

Bioinformatika III

Trimačių struktūrų analizė ir spėjimas

Paskaita 2
baltymų struktūrų klasifikacija

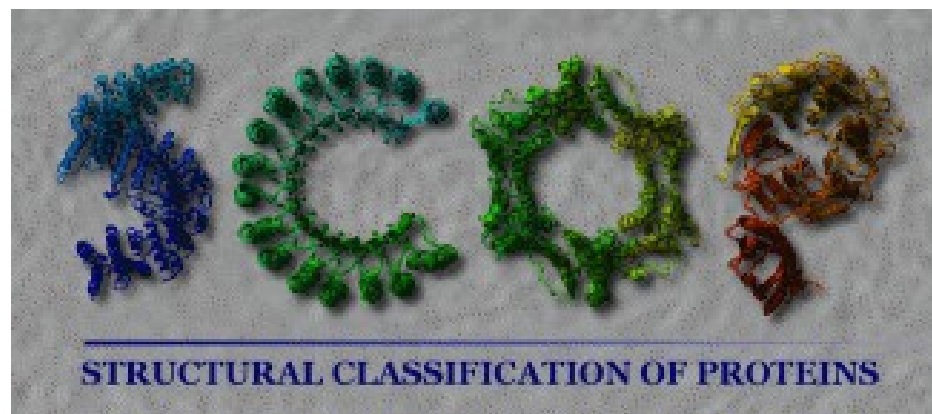
Saulius Gražulis
2022-02-15

Baltymų struktūrų klasifikacijos

- Klasifikacija SCOP
- Klasifikacija CATH
- Klasifikacija FSSP/Dali
- DNT autoenkoderiai?

SCOP klasifikacija

- Kuruojama žmonių
(Alexey G. Murzin, et al.,
Cyrus Chothia)
- Hierarchija:
 - Class
 - Fold
 - Superfamily
 - Family



<http://scop.mrc-lmb.cam.ac.uk/scop/>
<http://scop2.mrc-lmb.cam.ac.uk/>
<https://scop.berkeley.edu/>

SCOPe classes

SCOPe













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Stats & History

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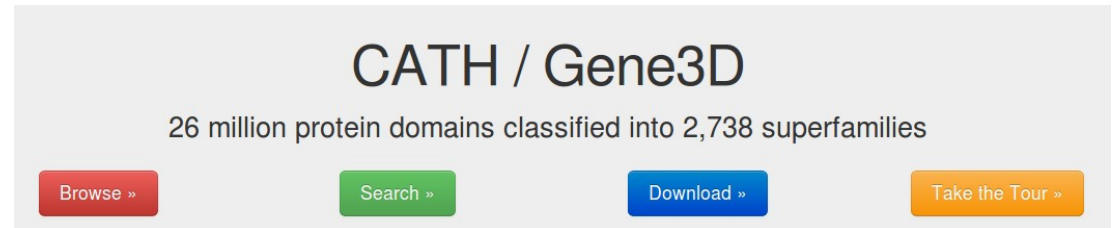
Classes in SCOPe 2.08:

1.  a: All alpha proteins [46456] (290 folds)
2.  b: All beta proteins [48724] (180 folds)
3.  c: Alpha and beta proteins (a/b) [51349] (148 folds)
4.  d: Alpha and beta proteins (a+b) [53931] (396 folds)
5.  e: Multi-domain proteins (alpha and beta) [56572] (74 folds)
6.  f: Membrane and cell surface proteins and peptides [56835] (69 folds)
7.  g: Small proteins [56992] (100 folds)
8.  h: Coiled coil proteins [57942] (7 folds)
9.  i: Low resolution protein structures [58117] (25 folds)
10.  j: Peptides [58231] (151 folds)
11.  k: Designed proteins [58788] (44 folds)
12.  l: Artifacts [310555] (1 fold)

<https://scop.berkeley.edu/>

CATH klasifikacija

- Beveik pilnai automatizēota
- Hierarchija:
 - Klasē
 - Architektūra
 - Topologija
 - Homologinē superšeima



<http://www.cathdb.info/>

(Sillitoe 2021 <https://doi.org/10.1093/nar/gkaa1079>)

Dali/FSSP



- PDBeFold links
 - [FAQ](#)
 - [Visualisation](#)
 - [Performance](#)
 - [Privacy](#)
 - [Version log](#)
 - [PDBeFold Links](#)
 - [Comparisons](#)
 - [Publications](#)
 - [PDBeFOLD](#)

PDBeFold. Structure Similarity.

PDBeFold functionality:

- pairwise comparison and 3D alignment of protein structures
- multiple comparison and 3D alignment of protein structures
- examination of a protein structure for similarity with the whole [PDB archive](#) or [SCOP archive](#)
- best C α -alignment of compared structures
- download and visualisation of best-superposed structures using [Rasmol](#) (Unix/Linux platforms), [Rastop](#) (Windows machines) and [Jmol](#) (platform-independent server-side java viewer)
- linking the results to other services - [PDBeMotif](#), [SCOP](#), [GeneCensus](#), [FSSP](#), [CATH](#), [PDBSum](#), [UniProt](#)

<https://www.ebi.ac.uk/msd-srv/ssm/>

- Original link dead?

(Holm 1997 <https://doi.org/10.1093/nar/25.1.231>)