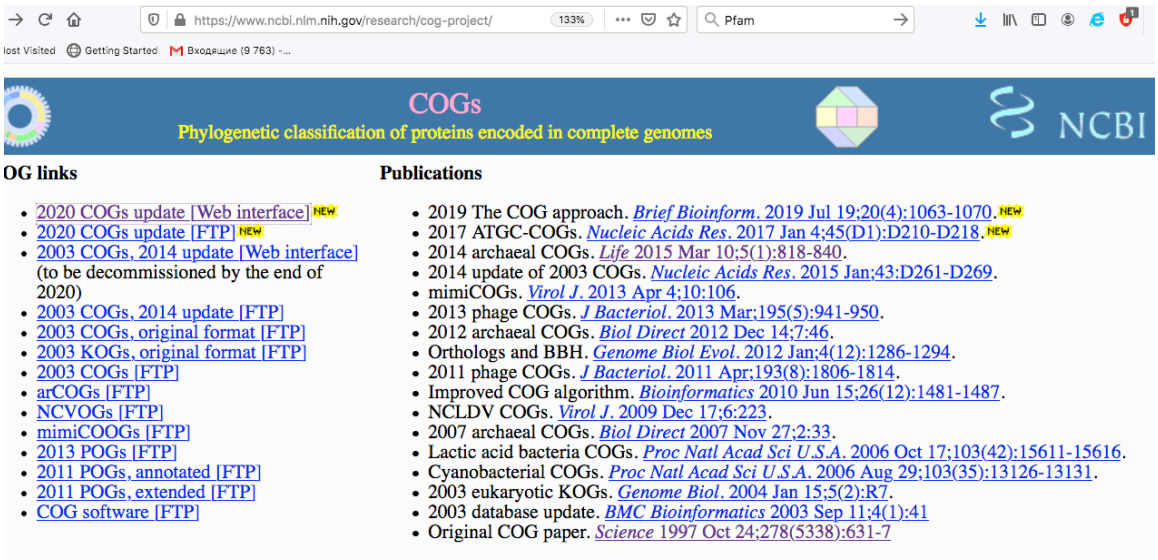
Семинар 10. Знакомство с базами данных ортологов и знакомство с 3-х мерной структурой белков по базе данных PDB.

Базы данных ортологов

COG database

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



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	COG0055	C	FoF1-type ATP synthase, beta subunit
1106	1194	COG0056	C	FoF1-type ATP synthase, alpha subunit
1109	1200	COG0224	C	FoF1-type ATP synthase, gamma subunit
1109	1216	COG0355	C	FoF1-type ATP synthase, epsilon subunit
1107	1203	COG0356	C	FoF1-type ATP synthase, membrane subunit a
1048	1172	COG0636	C	FoF1-type ATP synthase, membrane subunit c/Archaeal/vacuolar-type H+-ATPase, subunit K
1103	1471	COG0711	C	FoF1-type ATP synthase, membrane subunit b or b'
1095	1118	COG0712	C	FoF1-type ATP synthase, delta subunit
157	156	COG3312	C	FoF1-type ATP synthase accessory protein AtpI
278	279	COG5336	C	FoF1-type ATP synthase AtpZ/Atp1/AtpQ subunit, putative Ca2+/Mg2+ transporter
140	140	COG5387	O	Mitochondrial FoF1-type ATP synthase assembly chaperone ATP12
38	38	COG5756	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

