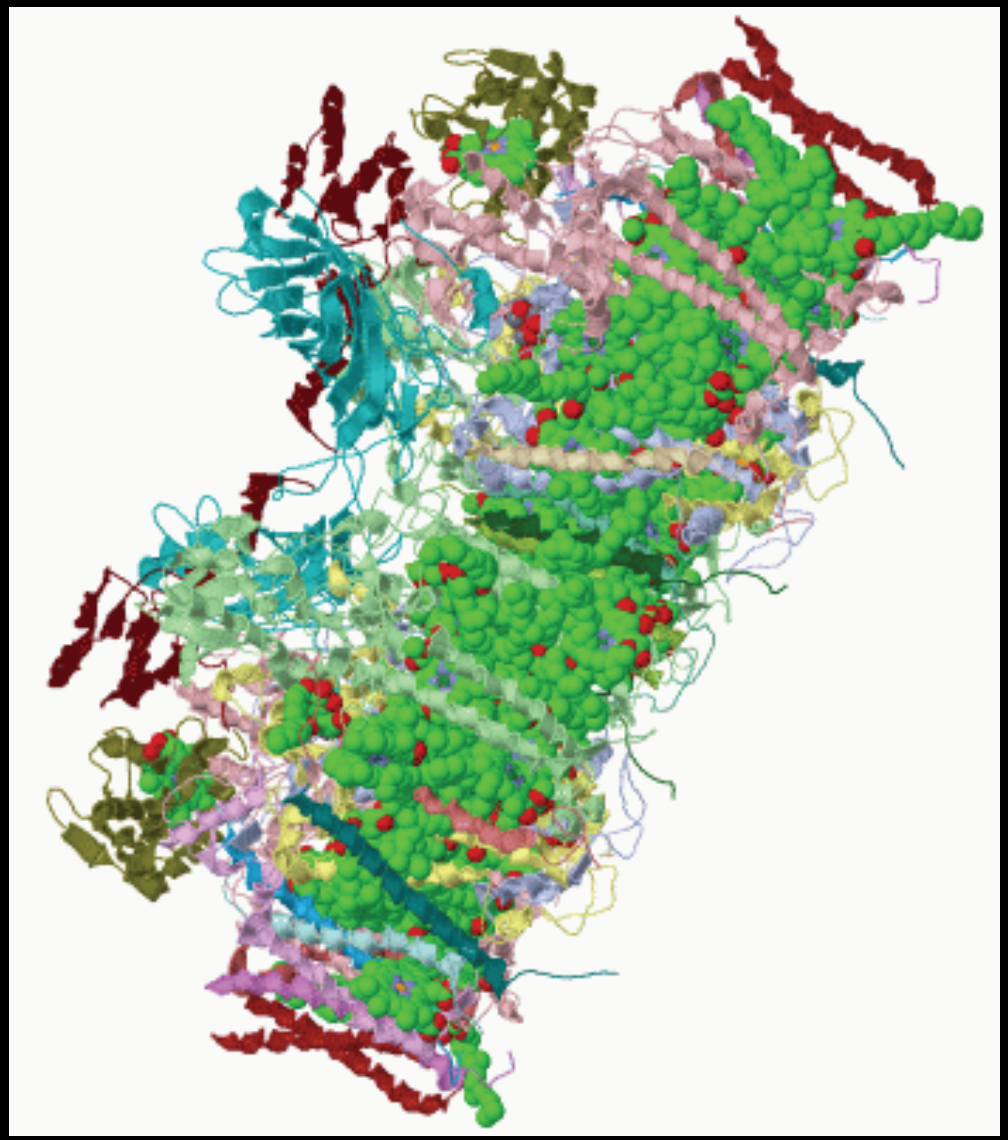


Prof. Karl Oberholser

Messiah College, PA

Student:

- **Ms. Emily Forscher**
  Photosystem II



Page by Ms Emily Forschler

Photosystem II

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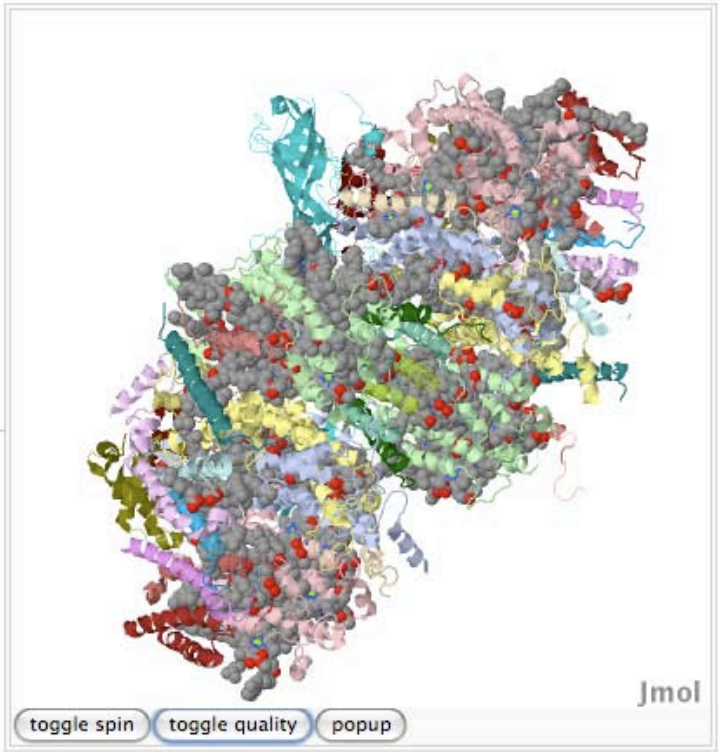


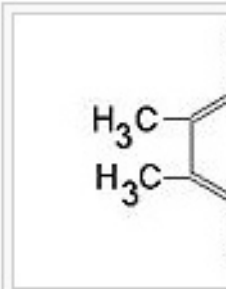
Background

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

A wiki for the scientific community

Names of contributors are listed on each page to give **credit** & add **responsibility**

Another important facet of Photosystem II is its ability to oxidize water to oxygen with its **oxygen evolving centers**. These centers are **cubane-like** structures with 3 **manganese**, 4 **oxygen** and a **calcium** linked to a fourth manganese.[1] Oxidation of water leaves 2 H^+ on the lumenal side of the membrane, helping to establish the proton gradient essential for ATP synthesis in the CF_1CF_0-ATP sythase protein. [edit]



reduced plastoqu

References [edit]

