Úloha 8

Predikce terciární struktury proteinů

Terciární struktura proteinů

- Konkrétní umístění jednotlivých atomů polypeptidového řetězce v prostoru

- **Absolutní souřadnice** – x, y, z

  pro N atomů je třeba 3N souřadnic

- **Relativní souřadnice** – vzdálenost, úhel, torzní úhel

  pro N atomů je třeba 3N – 3 souřadnic

- Komplikovaná hiearchie:

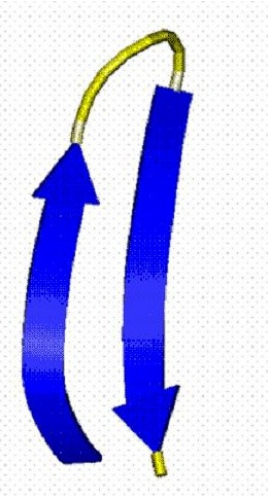
  Sekundární – (Supersekundární) – Terciární

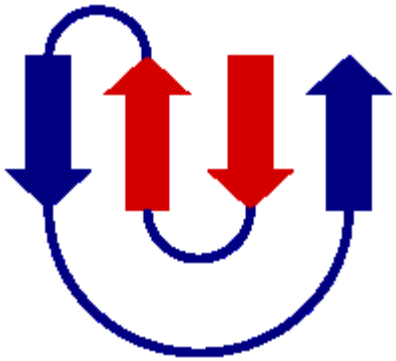
  Motivy – Foldy – Domény

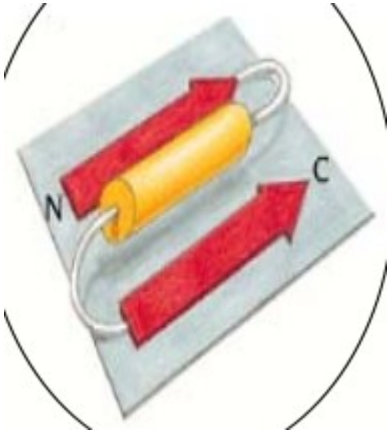
Strukturní motivy

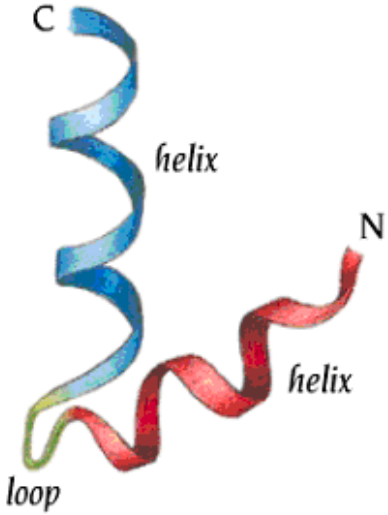
Způsob řazení úseků sekundární struktury, např:

- beta-vlásenka (beta-hairpin)
- Řecký klíč (Greek key)
- beta-alfa-beta
- Helix-otáčka-helix (helix-turn-helix)





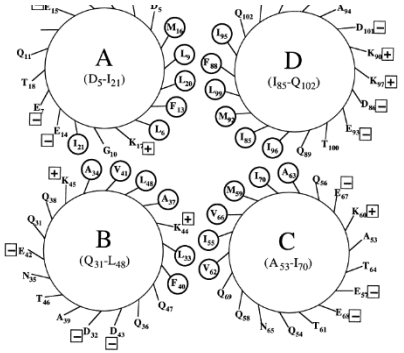


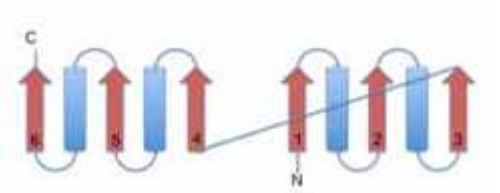


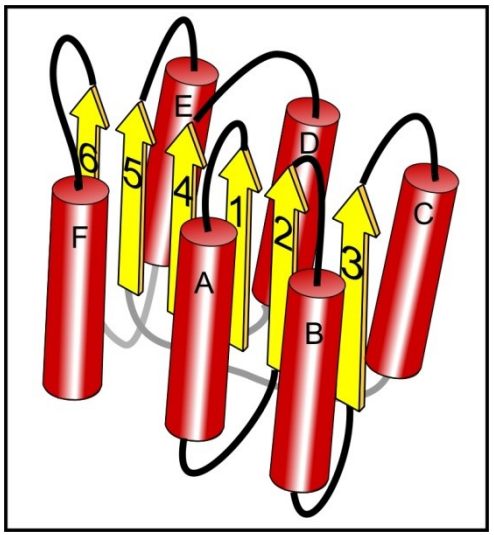
Proteinové foldy

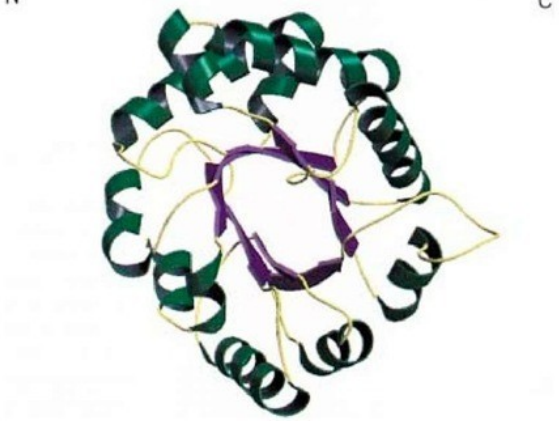
Vznikají kombinací několika motivů, např.:

