

Model building

the problem

Basic steps

0.- Map preprocessing

1.- Get the initial model (s)

2.- Rigid fitting of model(s) in map

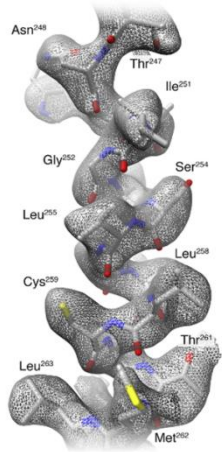
3.- Flexible fitting (refinement)
of model(s) in map

4.- Model(s) validation

Prediction & Processing

Docking

Rebuilding



Tools

1.- Get the initial model (s): Structure prediction (s)

de novo
modeling

AlphaFold
ModelAngelo
(template NOT needed)

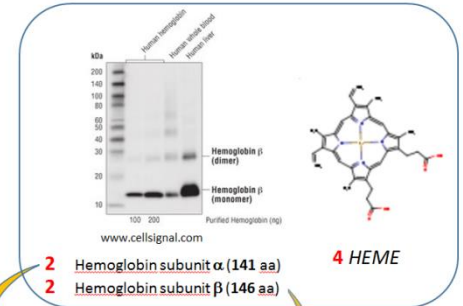
Homology
modeling

Our proteins borrow
the structure
of similar proteins
(template needed)

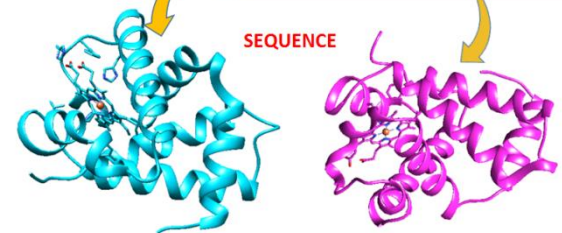
initial model \neq real model

1st clue:

Skeleton of α carbons
and
many side chains



SEQUENCE



Human ion channel TACAN isoform 1