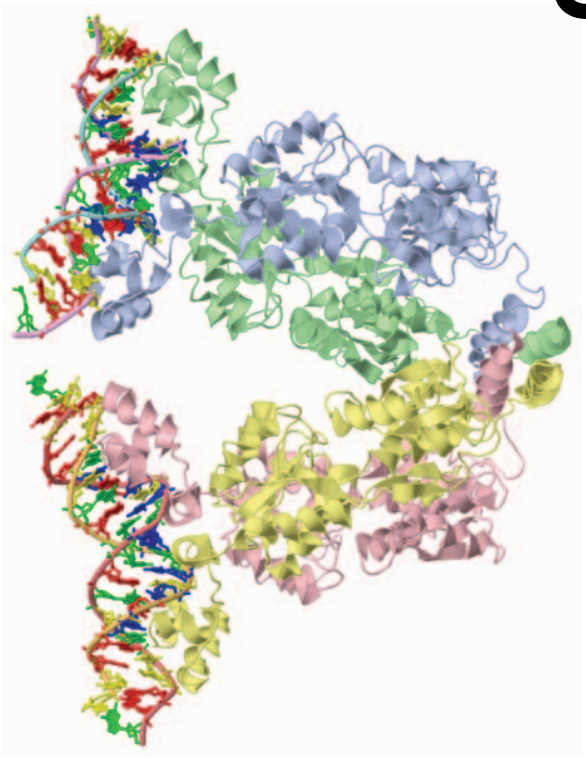
1. ↑ Ferreira, K.N., Iverson, T.M., Maghlaoui, K., Barber, J., Iwata, S. "Architecture of the photosynthetic oxygen-evolving center." Science, March 19, 2004, 303 (5665), 1831-8. PMID:14764885

2. Garrett, R.H., Grisham, C.M. *Biochemistry, 3rd Edition.* Belmont, CA: Thomson Brooks/ Cole, 2005.

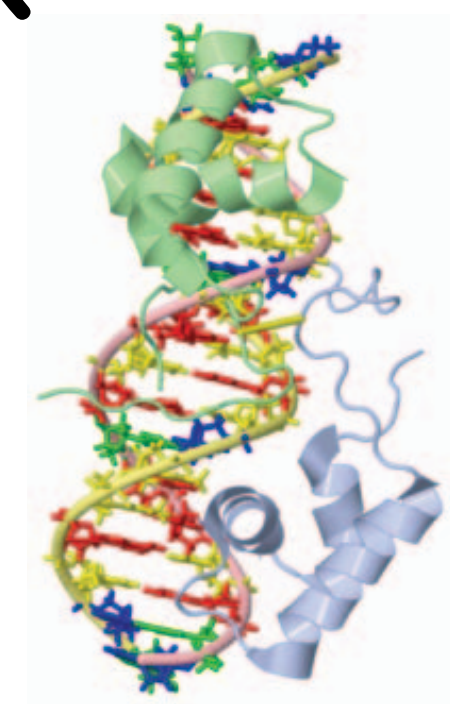
Contributors

Emily Forschler, Eran Hodis, Jaime Prilusky

Lac repressor/DNA complex



PDB-ID 1lbg
Crystal structure of the lactose operon repressor & its complexes with **cognate DNA**
Lewis *et al* & Lu *Science* (1996) **271**, 1247



PDB-ID 1osl
Solution structure of dimeric lactose DNA-binding domain complexed to a **nonspecific DNA seq**
Kalodimos *et al* & Kaptein *Science* (2004) **305**, 38

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Lac repressor

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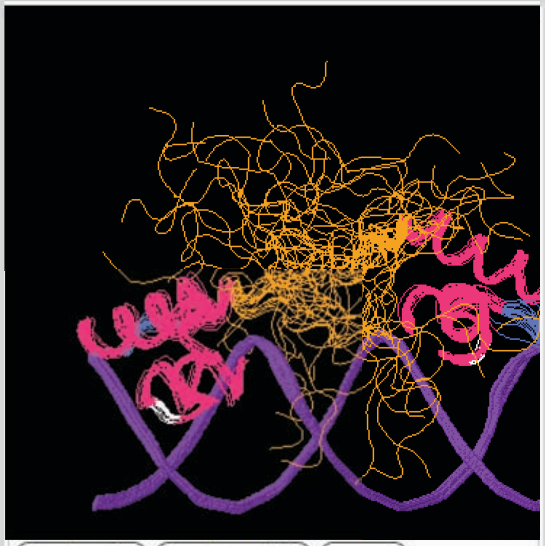

Morph of the lac repressor bending DNA as binding changes from non-specific to specific recognition of the operator sequence. Details Below.

What is the lac repressor? [edit]

Repressors are proteins that inhibit the expression of genes; that is, they inhibit the transcription of messenger RNA from their target genes. Each repressor targets a specific co-regulated group of genes by recognizing a specific sequence of DNA, called the *operator* in bacteria. Repressor proteins are coded for by *regulatory* genes.

Lewis *C.R. Biol* (2005) **328**, 521 [**X-ray**]
Kalodimos *et al* & Kaptein *Science* 2004, **305**, 386-9 [**NMR**]

Diseases & Drugs

David Canner

Pharmaceutical Drugs - Proteopedia, life in 3D

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Pharmaceutical Drugs

The Pharmaceutical industry is one of the world's largest industries, grossing well over $300 billion in the United States alone. Understanding how the drugs the pharma industry develops work and different characteristics of these compounds is important to nearly everyone as 50% of the US population takes at least one prescription medication regularly and nearly everyone takes a pharmaceutical pill at some point in their life.[1] The following is a growing list of pharmaceutical compounds organized by disorder.

AstraZeneca's Nexium

See Pharmaceutical Drug Targets for a list of drug targets organized by disease.

The majority of all modern medicinal drugs target members of the superfamily of proteins called the G protein-coupled receptors or GPCRs[2][3].

Treatments

The following is a list of pharmaceutical treatments for various diseases, organized by disorder. Each entry highlights general information about the therapeutic, pharmacokinetic data comparisons within its drug class, and a structural analysis explaining how the drug compound functions *in vivo*.

Alzheimer's Disease

Acetylcholinesterase Inhibitors
- Aricept - Generic: Donepezil
- Cognex - Generic: Tacrine
- Exelon - Generic: Rivastigmine
- Razadyne - Generic: Galantamine

Bacterial Infection

Macrolide Antibiotics
- Biaxin: - Generic: Clarithromycin
- Dynabac - Generic: Dirithromycin
- Ketek - Generic: Telithromycin
- Llosone - Generic: Erythromycin
- Rulide - Generic: Roxithromycin
- Zithromax - Generic: Azithromycin

Cancer

Anti-CD20 Monoclonal Antibody
- Arzerra - Generic: Ofatumumab
- Rituxan - Generic: Rituximab

B-Raf Kinase Inhibitor
- Zelboraf - Generic: Vemurafenib (Formerly: PLX-4032)

Chemotherapy
- Platinol - Generic: Cisplatin

Depression

Serotonin Transporter Inhibitors

Tricyclic Antidepressants
- Anafranil - Generic: Chlomipramine

Selective Serotonin Reuptake Inhibitors
- Prozac - Generic: Fluoxetine
- Xoloft - Generic: Sertraline

Diabetes

Dipeptidyl Peptidase-4 Inhibitor
- Galvus - Generic: Vildagliptin
- Januvia - Generic: Sitagliptin
- Onglyza - Generic: Saxagliptin

Peroxisome Proliferator-Activated Receptor Agonist
- Actos - Generic: Pioglitazone

Erectile Dysfunction

Phosphodiesterase Type 5 Inhibitor
- Cialis - Generic: Tadalafil
- Levitra - Generic: Vardenafil
- Viagra - Generic: Sildenafil

Looks like only a real ***Geek*** could do it(!)