- Helix-bundle
- Rossmanův fold
- TIM-barrel



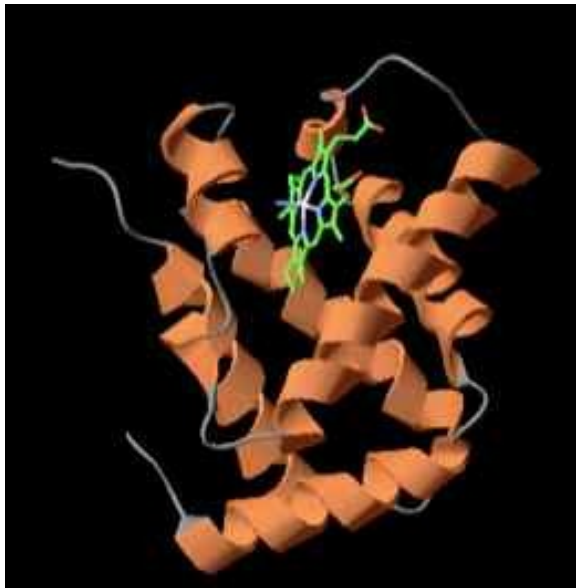






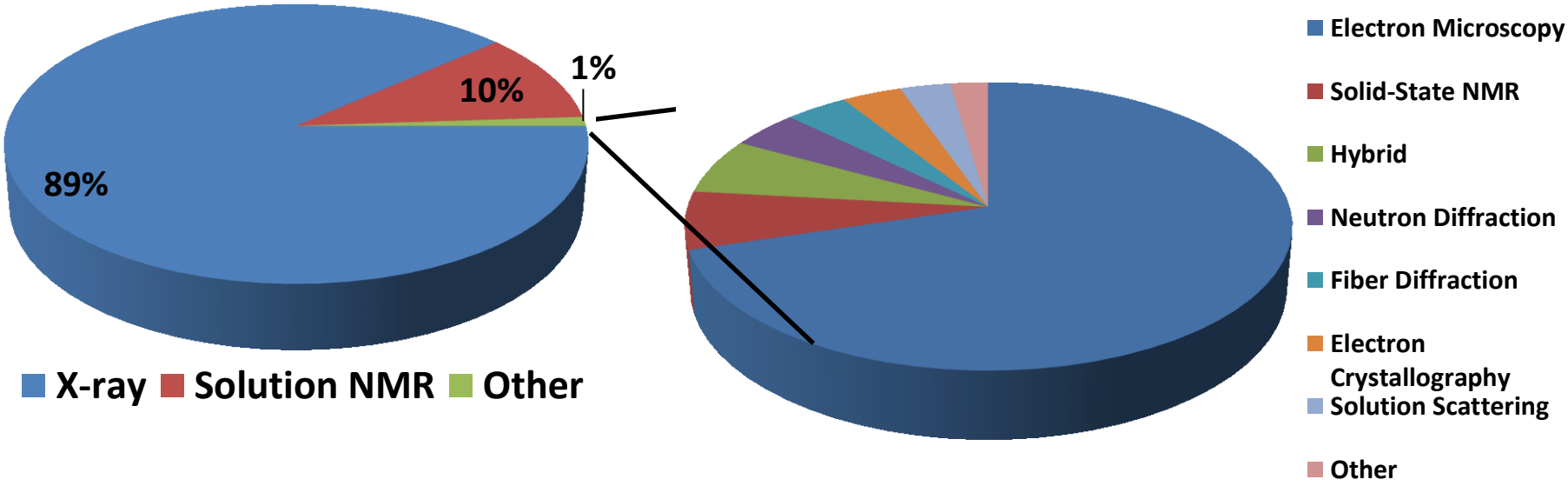
Proteinové domény

- Proteinová doména je prostorově vymezený úsek proteinu, obvykle s vlastní funkcí
- Známe proteiny jednodoménové i vícedoménové



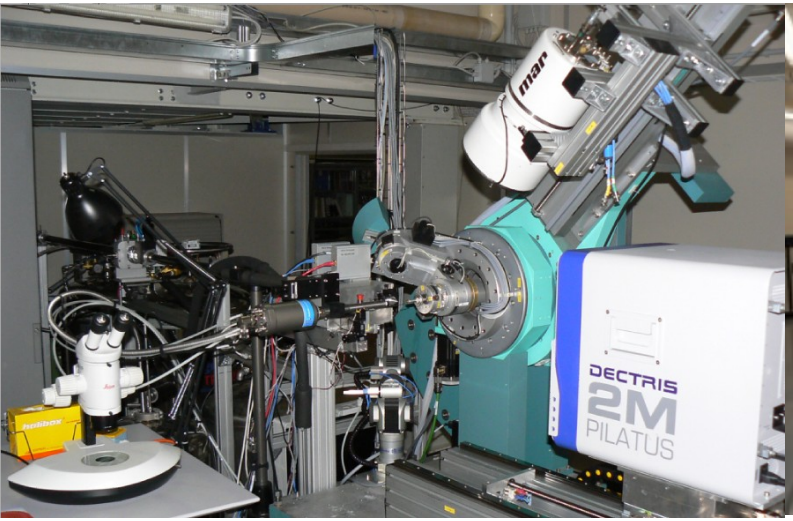
Metody určení 3D struktury

- Rentgenová difrakce - nejvíce struktur v PDB
- NMR
- Ostatní metody < 1%



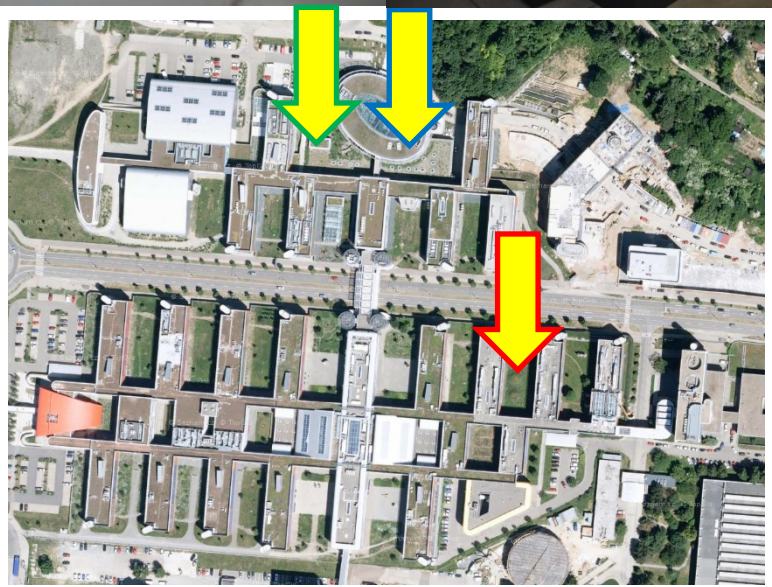
Metody určení 3D struktury

X-ray



NMR

Cryo-EM



Databáze 3D struktur

- **wwPDB** (http://www.wwpdb.org)

  RCSB PDB – Research Collaboratory for Structural Bioinformatics Protein Data Bank

  PDBe – Protein Data Bank Europe

  PDBj – Protein Data Bank Japan

  BMRB – Biological Magnetic Resonance Data Bank

- **SCOP** (http://scop.mrc-lmb.cam.ac.uk/scop/) – strukturní klasifikace proteinů

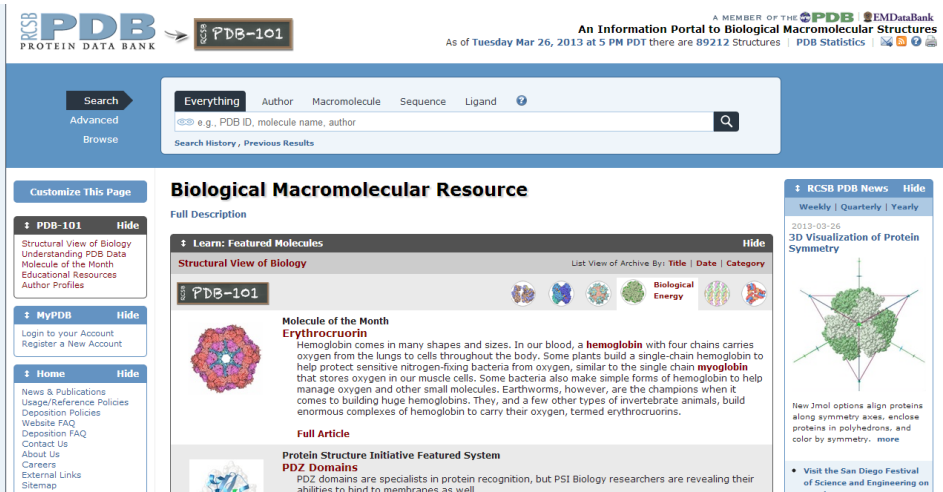
- **CATH** (http://www.cathdb.info/) – klasifikace proteinových domén z PDB

