CBMS workbench (virtual), Oct 13 2021

AlphaFold for MR

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Molecular replacement (MR)

Use a previously known structure to get phase estimates

The crystal

The search model

Rotation search

Translation search
AI scientists from Google DeepMind won CASP14 (Critical Assessment of Structural Prediction competition)

The average rmsd is ~1.6 Å!

The code is available on GitHub and can be run on google Colab:
- https://github.com/deepmind/alphafold
1) Do multiple sequence alignment (MSA)
   → find parts of the sequence more likely to mutate and correlations between them
   → find proteins that may have a similar structure ("templates")
   → guess which amino acids are likely to be in contact with each other

2) Neural network 1: identify which parts of the MSA are more informative

3) Neural network 2: build a model

Amino acid sequence → Structural model
Use AlphaFold model for MR
AlphaFold for MR

Use the tutorial data for the A2U-globulin structure (MR tutorial)

1) Run the tutorial with supplied search model

2) With the sequence, do a prediction and run MR again
An NIH/NIGMS funded Program Project

The Phenix Project

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