Adding molecular scenes is easy!

1ACJ* shows the crystal structure of *Torpedo californica* acetylcholinesterase (TcAChE) complexed with tacrine.

Tacrine was the first cholinesterase inhibitor approved for the treatment of **Alzheimer's disease**.

Tacrine's ringed structure is stacked between the aromatic rings of Trp84 and Phe330.

---

*Harel *et al* Silman & Sussman (1993) "Quaternary ligand binding to aromatic residues in the active-site gorge of acetylcholinesterase" *PNAS*, **90**, 9031-5.

http://proteopedia.org/w/Sandbox_780

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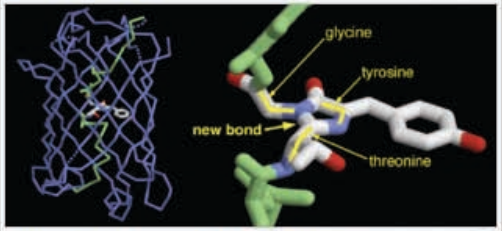
Sandbox 780

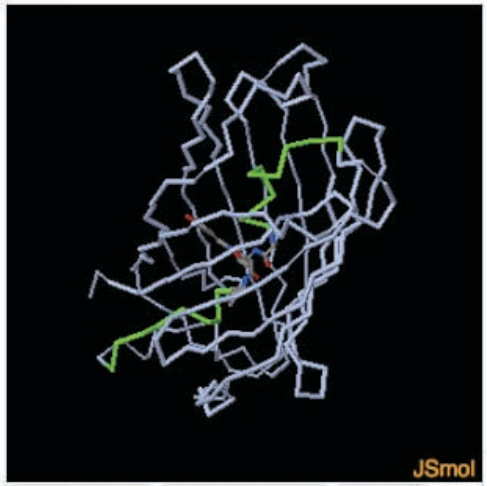
Example page for Green fluorescent protein (**GFP**) [edit]



Green fluorescent protein (1ema)

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish Aequorea victoria (PDB entry 1ema), fluorsceses green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure



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GFP (PDB entry 1ema)

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the

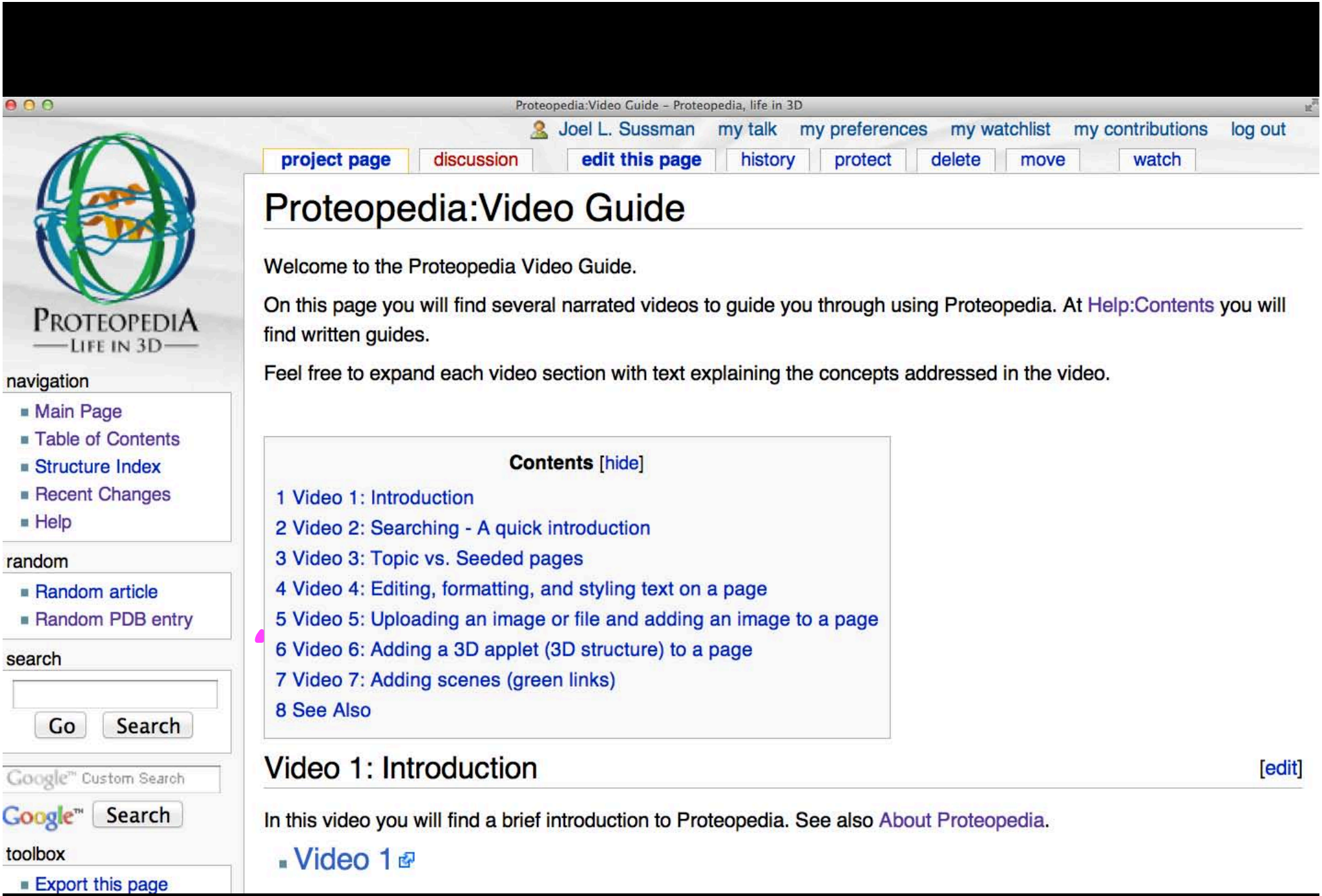
References [edit]

1. ↑ Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the Aequorea victoria green fluorescent protein. Science. 1996 Sep 6;273(5280):1392-5. PMID:8703075

Quiz

1. How many alpha helices are in this structur
   - One
   - None

Page you can make in ~10 min, see lecture notes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3 Video 3: Topic vs. Seeded pages
4 Video 4: Editing, formatting, and styling text on a page
5 Video 5: Uploading an image or file and adding an image to a page
6 Video 6: Adding a 3D applet (3D structure) to a page
7 Video 7: Adding scenes (green links)
8 See Also
Video 1: Introduction [edit]
In this video you will find a brief introduction to Proteopedia. See also About Proteopedia.
Video 1

www.proteopedia.org

- English is the *official* language of *Proteopedia*, however, some pages are also being translated into other languages.