- **EMDataBank** (http://www.emdatabank.org/) – struktury z elektronové mikroskopie

Formáty uložení 3D struktury

PDB (Protein Data Bank)

- PDB File Format (http://www.wwpdb.org/documentation/file-format)
- mmCIF File Format and PDB Exchange Dictionary
- PDBML - XML File Format



PDB

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ATOM      7  CD  ARG A   7     -24.396 -12.945  52.578  1.00 59.72           C
ATOM      8  NE  ARG A   7     -25.048 -12.736  53.869  1.00 61.30           N
ATOM      9  CZ  ARG A   7     -24.413 -12.499  55.014  1.00 61.72           C
ATOM     10 NH1 ARG A   7     -23.087 -12.440  55.065  1.00 61.05           N
ATOM     11 NH2 ARG A   7     -25.115 -12.320  56.126  1.00 63.61           N
ATOM     12  N   TYR A   8     -24.055  -9.007  49.545  1.00 50.83           N
ATOM     13  CA  TYR A   8     -23.096  -8.100  48.940  1.00 48.87           C
ATOM     14  C   TYR A   8     -21.680  -8.609  49.201  1.00 47.84           C
ATOM     15  O   TYR A   8     -21.378  -9.123  50.279  1.00 47.98           O
ATOM     16  CB  TYR A   8     -23.287  -6.680  49.481  1.00 47.56           C
ATOM     17  CG  TYR A   8     -24.700  -6.147  49.294  1.00 48.37           C
ATOM     18  CD1 TYR A   8     -25.123  -5.630  48.067  1.00 49.00           C
ATOM     19  CD2 TYR A   8     -25.619  -6.180  50.332  1.00 48.91           C
ATOM     20  CE1 TYR A   8     -26.419  -5.156  47.889  1.00 48.83           C
ATOM     21  CE2 TYR A   8     -26.918  -5.707  50.160  1.00 50.24           C
ATOM     22  CZ  TYR A   8     -27.306  -5.192  48.936  1.00 49.98           C
ATOM     23  OH  TYR A   8     -28.589  -4.719  48.773  1.00 51.15           O
ATOM     24  N   LYS A   9     -20.837  -8.493  48.178  1.00 46.89           N
ATOM     25  CA  LYS A   9     -19.429  -8.849  48.240  1.00 45.81           C
ATOM     26  C   LYS A   9     -18.589  -7.576  48.327  1.00 43.61           C
ATOM     27  O   LYS A   9     -19.052  -6.506  47.921  1.00 42.40           O
ATOM     28  CB  LYS A   9     -19.034  -9.623  46.986  1.00 47.08           C
ATOM     29  CG  LYS A   9     -19.825 -10.894  46.763  1.00 49.32           C
ATOM     30  CD  LYS A   9     -19.594 -11.448  45.365  1.00 51.43           C
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ATOM     33  N   PRO A  10     -17.364  -7.701  48.849  1.00 42.21           N
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ATOM     35  C   PRO A  10     -15.637  -6.210  47.808  1.00 40.77           C
ATOM     36  O   PRO A  10     -14.406  -6.346  47.819  1.00 40.13           O
ATOM     37  CB  PRO A  10     -15.542  -7.084  50.158  1.00 40.95           C
ATOM     38  CG  PRO A  10     -15.397  -8.529  49.837  1.00 42.10           C
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ATOM     40  N   ASP A  11     -16.313  -5.778  46.748  1.00 40.65           N
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ATOM     43  O   ASP A  11     -17.804  -4.241  45.194  1.00 40.53           O
ATOM     44  CB  ASP A  11     -15.159  -6.174  44.567  1.00 42.62           C
ATOM     45  CG  ASP A  11     -16.278  -6.799  43.791  1.00 45.99           C
ATOM     46 OD1 ASP A  11     -16.825  -7.814  44.274  1.00 50.77           O
ATOM     47 OD2 ASP A  11     -16.673  -6.360  42.684  1.00 49.06           O
ATOM     48  N   TRP A  12     -16.044  -3.075  44.451  1.00 38.94           N
```

mmCIF

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ATOM   1    N  N    . GLU A 1 1   ? 7.254   11.020 4.888  1.00 61.38 ? ? ? ? ? ? 546 GLU A N   1
ATOM   2    C  CA   . GLU A 1 1   ? 6.404   12.200 5.071  1.00 67.04 ? ? ? ? ? ? 546 GLU A CA  1
ATOM   3    C  C    . GLU A 1 1   ? 7.111   13.526 4.729  1.00 59.60 ? ? ? ? ? ? 546 GLU A C   1
ATOM   4    O  O    . GLU A 1 1   ? 6.576   14.360 3.999  1.00 64.05 ? ? ? ? ? ? 546 GLU A O   1
ATOM   5    C  CB   . GLU A 1 1   ? 5.842   12.232 6.500  1.00 74.02 ? ? ? ? ? ? 546 GLU A CB  1
ATOM   6    C  CG   . GLU A 1 1   ? 5.625   13.627 7.094  1.00 74.52 ? ? ? ? ? ? 546 GLU A CG  1
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ATOM   10   N  N    . ASP A 1 2   ? 8.299   13.714 5.287  1.00 44.26 ? ? ? ? ? ? 547 ASP A N   1
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ATOM   12   C  C    . ASP A 1 2   ? 10.508  14.039 4.527  1.00 30.06 ? ? ? ? ? ? 547 ASP A C   1
ATOM   13   O  O    . ASP A 1 2   ? 11.245  13.650 5.424  1.00 29.92 ? ? ? ? ? ? 547 ASP A O   1
ATOM   14   C  CB   . ASP A 1 2   ? 9.460   15.735 6.039  1.00 34.15 ? ? ? ? ? ? 547 ASP A CB  1
ATOM   15   C  CG   . ASP A 1 2   ? 10.399  16.909 5.672  1.00 36.09 ? ? ? ? ? ? 547 ASP A CG  1
ATOM   16   O  OD1  . ASP A 1 2   ? 11.138  16.835 4.665  1.00 33.05 ? ? ? ? ? ? 547 ASP A OD1 1
ATOM   17   O  OD2  . ASP A 1 2   ? 10.397  17.917 6.418  1.00 36.96 ? ? ? ? ? ? 547 ASP A OD2 1
ATOM   18   N  N    . LEU A 1 3   ? 10.778  13.854 3.239  1.00 32.19 ? ? ? ? ? ? 548 LEU A N   1
ATOM   19   C  CA   . LEU A 1 3   ? 11.922  13.061 2.787  1.00 30.81 ? ? ? ? ? ? 548 LEU A CA  1
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ATOM   22   C  CB   . LEU A 1 3   ? 11.876  12.852 1.272  1.00 34.20 ? ? ? ? ? ? 548 LEU A CB  1
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ATOM   26   N  N    . PHE A 1 4   ? 13.292  15.008 3.199  1.00 29.71 ? ? ? ? ? ? 549 PHE A N   1
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ATOM   35   C  CE2  . PHE A 1 4   ? 17.430  19.281 2.954  1.00 28.10 ? ? ? ? ? ? 549 PHE A CE2 1
ATOM   36   C  CZ   . PHE A 1 4   ? 17.586  19.769 4.244  1.00 21.53 ? ? ? ? ? ? 549 PHE A CZ  1
ATOM   37   N  N    . LYS A 1 5   ? 13.825  15.663 5.896  1.00 24.70 ? ? ? ? ? ? 550 LYS A N   1
ATOM   38   C  CA   . LYS A 1 5   ? 13.979  15.407 7.317  1.00 26.90 ? ? ? ? ? ? 550 LYS A CA  1
ATOM   39   C  C    . LYS A 1 5   ? 14.403  13.966 7.541  1.00 28.64 ? ? ? ? ? ? 550 LYS A C   1
```