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

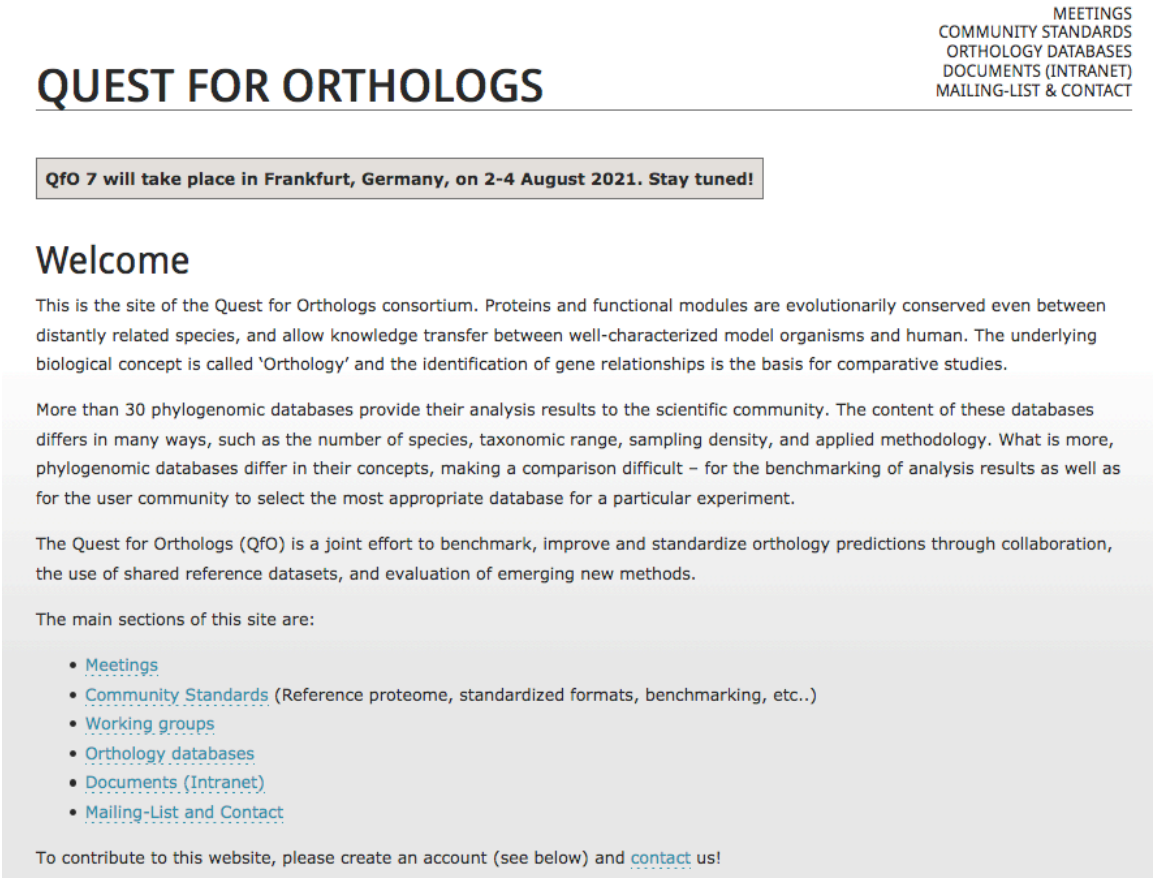
SEQUENCE SEARCH	Analyze your protein sequence for Pfam matches
VIEW A PFAM ENTRY	View Pfam annotation and alignments
VIEW A CLAN	See groups of related entries
VIEW A SEQUENCE	Look at the domain organisation of a protein sequence
VIEW A STRUCTURE	Find the domains on a PDB structure
KEYWORD SEARCH	Query Pfam by keywords
JUMP TO	enter any accession or ID 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