http://proteopedia.org/w/1vot_(Chinese)

Dr. Yechun Xu

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Aricept

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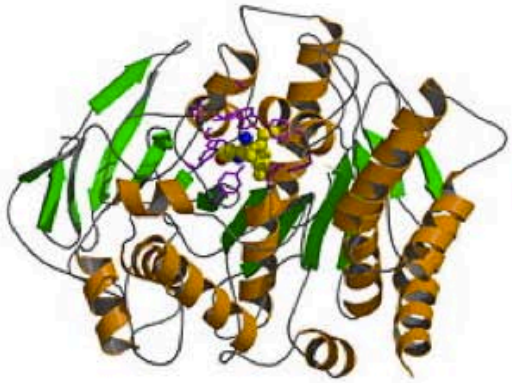

石杉碱甲与乙酰胆碱酯酶复合物的三维结构

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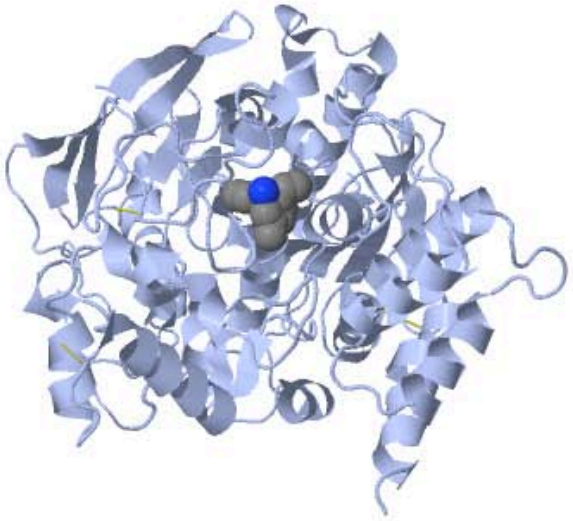
3 关于此结构
4 参考文献

背景介绍 [edit]

中国科研工作者在20世纪80年代从**中药**[1]千层塔中分离得到天然产物**石杉碱甲**被证实是乙酰胆碱酯酶的可逆抑制剂，对该酶具有特定、高效的抑制活性。早在1000多年前，中国人已将千层塔用于擦伤、疲惫、肿胀、精神分裂症以及重症肌无力等疾病的治疗。从1996年开始，药品名为双益平[2]的石杉碱甲已在中国广泛用于早老年痴呆症的治疗。与美国食品药品管理局（FDA）批准的目前用于老年痴呆症治疗的多奈哌齐（Donepezil，商品名Aricept）、利伐司替明（Rivastigmine，商品名Exelon）和加兰他敏（Galanthamine，商品名Reminyl）三个药相比，石杉碱甲具有能更好渗透血脑屏障、生物口服利用度更高和对乙酰胆碱酯酶抑制时效更长的特点。



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Sites:	AC1 and ACT
Ligands:	HUP
Activity:	Acetylcholinesterase, with EC number 3.1.1.7
Structural annotation:	[show]
Functional annotation:	[show]
Evolutionary conservation:	
Resources:	FirstGlance, OCA, PDBsum, RCSB

http://proteopedia.org/w/1eve_(Arabic)

Muneef Ayyash

1eve (Arabic) - Proteopedia, life in 3D

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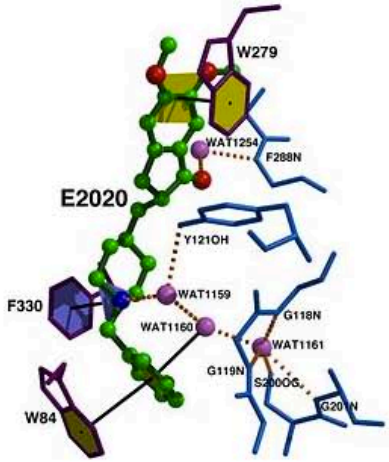

الشكل المركب الثلاثي الأبعاد للدواء المضاد للأزهايمر Aricept مرتبط مع acetylcholinesterase (أنظر أيضا AChE bivalent inhibitors (Part II))

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1eve, resolution 2.50Å (default scene)

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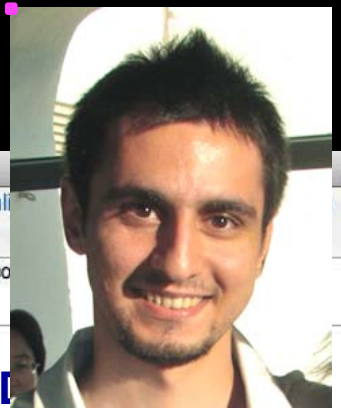
Functional annotation:	[show]
Evolutionary conservation:	

مقدمة [edit]

هنالك عدة مثبطات للكولين إما يجري استخدامها للعلاج من أعراض مرض الزهايمر أو هي في تجارب سريرية متقدمة. الدواء **E2020** ويسوق بإسم **Aricept** هو عضو في عائلة كبيرة من N-benzylpiperidine مثبطات أستيلكولينستراز (AChE)، الذي تم تركيبه وتطويره وتقييمه من قبل شركة ايساي في اليابان. وقد صممت هذه المثبطات على أساس دراسات QSAR قبل الكشف عن الشكل الثلاثي الأبعاد لمثبط أستيلكولينستراز "Torpedo californica (1ea5 AChE "TcAChE . ويعزز دواء ال Aricept إلى حد كبير في أداء حيوانات مخبرية تعاني من قصور وظيفي مرتبط بالكولين ولهذا الدواء قابلية عالية للربط مع الأستيلكولينستراز لكل من الانقليس الكهربائي والفأر في نطاق ضئيل "nanomolar".

http://proteopedia.org/w/1eve_(Turkish)



Samet Serdar Yildirim

1eve (Turkish) – Proteopedia, life in 3D

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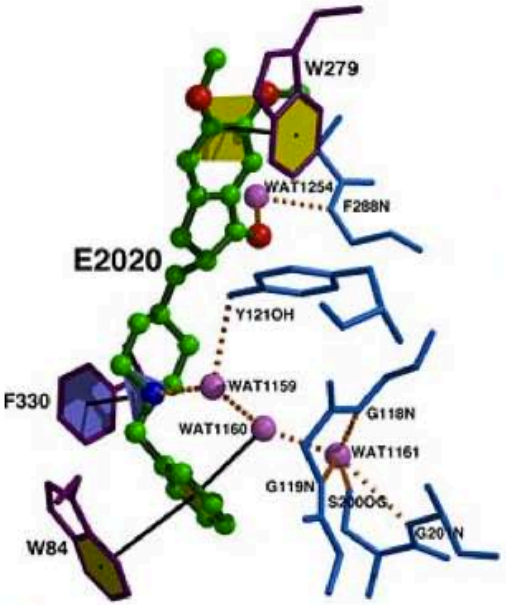