Úkol 1

Seznamte se s formátem .pdb - otevřete soubor **4AGT.pdb** v textovém prohlížeči a uveďte:

- O jaký protein se jedná?
- Jakou technikou byla struktura získána?
- V kterém časopisu byla struktura publikována?
- Kolik řetězců proteinu obsahuje kompletní struktura?
- Kolik úseků struktury helixu obsahuje každý monomer daného proteinu?
- Je ve struktuře přítomen nějaký kov?

In silico predikce 3D struktury

- ***Ab initio***

- **Homologní modelování**

- **Threading („navlékání“)**

1) *Ab initio* - Quark

- Nevyžaduje existenci homologního proteinu
- Predikuje 2D strukturu, modeluje fragmenty a kombinuje je navzájem
- Nízká spolehlivost zejm. pro větší proteiny

QUARK http://zhanglab.ccmb.med.umich.edu/QUARK/

QUARK Ab Initio Results for Job Q12270

Submitted Primary Sequence

```
>Length 71
HVKRPMNAFMVWAQAARRKLADQYPHLHNAELSKTLGKLWRLLNEVEKRPFVEEAERLRVQHKKDHPDYKY
12345678901234567890123456789012345678901234567890123456789012345678901
--------10--------20--------30--------40--------50--------60--------70
```

Predicted Secondary Structure

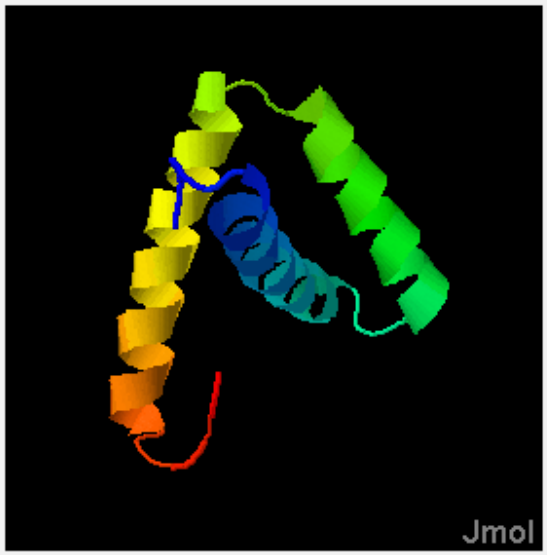
```
>C-coil;H-helix;E-sheet;T-beta turn
HVKRPMNAFMVWAQAARRKLADQYPHLHNAELSKTLGKLWRLLNEVEKRPFVEEAERLRVQHKKDHPDYKY
CTTTTCHHHHHHHHHHHHHHHHTTTTCHHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHHHTTTTTT
12345678901234567890123456789012345678901234567890123456789012345678901
--------10--------20--------30--------40--------50--------60--------70
```

Download Predicted 3-state Secondary Structure Types
Download Predicted Starting Beta-turn Position
Download Predicted Real-value Phi-angle
Download Predicted Real-value Psi-angle
Download Distance Profile from Fragments
Download Clustered Torsion Angle Pairs from Fragments

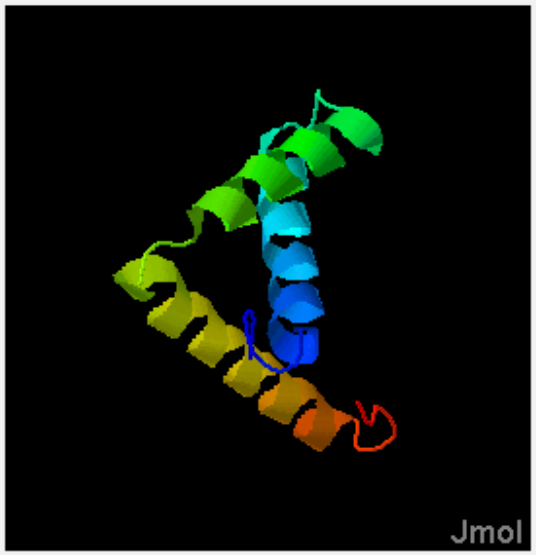
Predicted Solvent Accessibility

```
>0-buried to 9-exposed
HVKRPMNAFMVWAQAARRKLADQYPHLHNAELSKTLGKLWRLLNEVEKRPFVEEAERLRVQHKKDHPDYKY
54420110100002101220143124121120020013004312321122013203301220353123143
12345678901234567890123456789012345678901234567890123456789012345678901
--------10--------20--------30--------40--------50--------60--------70
```

