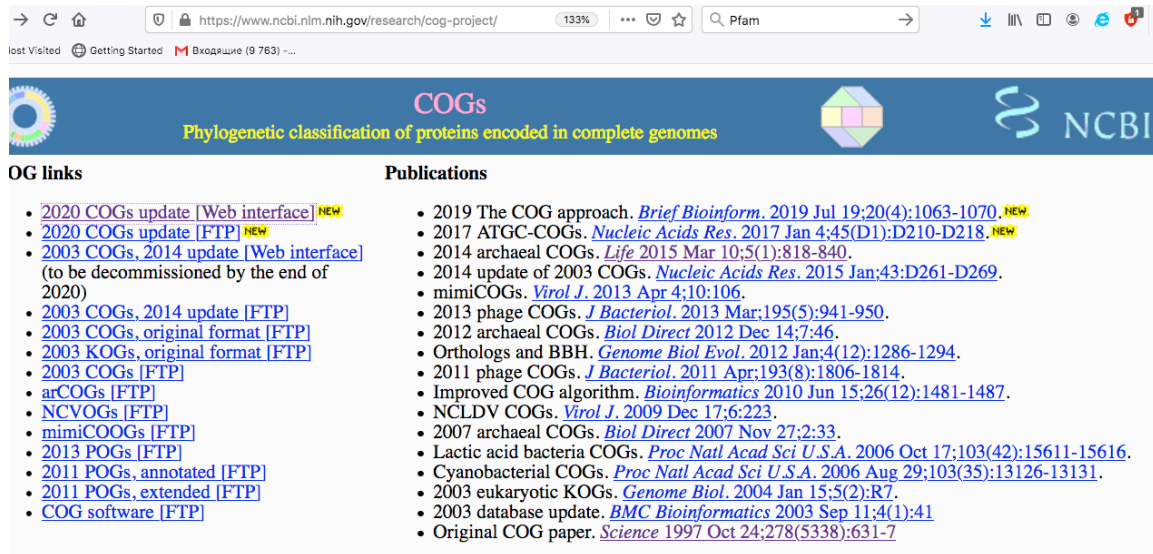


**Семинар 10.** Знакомство с базами данных ортологов и знакомство с 3-х мерной структурой белков по базе данных PDB.

## Базы данных ортологов

### COG database

<https://www.ncbi.nlm.nih.gov/research/cog-project/>



**OG links**

- [2020 COGs update \[Web interface\]](#) **NEW**
- [2020 COGs update \[FTP\]](#) **NEW**
- [2003 COGs, 2014 update \[Web interface\]](#) (to be decommissioned by the end of 2020)
- [2003 COGs, 2014 update \[FTP\]](#)
- [2003 COGs, original format \[FTP\]](#)
- [2003 KOGs, original format \[FTP\]](#)
- [2003 COGs \[FTP\]](#)
- [arCOGs \[FTP\]](#)
- [NCVOGs \[FTP\]](#)
- [mimiCOGs \[FTP\]](#)
- [2013 POGs \[FTP\]](#)
- [2011 POGs, annotated \[FTP\]](#)
- [2011 POGs, extended \[FTP\]](#)
- [COG software \[FTP\]](#)

**Publications**

- 2019 The COG approach. *Brief Bioinform.* 2019 Jul 19;20(4):1063-1070. **NEW**
- 2017 ATGC-COGs. *Nucleic Acids Res.* 2017 Jan 4;45(D1):D210-D218. **NEW**
- 2014 archaeal COGs. *Life* 2015 Mar 10;5(1):818-840.
- 2014 update of 2003 COGs. *Nucleic Acids Res.* 2015 Jan;43:D261-D269.
- mimiCOGs. *Virol J.* 2013 Apr 4;10:106.
- 2013 phage COGs. *J Bacteriol.* 2013 Mar;195(5):941-950.
- 2012 archaeal COGs. *Biol Direct* 2012 Dec 14;7:46.
- Orthologs and BBH. *Genome Biol Evol.* 2012 Jan;4(12):1286-1294.
- 2011 phage COGs. *J Bacteriol.* 2011 Apr;193(8):1806-1814.
- Improved COG algorithm. *Bioinformatics* 2010 Jun 15;26(12):1481-1487.
- NCLDV COGs. *Virol J.* 2009 Dec 17;6:223.
- 2007 archaeal COGs. *Biol Direct* 2007 Nov 27;2:33.
- Lactic acid bacteria COGs. *Proc Natl Acad Sci U.S.A.* 2006 Oct 17;103(42):15611-15616.
- Cyanobacterial COGs. *Proc Natl Acad Sci U.S.A.* 2006 Aug 29;103(35):13126-13131.
- 2003 eukaryotic KOGs. *Genome Biol.* 2004 Jan 15;5(2):R7.
- 2003 database update. *BMC Bioinformatics* 2003 Sep 11;4(1):41
- Original COG paper. *Science* 1997 Oct 24;278(5338):631-7