Asetilkolinesteraz ile kompleks oluşturan, anti-Alzheimer ilacı, Aricept'in 3 boyutlu yapısı (Ayrıca bakınız: AChE bivalent inhibitors (Part II))

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Önbilgi [edit]

Bazı kolinesteraz inhibitörleri, Alzheimer hastalığının semptomik tedavisinde veya ileri klinik çalışmalarda kullanılmaktadır. **Aricept** olarak pazarlanan, N-benzilpiperidin tabanlı asetilkolinesteraz (AChE) inhibitörleri ailesinin bir üyesi olan **E2020**, Japonya'da bulunan Eisai şirketi tarafından geliştirilmekte, sentezlenmekte ve değerlendirilmektedir. Bu inhibitörler, *Torpedo californica* AChE (*Tc*AChE) (1ea5) 'nin 3 boyutlu yapısının izahından önce, QSAR çalışmaları temel alınarak dizayn edilmiştir. Bu inhibitör hayvan modellerinde kolinerjik hipofonksiyonun performansını anlamlı şekilde artırmaktadır ve AChE için yüksek afiniteye sahiptir; nanomolar düzeyde, elektrik yılan balığı ve fare AChElerinin her ikisine bağlanmaktadır.

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Ligands:	**E20, NAG**
Activity:	Acetylcholinesterase, with EC number 3.1.1.7
Structural annotation:	[show]
Functional annotation:	
Evolutionary conservation:	[show]

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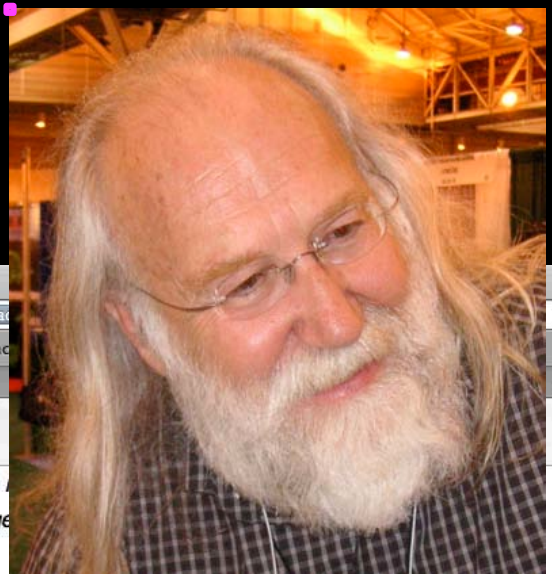
How can **high school** students contribute something **useful**?



Tim Herman

Group:SMART:Teams – Proteopedia, life in 3D

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Group:SMART:Teams

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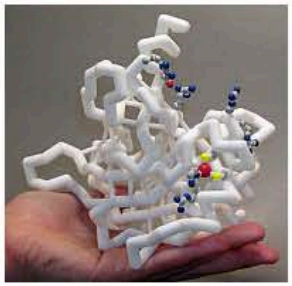
Overview of the Program



What do you get when you combine enthusiastic high school teachers and their students, scientists excited about their research, and Rapid Prototyping technology? SMART (Students Modeling A Research Topic) Teams! In this multi-faceted program, students develop teamwork as they delve into the molecular world, explore science as a process and not just a collection of facts, and work closely with a researcher to understand and model the structure-function relationship of a protein the researcher studies. After designing and building a model of the protein using Rapid Prototyping technology, SMART teams create an oral presentation explaining their work to a lay audience and a poster which is presented to a scientific audience.

SMART Teams consist of a teacher who has participated in the Center for BioMolecular Modeling's summer course, Modeling the Molecular World, Part I (or its predecessor, Genes, Schemes and Molecular Machines), students, and a research mentor.

Qualification, Research, and Presentation Phases

Teams work to complete the three phases of the program:

Group:SMART:A Physical Model of the β2-Adrenergic Receptor - Proteopedia, life in 3D

http://www.proteopedia.org/w/Group:SMART:A_Physical_Model_of_the_β2-Adrenergic_Receptor

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Group:SMART:A Physical Model of the β2-Adrenergic Receptor

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A SMART Team Mole

ison West High School 2008 SMART

ong, Esther Yoon, Xiao Zhu:

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Center for BioMolecular Modeling

NYC high school students publish paper on their *Proteopedia* page

Multimedia in Biochemistry and Molecular Biology Education

Acetylcholinesterase: Substrate Traffic and Inhibition

Received for publication, January 9, 2012; accepted 1 February 2012

Mary Acheampong,‡ Daviana Dueño,‡ Bobby Glover,‡ Alafia Henry,‡ Randol Mata,‡ Marisa VanBrakle,‡ Lars Westblade,§ Joel Sussman,¶ and Allison Granberry‡*

From the ‡Hostos-Lincoln Academy, Bronx, New York, §Touro College of Pharmacy, New York, ¶Department of Structural Biology, The Weizmann Institute of Science, Rehovot 76100 Israe

In 1991, the laboratory of Joel L. Sussman and Israel Silman determined the 3D structure of the enzyme acetylcholinesterase (AChE) isolated from the Pacific electric ray (*Torpedo californica*). Later, in 1995, the structure of AChE in complex with the snake toxin fasciculin-II (FAS-II) was solved by Sussman, Silman, Bourne, Taylor, and Marchot. This *Proteopedia* page, (http://www.proteopedia.org/w/Acetylcholinesterase:_Substrate_Traffic_and_Inhibition) with the use of two physical models, compares the structure of the AChE/acetylcholine (ACh) complex to illustrate the process of ACh hydrolysis; which we term the substrate traffic story, and the structure of the AChE/FAS-II complex to illustrate the process of AChE inhibition by FAS-II; which we refer to as the inhibition story. Visitors to this page may view video clips of these physical models, demonstrating the substrate traffic story and the inhibition story as well as comparative computer models of how the physical models were designed.

AChE, embedded in the postsynaptic membrane, is essential for termination of the nerve impulse at the cholinergic synapse. Unlike other enzymes that have active

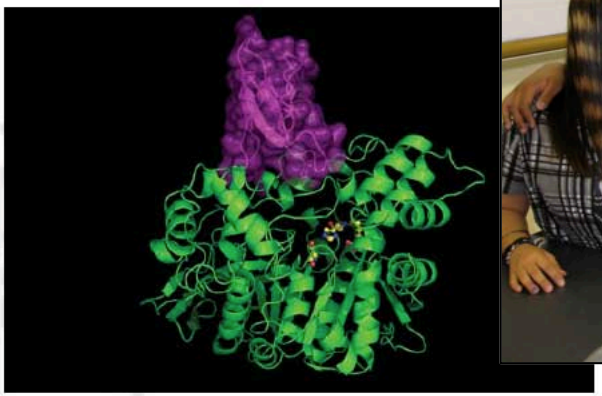

FIG. 1. **Structure of the AChE/FAS-II complex.** AChE is colored green and is shown as a ribbon diagram, whereas FAS-II is colored magenta and is shown as a ribbon diagram with the molecular surface highlighted. Residues that form the AChE active site: serine at position 200, glutamic acid at position 327 and histidine at position 440, are shown in ball and stick format (carbon atoms, yellow; nitrogen atoms, blue; oxygen atoms, red).