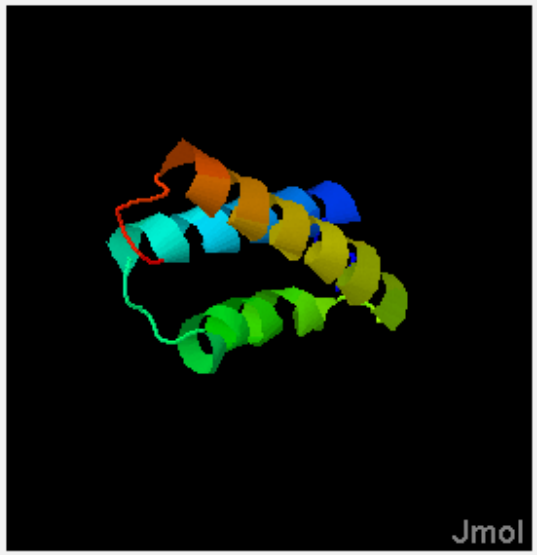
Predicted Tertiary Structure



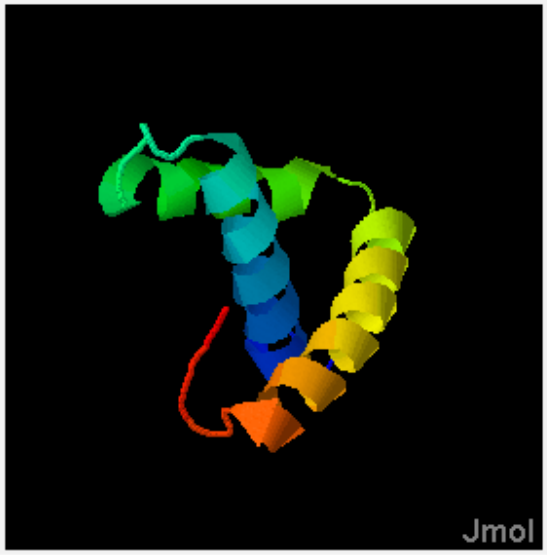
Download Model 1

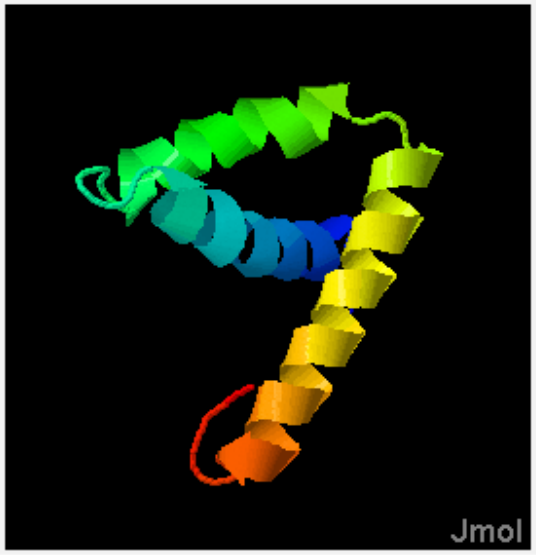


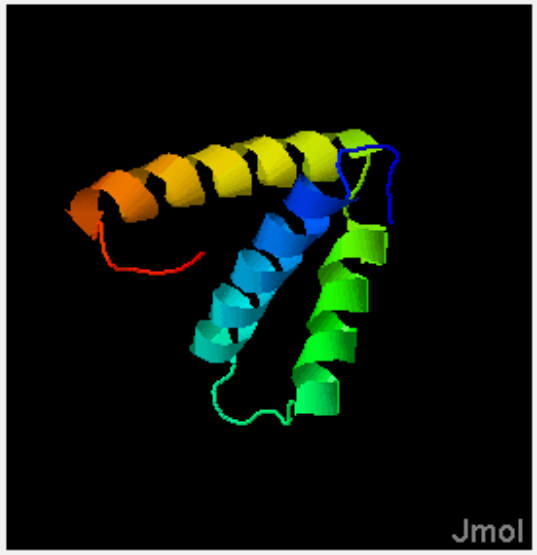
Download Model 2



Download Model 3



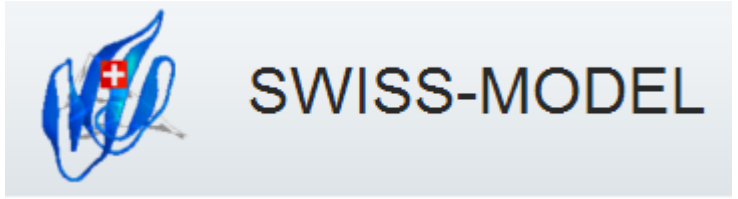




2) Homologní modelování

- Využívá skutečnosti, že dva proteiny ze stejné rodiny a s podobnou sekvencí mají i podobnou 3D strukturu
- Nutno znát strukturu homologního proteinu = templát

SWISS-MODEL http://swissmodel.expasy.org/



Úkol 2

- Pokuste se vytvořit model struktury pro zadaný protein pomocí serveru **SWISS-MODEL** (http://swissmodel.expasy.org/). Použijte automatický mód.

Sekvence proteinu[Penicillium camemberti]:
MPSNGAHDIVFRTSIAACNSNSRLRVYMQDVLGKIRESKYEDKWSNGTEKN
VIASAKLYSPVACTSSELDNIRVYYLSTENIMKDMAYDKSKGWHEGNLGKK
RFMTAPYSNLAACNLKGPGMTISVYCQIADNTIQEYGVKDDGNWEKMSNLG
LAMPGTDIACTVLKTSEPKIRVYFQHMEHGIIEKCYDNKHGWYDGAAKFPK
VQPRTSIACTSYMAGSETLGIRVFFNAANMVLEMVYDGMSWTEGHFHADCI
PGTQIACIS

Swiss-Model

Welcome to SWISS-MODEL

SWISS-MODEL is a fully automated protein structure homology-modelling server, accessible via the ExPASy web server, or from the program DeepView (Swiss Pdb-Viewer). The purpose of this server is to make Protein Modelling accessible to all biochemists and molecular biologists worldwide.

Start Modelling

SWISS-MODEL has recently had a face lift! You can still access the familiar version here.

Protein Structure Bioinformatics Group
c/o Prof. Torsten Schwede
Swiss Institute of Bioinformatics
Biozentrum, University of Basel
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CH-4056 Basel / Switzerland
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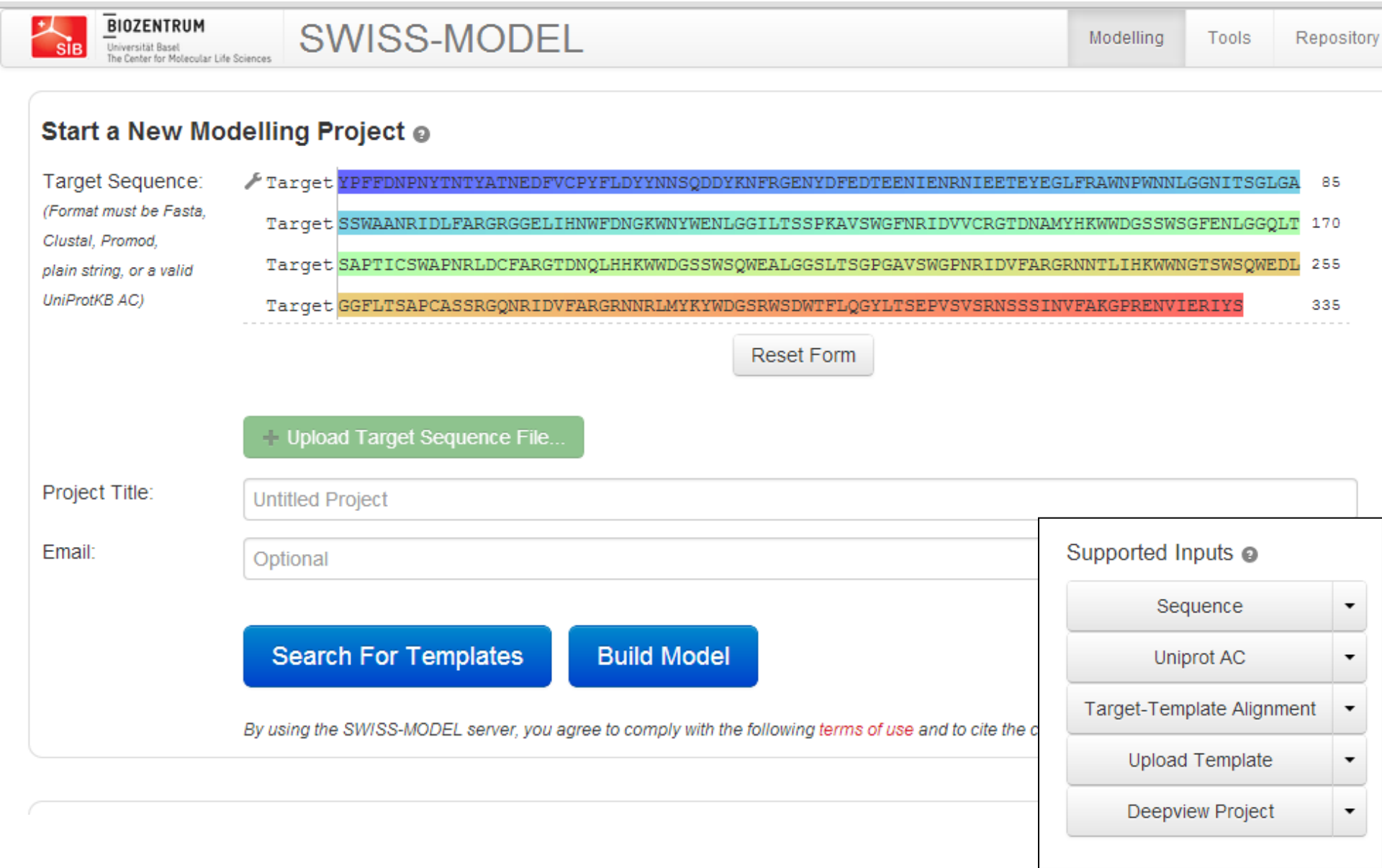
SIB Swiss Institute of Bioinformatics