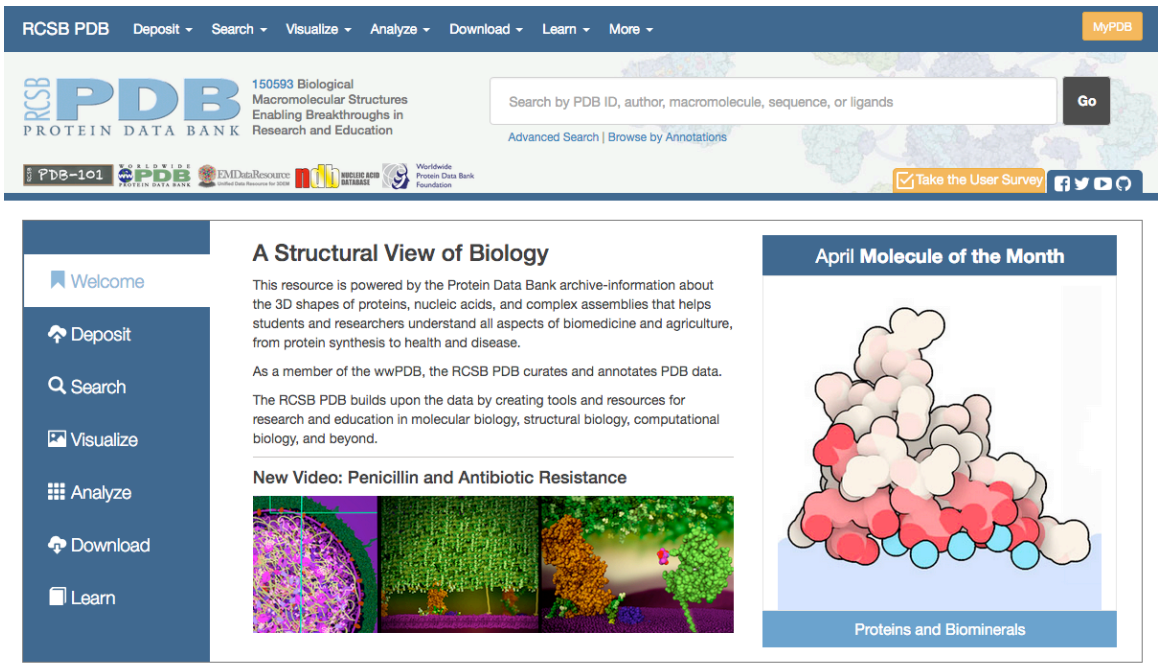


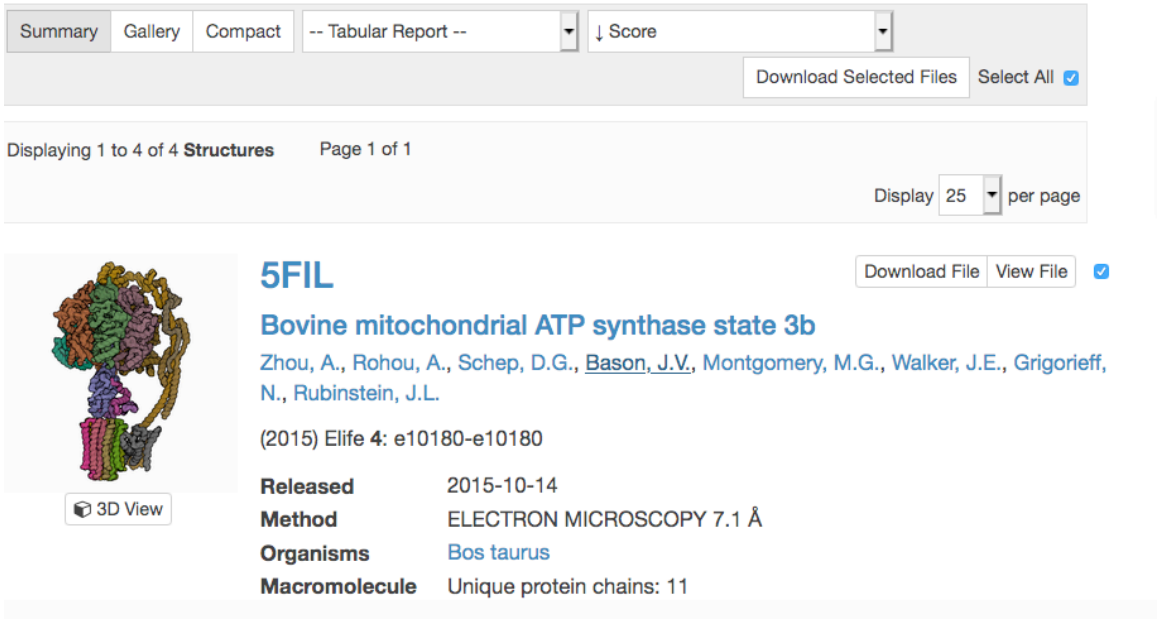
Смотрим, какие там базы данных, какие организмы представлены.

