EXPERIMENT 11: STRUCTURE MODELING

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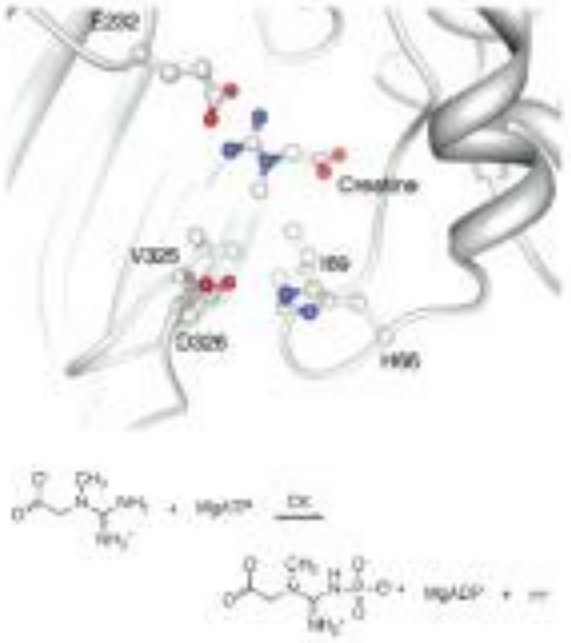
SUSTC

From sequence to structure

Sequence → Structure → Function

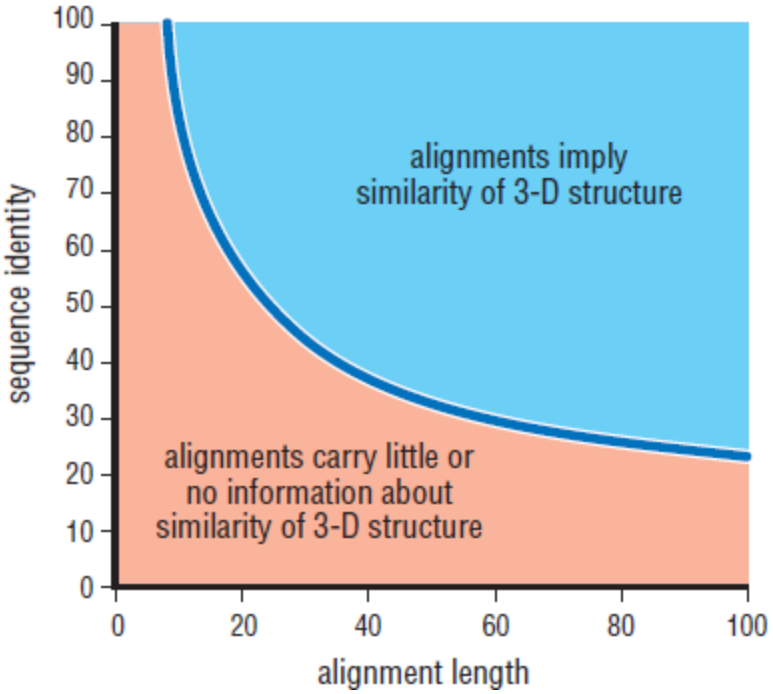
MPFGNTHNKFKL
NYKPEEEYPDLSK
HNNHMAKVLTLE
LYKKLRDKETPSGF
TVDDVIQTGVDNP
GHPFIMTVGCVAG
DEESYEVFKELFDPI
ISDRHGGYKPTD...



Methods

- Homology modeling
  - **SWISS-MODEL** (http://swissmodel.expasy.org/)
  - Modeller (https://salilab.org/modeller/)
- Profile-based threading
  - Hhpred (http://toolkit.tuebingen.mpg.de/hhpred)
- *De novo* modeling
  - Robetta (http://robetta.bakerlab.org/)

The basis for homology modeling



SWISS-MODEL protocol

- http://swissmodel.expasy.org/docs/examples

Tasks

1. Find the amino acid sequence of human KANK1
2. Predict the ANK repeat region in KANK1
   - Using SMART
3. Predict the 3D structure of the ANK repeat region of KANK1
   - Using SWISS-MODEL
4. Analyze the prediction results
   - Reliable or not?
5. Predict the KN motif in KANK1
6. Predict the 3D structure of the KN motif of KANK1
   - Try to use different prediction methods

PyMOL Addition - Movie

- PyMOL Wiki's Movie School
  - http://www.pymolwiki.org/index.php/MovieSchool

Lab report format

- Title
- Your name and student No.
- Introduction
- Methods
- Results
- Conclusions