Acheampong *et al* Sussman & Granberry *BAMBED* (2012) **40**, 144

Allison Granberry

SMART Team @Hostos-Lincoln Academy guided by Ms. Allison Granberry

More than just pretty pictures

EMBO Member Joel L. Sussman makes students love structural biology

Used for teaching biology in high-school classrooms around the world; applied as an interactive three-dimensional article supplement in a journal of chemistry; and, most recently, elected as the best web-based multimedia tool by *The Scientist*. *Proteopedia* (www.proteopedia.org) is the first free, collaborative three-dimensional online encyclopedia of molecules – and yet another example of how scientists bring science to the public. "This website gives students and other users a chance to view protein structures, which turn out to be extraordinarily appealing to them," explains project initiator and EMBO Member *Joel L. Sussman* from the Weizmann Institute of Science in Israel, who co-develo the tool with *Jaime Prilusky & Eran H* also at the Weizmann.

Bobby Glover - National Scholar for Coca-Cola

The visual effects are amazing: Upon c ing on one of the green links attached page in *Proteopedia*, a multicoloured pic appears which can then be rotated by sir pulling the computer mouse – as if the were holding the model in his own hands. *Proteopedia* is more than just pretty pictu It helps identify the features of molecul explains Sussman. Even senior researc appreciate how their own research find are visualized on the website.

Earlier this year, his team visite high-school classroom at the Ho Lincoln Academy in South Bronx, New Y "The students were crazy about it," re Sussman. Their teacher also found it us develop- . To make pages in Russian, es of the

Marisa VanBrakle Gates Millennium Scholarship

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- as media for Final Projects/Thesis
- as driving topic for Student's Clubs

Researchers:
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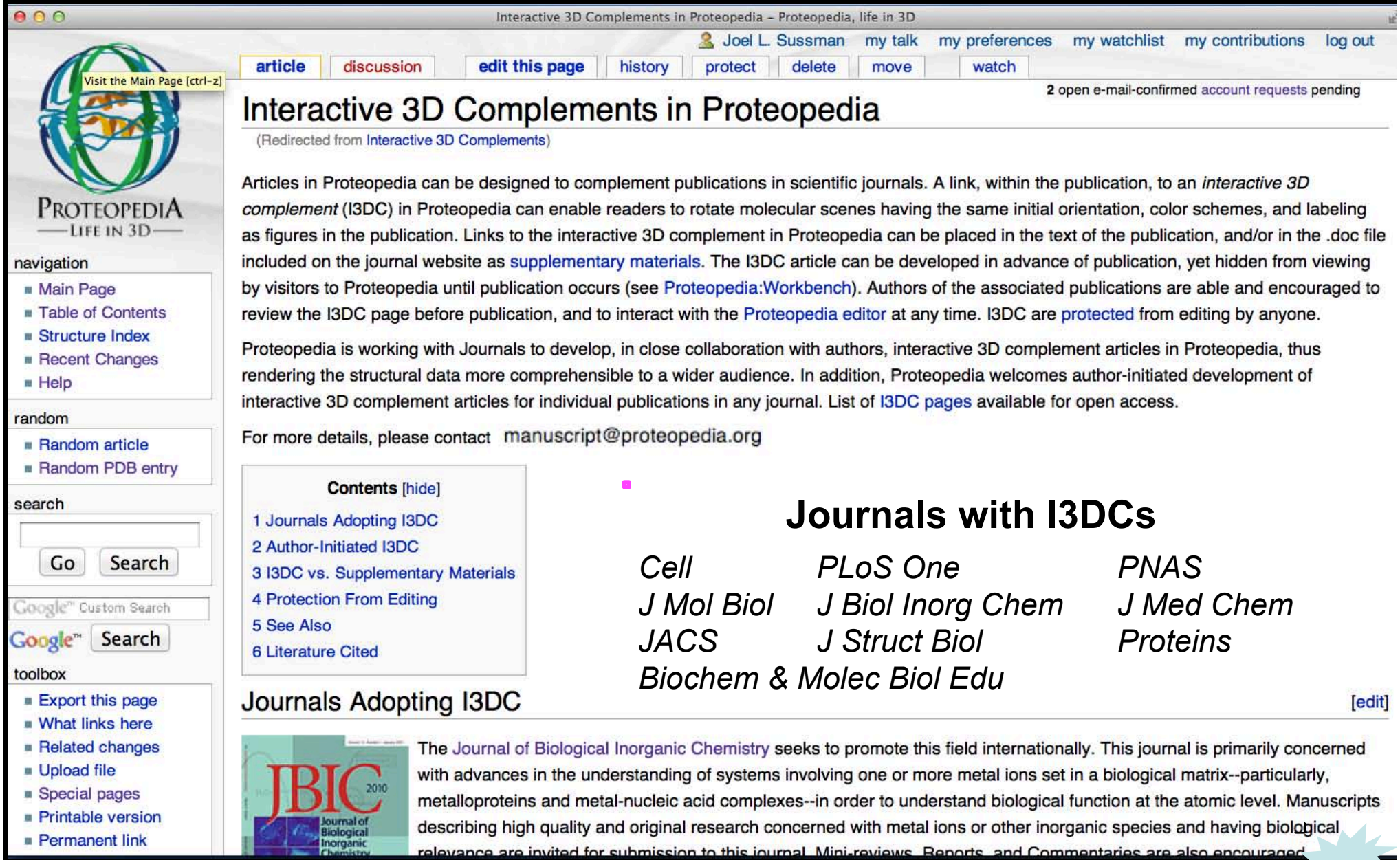
- as a shared secure shared collaboration site

Journals:
- as an Interactive 3D Complement (I3DC)

Interactive 3D Complements (I3DCs)