Идем на [2020 COGs update \[Web interface\]](#)

<https://www.ncbi.nlm.nih.gov/research/cog>

Ищем печатную денежную машинку «ATP synthase»

Разбираемся в представленности в разных видах и пробуем скачать какое-нибудь семейство –

## Results

12 COG definitions

2 pathways

### COGs

[Download](#)

Organism	Protein	COG	Cat	Annotation
1106	1196	<a href="#">COG0055</a>	C	FoF1-type ATP synthase, beta subunit
1106	1194	<a href="#">COG0056</a>	C	FoF1-type ATP synthase, alpha subunit
1109	1200	<a href="#">COG0224</a>	C	FoF1-type ATP synthase, gamma subunit
1109	1216	<a href="#">COG0355</a>	C	FoF1-type ATP synthase, epsilon subunit
1107	1203	<a href="#">COG0356</a>	C	FoF1-type ATP synthase, membrane subunit a
1048	1172	<a href="#">COG0636</a>	C	FoF1-type ATP synthase, membrane subunit c/Archaeal/vacuolar-type H <sup>+</sup> -ATPase, subunit K
1103	1471	<a href="#">COG0711</a>	C	FoF1-type ATP synthase, membrane subunit b or b'
1095	1118	<a href="#">COG0712</a>	C	FoF1-type ATP synthase, delta subunit
157	156	<a href="#">COG3312</a>	C	FoF1-type ATP synthase accessory protein AtpI
278	279	<a href="#">COG5336</a>	C	FoF1-type ATP synthase AtpZ/Atp1/AtpQ subunit, putative Ca <sup>2+</sup> /Mg <sup>2+</sup> transporter
140	140	<a href="#">COG5387</a>	O	Mitochondrial FoF1-type ATP synthase assembly chaperone ATP12
38	38	<a href="#">COG5756</a>	C	FoF1-type ATP synthase subunit Atp1, cyanobacterial family

## Protein family database

<https://pfam.xfam.org/>

[HOME](#) | [SEARCH](#) | [BROWSE](#) | [FTP](#) | [HELP](#) | [ABOUT](#)

### Pfam 33.1 (May 2020, 18259 entries)

The Pfam database is a large collection of protein families, each represented by **multiple sequence alignments** and **hidden Markov models (HMMs)**. [More...](#)

#### QUICK LINKS

[SEQUENCE SEARCH](#)

[VIEW A PFAM ENTRY](#)

[VIEW A CLAN](#)

[VIEW A SEQUENCE](#)

[VIEW A STRUCTURE](#)

[KEYWORD SEARCH](#)

[JUMP TO](#)

#### YOU CAN FIND DATA IN PFAM IN VARIOUS WAYS...

Analyze your protein sequence for Pfam matches

View Pfam annotation and alignments

See groups of related entries

Look at the domain organisation of a protein sequence

Find the domains on a PDB structure

Query Pfam by keywords

[Go](#)

[Example](#)

Enter any type of accession or ID to jump to the page for a Pfam entry or clan, UniProt sequence, PDB structure, etc.

Or view the [help](#) pages for more information

Ищем там “ATP synthase” – смотрим представленность видов.

## Quest for orthologs

# QUEST FOR ORTHOLOGS

**QfO 7 will take place in Frankfurt, Germany, on 2-4 August 2021. Stay tuned!**

## Welcome

This is the site of the Quest for Orthologs consortium. Proteins and functional modules are evolutionarily conserved even between distantly related species, and allow knowledge transfer between well-characterized model organisms and human. The underlying biological concept is called 'Orthology' and the identification of gene relationships is the basis for comparative studies.

More than 30 phylogenomic databases provide their analysis results to the scientific community. The content of these databases differs in many ways, such as the number of species, taxonomic range, sampling density, and applied methodology. What is more, phylogenomic databases differ in their concepts, making a comparison difficult – for the benchmarking of analysis results as well as for the user community to select the most appropriate database for a particular experiment.

The Quest for Orthologs (QfO) is a joint effort to benchmark, improve and standardize orthology predictions through collaboration, the use of shared reference datasets, and evaluation of emerging new methods.

The main sections of this site are:

- [Meetings](#)
- [Community Standards](#) (Reference proteome, standardized formats, benchmarking, etc..)
- [Working groups](#)
- [Orthology databases](#)
- [Documents \(Intranet\)](#)
- [Mailing-List and Contact](#)

To contribute to this website, please create an account (see below) and [contact](#) us!

Смотрим, какие там базы данных, какие организмы представлены.

## База данных PDB

<https://www.rcsb.org/>

Смотрим, как последовательности превращаются в 3-х мерные структуры. Ищем структуры для известных белков – ATP synthase, DNA polymerase, RNA polymerase, tRNA synthase, ribosomal proteins, gyrases.