BIOZENTRUM
Universität Basel
The Center for Molecular Life Sciences

When you publish or report results using SWISS-MODEL, please cite the relevant publications:

- Arnold K., Bordoli L., Kopp J., and Schwede T. (**2006**). The SWISS-MODEL Workspace: A web-based environment for protein structure homology modelling. *Bioinformatics*, 22,195-201.
- Kiefer F, Arnold K, Künzli M, Bordoli L, Schwede T (**2009**). The SWISS-MODEL Repository and associated resources. *Nucleic Acids Research*. 37, D387-D392.
- Guex, N.; Peitsch, M.C.; Schwede, T. **(2009)** SWISS-MODEL and Swiss PdbViewer. Automated comparative protein structure modeling with SWISS-MODEL and Swiss-PdbViewer: A historical perspective. *Electrophoresis*, 30(S1), S162-S173.

Swiss-Model


BIOZENTRUM
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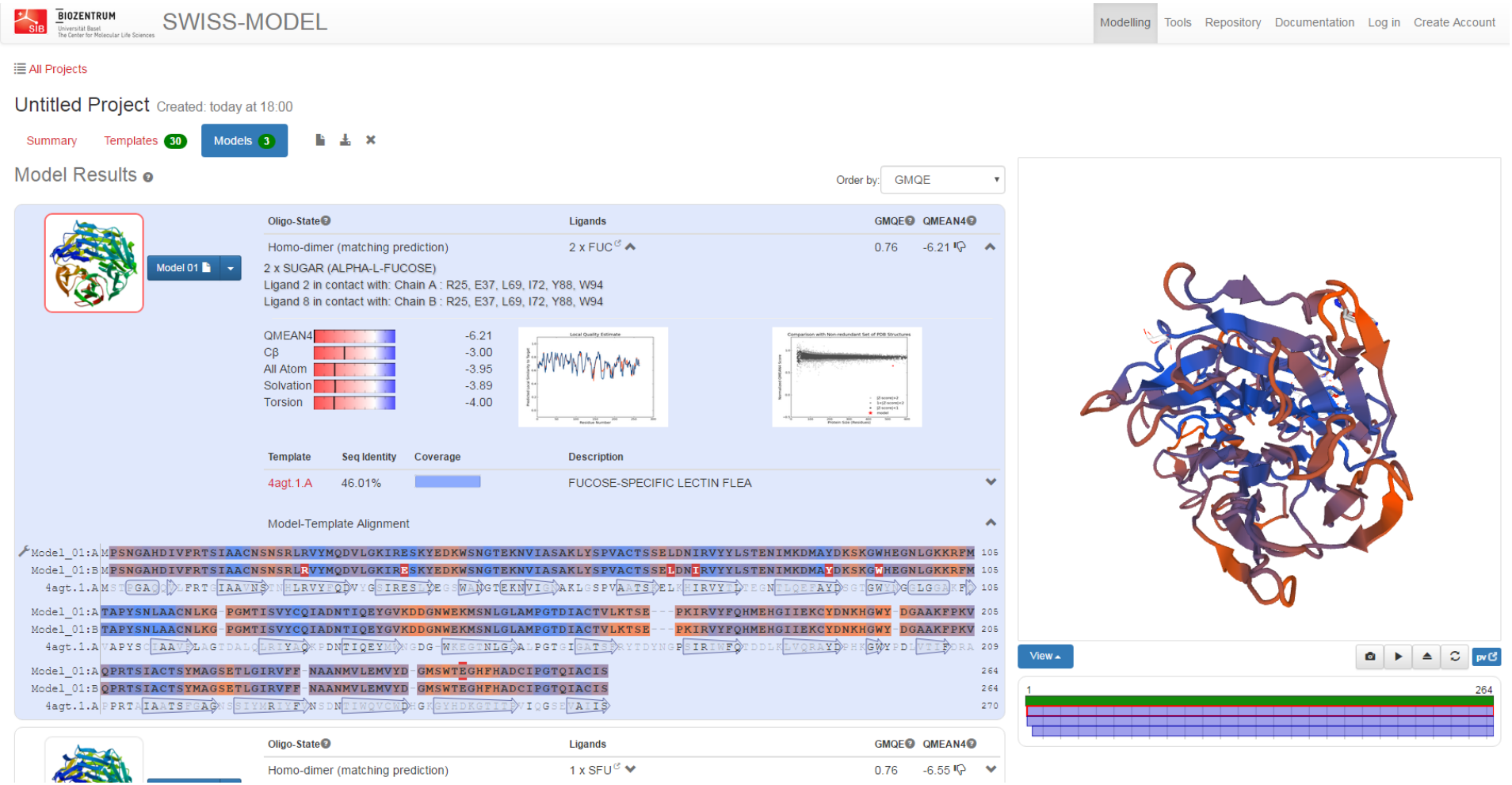
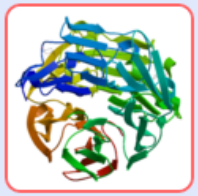
The Center for Molecular Life Sciences
SWISS-MODEL
Modelling
Tools
Repository
Start a New Modelling Project
Target Sequence:
(Format must be Fasta, Clustal, Promod, plain string, or a valid UniProtKB AC)
Target YPFFDNPNYTNTYATNEDFVCPYFLDYYNNSQDDYKNFRGENYDFEDTEENIENRNIEETEYEGLFRAWNPWNNLGGNITSGLGA 85
Target SSWAANRIDLFARGRGGELIHNWFDNGKWNYWENLGGILTSSPKAVSWGFNRIDVVCRGTDNAMYHKWWDGSSWSGFENLGGQLT 170
Target SAPTICSWAPNRLDCFARGTDNQLHHKWWDGSSWSQWEALGGSLTSGPGAVSWGPNRIDVFARGRNNTLIHKWWNGTSWSQWEDL 255
Target GGFLTSAPCASSRGQNRIDVFARGRNNRLMYKYWDGSRWSDWTFLQGYLTSEPVSVSRNSSSINVFAKGPRENVIERIYS 335
Reset Form
Upload Target Sequence File...
Project Title:
Untitled Project
Email:
Optional
Search For Templates
Build Model
By using the SWISS-MODEL server, you agree to comply with the following terms of use and to cite the c
Supported Inputs
Sequence
Uniprot AC
Target-Template Alignment
Upload Template
Deepview Project