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2) Creating 3D figures for publications
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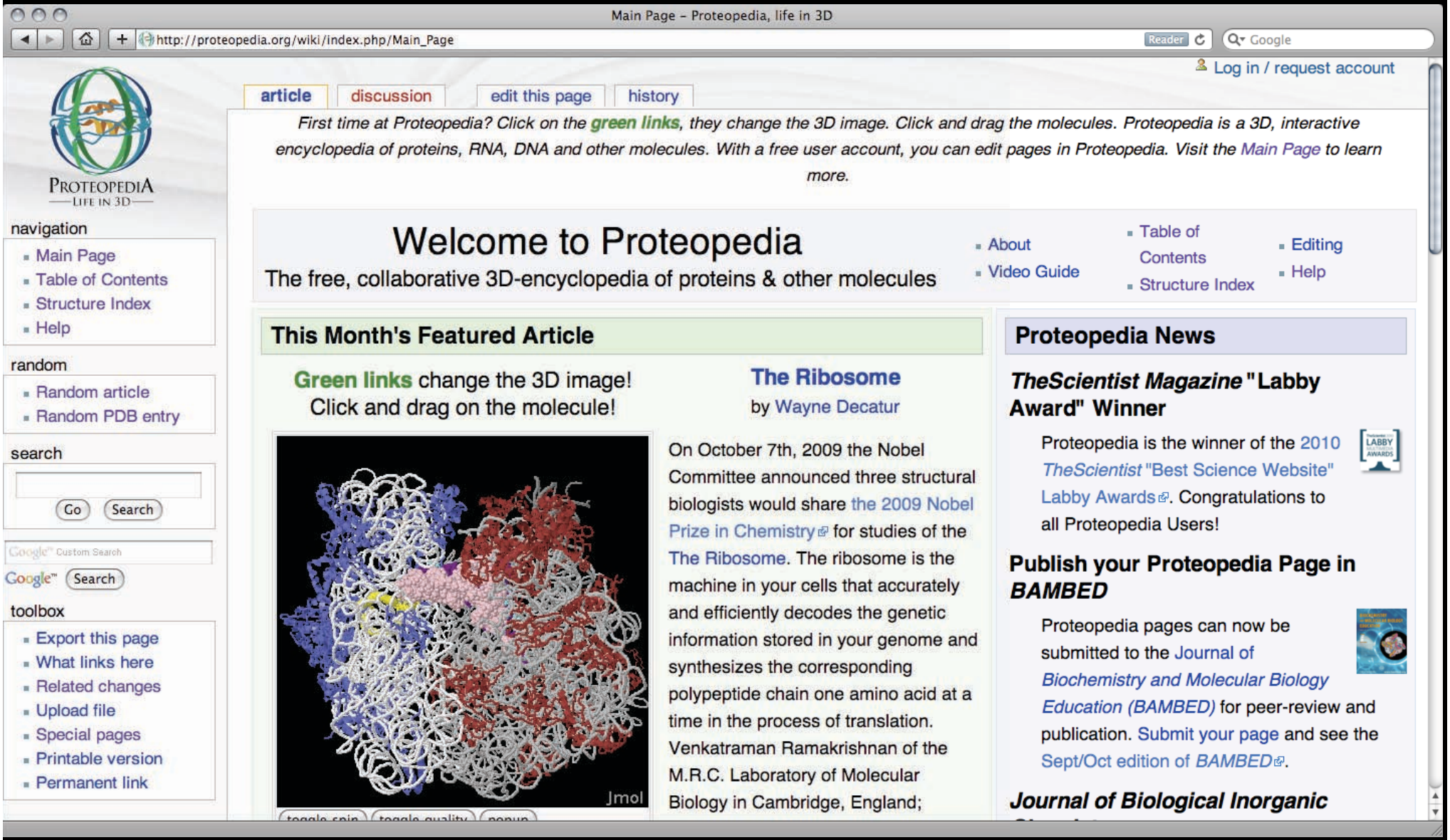
http://proteopedia.org



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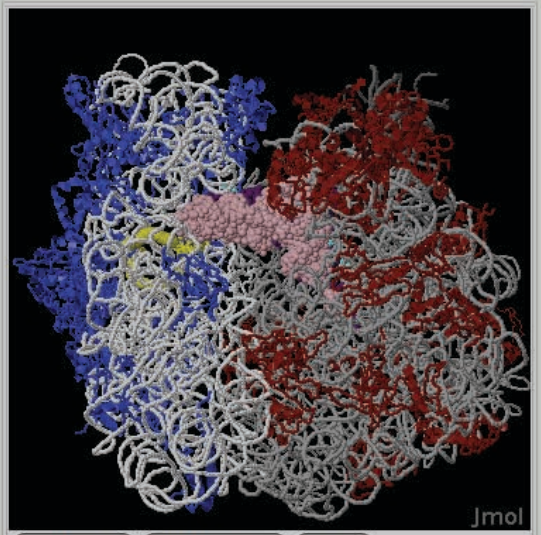

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The Ribosome
by Wayne Decatur

On October 7th, 2009 the Nobel Committee announced three structural biologists would share the 2009 Nobel Prize in Chemistry for studies of the The Ribosome. The ribosome is the machine in your cells that accurately and efficiently decodes the genetic information stored in your genome and synthesizes the corresponding polypeptide chain one amino acid at a time in the process of translation. Venkatraman Ramakrishnan of the M.R.C. Laboratory of Molecular Biology in Cambridge, England;

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Journal of Biological Inorganic

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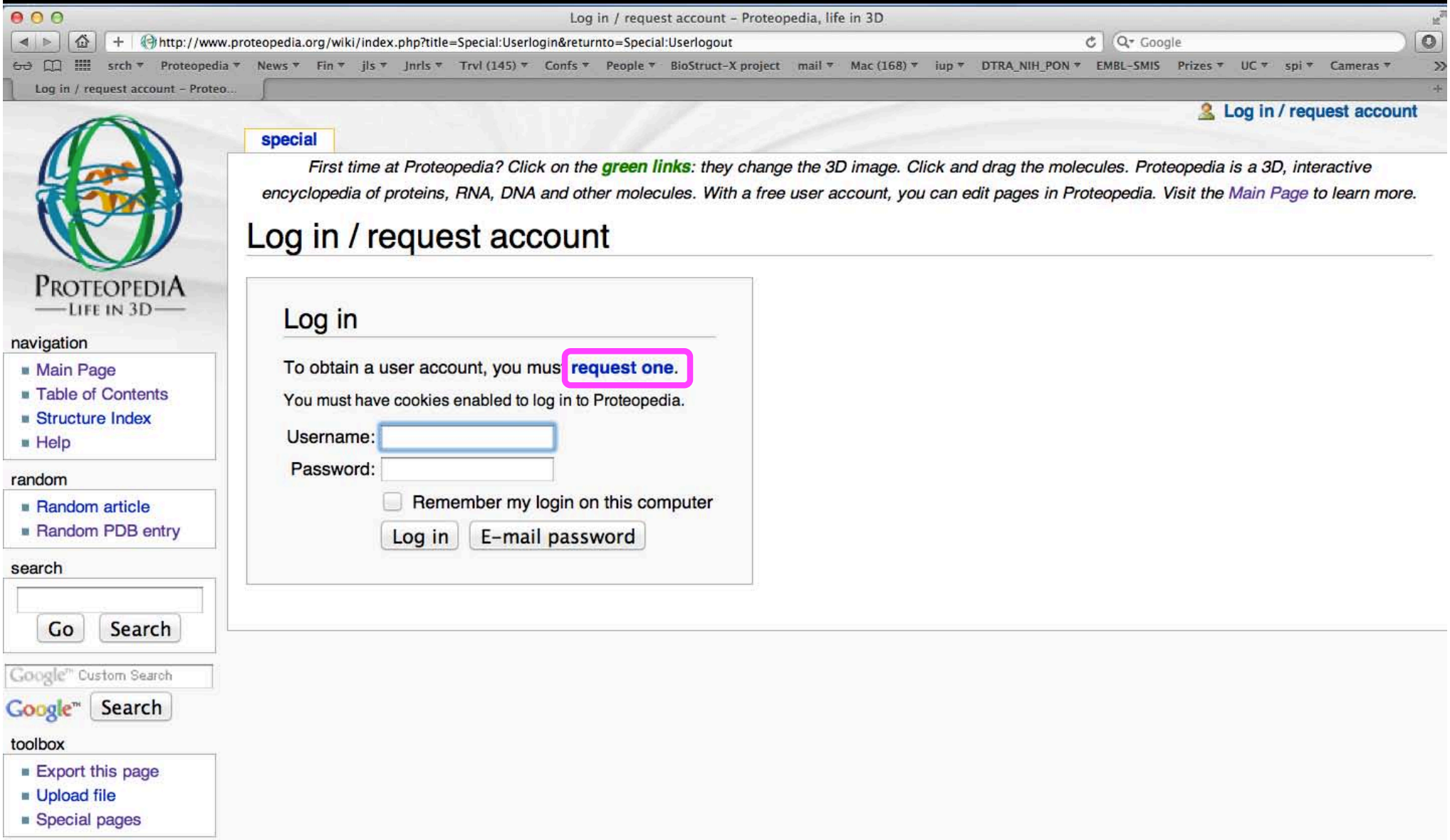