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.





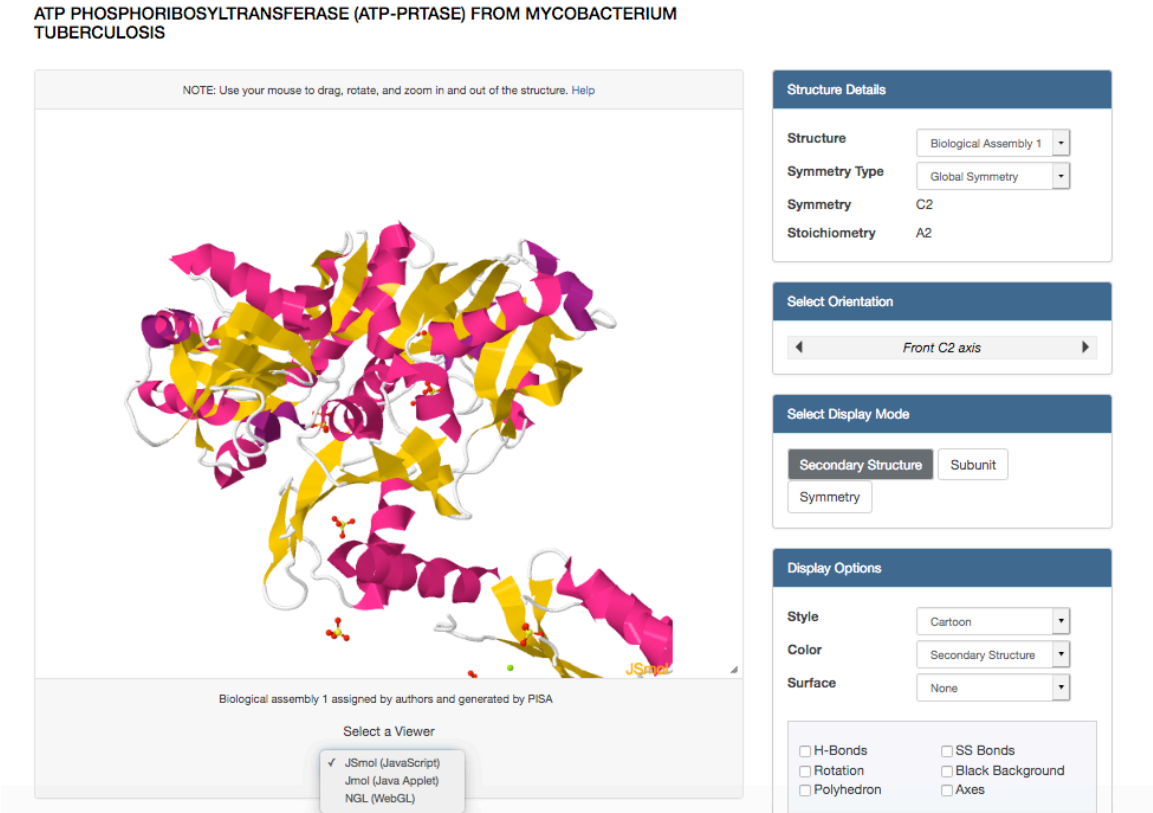
Обратить внимание, каким методом построена структура.

Поизучать разные отображения

Jmol/NGS (Jmol- более распространенная)

Style – Cartoon/Backbone/Space Fill

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



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