Swiss-Model

- Několik templátů, několik modelů



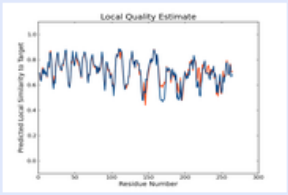


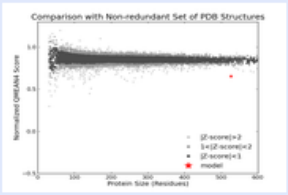
Model 01

Oligo-State	Ligands	GMQE	QMEAN4
Homo-dimer (matching prediction)	2 x FUC	0.76	-6.21

2 x SUGAR (ALPHA-L-FUCOSE)
Ligand 2 in contact with: Chain A : R25, E37, L69, I72, Y88, W94
Ligand 8 in contact with: Chain B : R25, E37, L69, I72, Y88, W94

QMEAN4	-6.21
Cβ	-3.00
All Atom	-3.95
Solvation	-3.89
Torsion	-4.00





Template	Seq Identity	Coverage	Description
4agt.1.A	46.01%		FUCOSE-SPECIFIC LECTIN FLEA

Oligo-state	Method	Seq Similarity	Range	Coverage
homo-dimer	X-ray, 2.00 Å	0.43	2 - 264	1.00

Ligand	Added to Model	Description
FUC	✓	SUGAR (ALPHA-L-FUCOSE)
FUC	✓	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Clashing with protein.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC	✕ - Binding site not conserved.	SUGAR (ALPHA-L-FUCOSE)
FUC-NAG-NDG	✕ - Clashing with protein.	SUGAR (3-MER)
FUC-NDG	✕ - Binding site not conserved.	SUGAR (2-MER)
NA	✕ - Not biologically relevant.	SODIUM ION

3) Threading

- Modelování při nízké homologii s proteiny se známou strukturou
- Porovnává možnost přiložení sekvence na proteiny známých foldů

Phyre2 http://www.sbg.bio.ic.ac.uk/phyre2/

Phyre2

ARDLVIPMIYCGHGY

PSI-Blast

HMM

HMM-HMM matching

Hidden Markov Model DB of **KNOWN STRUCTURES**

Very powerful – able to reliably detect extremely remote homology

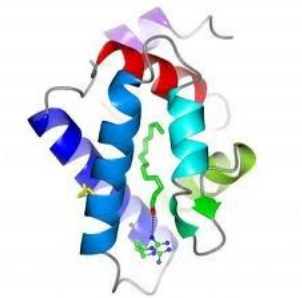
Routinely creates accurate models even when sequence identity is <15%

ARDL--VIPMIYCGHGY

AFDLCDLIPV--CGMAY

Sequence of known structure

3D-Model



Phyre2

Protein Homology/analogY Recognition Engine V 2.0

Subscribe to Phyre at Google Groups

Email: Subscribe

Visit Phyre at Google Groups

What's New in Phyre2

E-mail Address	houser@mail.muni.cz
Optional Job description	CBL
Amino Acid Sequence	MYPFFDNPNYTNTYATNEDFVCPYFLDYYNNSQDDYKNFRGENYDFEDTEENIENRNI EETEYEGLFRAWNPWNNLGGNITSGLGASSWAANRIDLFARGRGGELIHNWFDNGKWN YWENLGGILTSSPKAVSWGFNRIDVVCRGTDNAMYHKWWDGSSWSGFENLGGQLTSAP TICSWAPNRLDCFARGTDNQLHHKWWDGSSWSQWEALGGSLTSGPGAVSWGPNRIDVF ARGRNNTLIHKWWNGTSWSQWEDLGGFLTSAPCASSRGQNRIDVFARGRNNRLMYKYW DGSRWSDWTFLQGYLTSEPVSVSRNSSSINVFAKGPRENVIERIYS
Modelling Mode	Normal ◉ Intensive ○
	Phyre Search Reset

Phyre2

Job Status

Email	houser@mail.muni.cz
Job Description	CBL_____
Unique Job ID	6ae742ede312f99d
Date	Mon Feb 4 14:20:24 GMT 2013

Estimated total processing time: 2.2 hours ± 1.9 hours

Your job has entered the queue....*Waiting for job to start.*

171 jobs running **0** jobs queued

This page auto-refreshes every 30 seconds until job completion ....

Summary

Top model

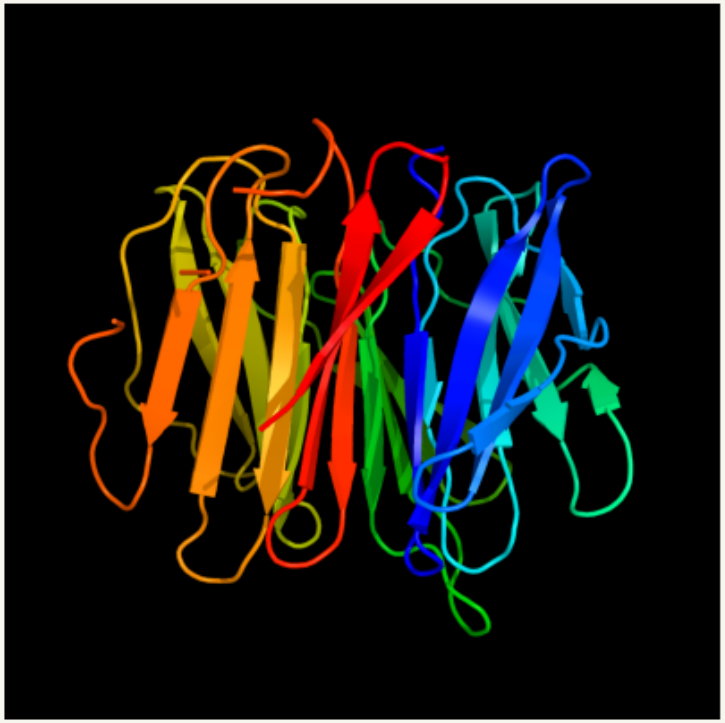


Image coloured by rainbow N → C terminus

Model (left) based on template d1ofza_

Top template information

Fold:6-bladed beta-propeller
Superfamily: Fucose-specific lectin
Family: Fucose-specific lectin

Confidence and coverage

Confidence:	100.0%	Coverage:	76%

255 residues (76% of your sequence) have been modelled with 100.0% confidence by the single highest scoring template.