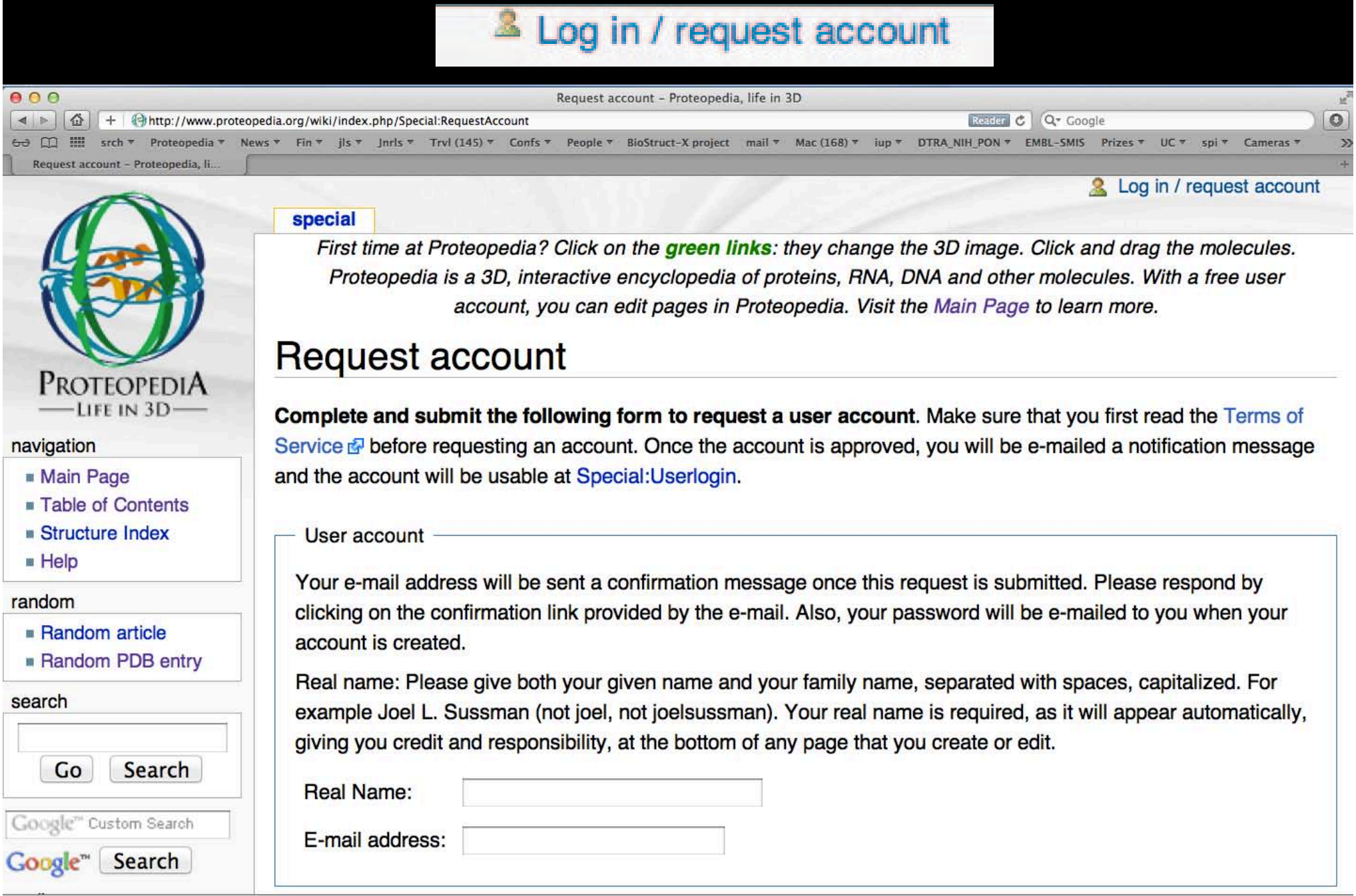
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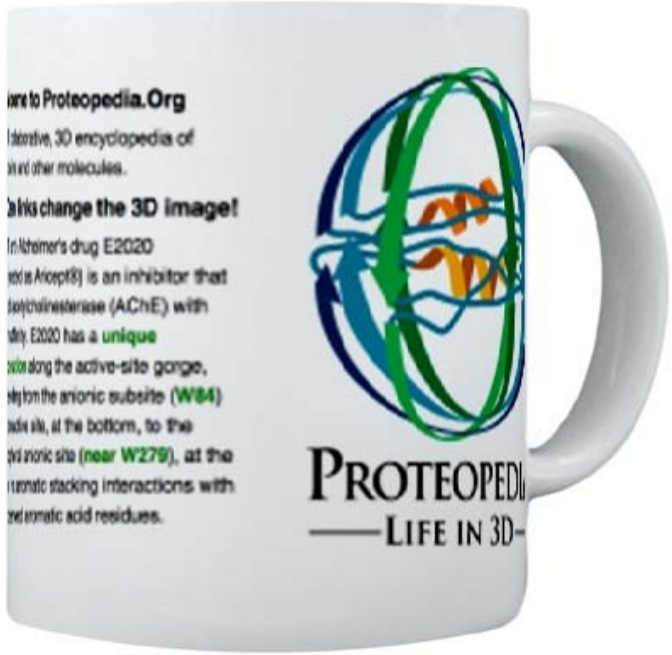


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