Welcome

Deposit

Search

Visualize

Analyze

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Learn

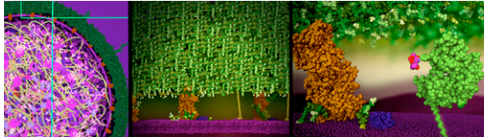
### A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

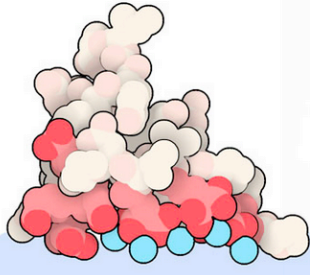
As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

**New Video: Penicillin and Antibiotic Resistance**



### April Molecule of the Month




Proteins and Biomaterials

Summary Gallery Compact -- Tabular Report -- ↓ Score

Download Selected Files Select All ☒

Displaying 1 to 4 of 4 Structures Page 1 of 1

Display 25 per page



3D View

## 5FIL

### Bovine mitochondrial ATP synthase state 3b

Zhou, A., Rohou, A., Schep, D.G., Bason, J.V., Montgomery, M.G., Walker, J.E., Grigorieff, N., Rubinstein, J.L.

(2015) Elife 4: e10180-e10180

<b>Released</b>	2015-10-14
<b>Method</b>	ELECTRON MICROSCOPY 7.1 Å
<b>Organisms</b>	<a href="#">Bos taurus</a>
<b>Macromolecule</b>	Unique protein chains: 11

Download File View File ☒

Обратить внимание, каким методом построена структура.

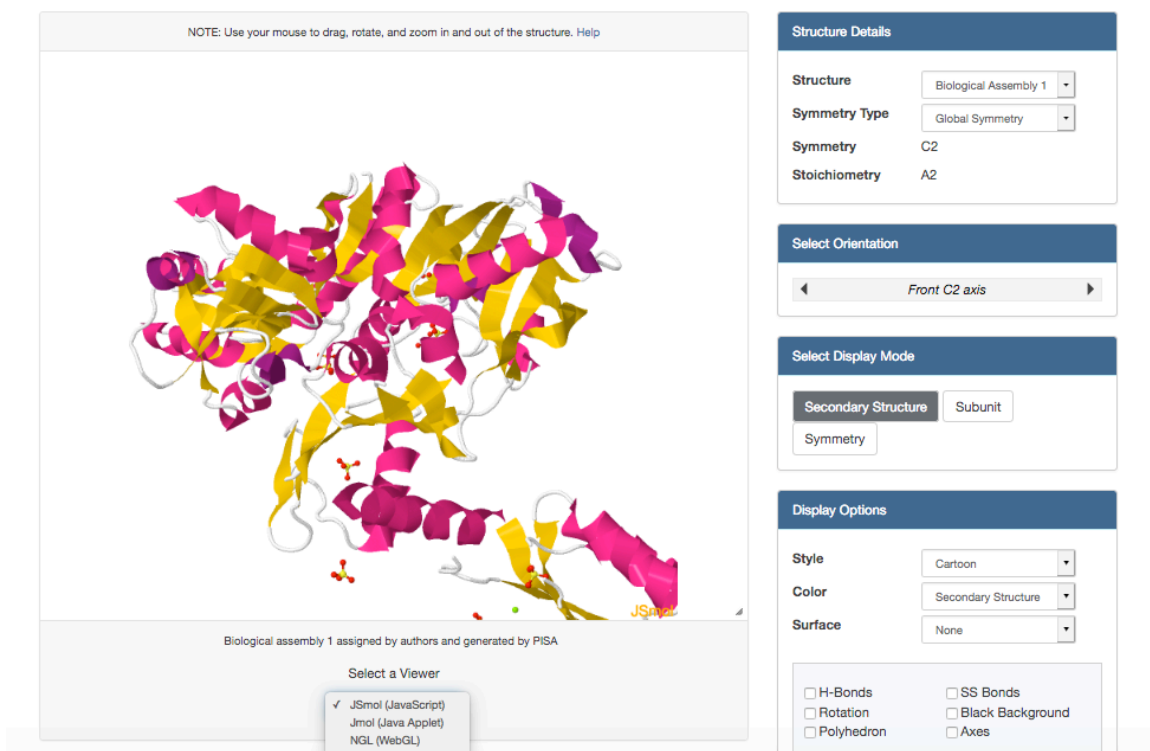
Поизучать разные отображения

Jmol/NGS (Jmol- более распространенная)

Style – Cartoon/Backbone/Space Fill

Color – Sequence/Hydrophobicity/By amino acid и т.д.

ATP PHOSPHORIBOSYLTRANSFERASE (ATP-PRTASE) FROM MYCOBACTERIUM TUBERCULOSIS



Обратить внимание на лиганды (небольшие молекулы, которые соединяются с белком). Есть, например, у 1NH7 ATP PHOSPHORIBOSYLTRANSFERASE (ATP-PRTASE) FROM MYCOBACTERIUM TUBERCULOSIS

Можно включить вращение – Rotation справа внизу.

В правом верхнем углу – Display Files, Download Files