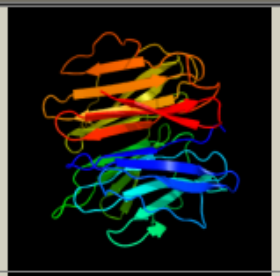
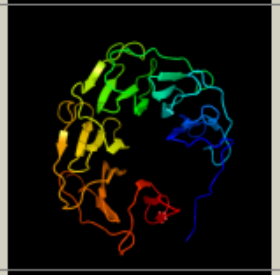
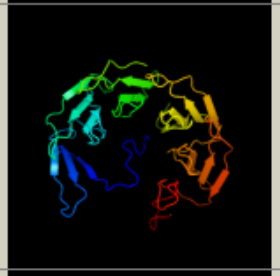
3D viewing

Interactive 3D view in Jmol

Sequence analysis

View PSI-Blast Pseudo-Multiple Sequence Alignment

Secondary structure and disorder prediction

#	Template	Alignment Coverage	3D Model	Confidence	% i.d.	Template Info
1	d1ofza_	Alignment		100.0	20	**Fold:**6-bladed beta-propeller **Superfamily:**Fucose-specific lectin **Family:**Fucose-specific lectin
2	c2xbgA_	Alignment		97.9	13	**PDB header:**photosynthesis **Chain:** A: **PDB Molecule:**ycf48-like prote **PDBTitle:** crystal structure of ycf48 from
3	c2c4dA_	Alignment		95.6	16	**PDB header:**lectin **Chain:** A: **PDB Molecule:**psathyrella velu **PDBTitle:** 2.6a crystal structure of psathy with n-acetylglucosamine
4	c2xcyA_	Alignment		95.3	14	**PDB header:**hydrolase **Chain:** A: **PDB Molecule:**extracellular sia **PDBTitle:** crystal structure of aspergillus f

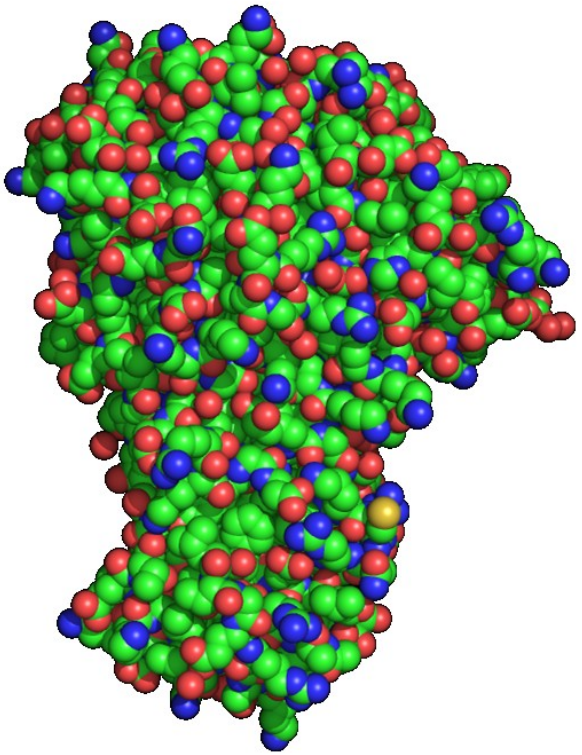
Analýza 3D struktur

- Určení **strukturních prvků** (sekundární struktura, motivy, foldy) a zařazení do příslušných nadrodin
- **Povrchy** – přístupnost pro solvent, hydrofobicita, analýza kavit a tunelů
- **Vazebná místa** – predikce funkce
- **Interakce** (protein-protein – 4D, protein-DNA, protein-ligand) – plochy, energie, vazby
- **Homology** – hledání, porovnávání

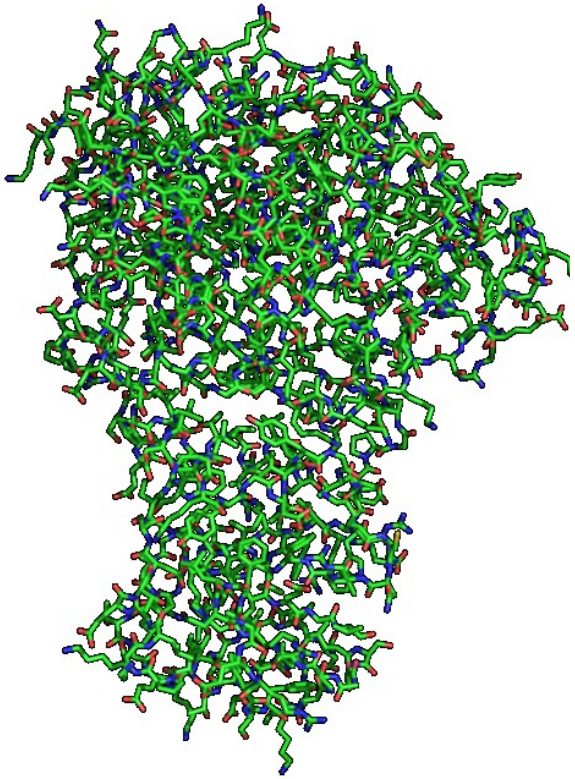
Zobrazení 3D struktury

- Zobrazovací SW: **PyMol**, Jmol, RasMol, VMD, Chimera, Cn3D,…

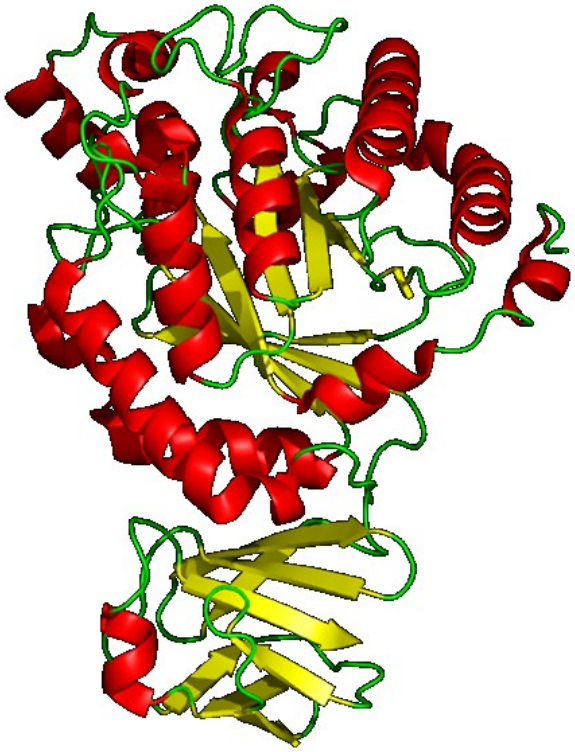
spheres, surface



sticks/balls and sticks



cartoon/ribbon



Úkol 3

➢ Zpracujte strukturní model v programu **PyMol**:

- Otevřete homologní model a originální templát (model01.pdb, 4agt.pdb)
- Zobrazte obě struktury jako cartoon a jako sticks a uložte jako obrázek s vysokým rozlišením (1200x1200 dpi)
- Extrahujte řetězce A, proveďte alignment
- Porovnejte strukturu vazebného místa v okolí ligandů Fuc910, 920 a 950 v řetězci A

Doplňková literatura a další zdroje

- http://www.wikipedia.org ☺
- http://www.proteinstructures.com/
- http://cssb.biology.gatech.edu/resources#services
- http://www.ebi.ac.uk/services/structures
- Odborné články ve studijních materiálech