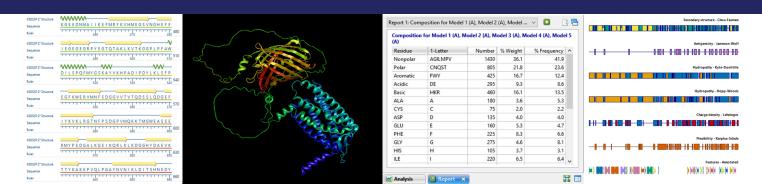# NovaFold AI
Protein Structure Prediction Software

Easy and robust structure prediction in minutes

NovaFold AI software incorporates the award-winning AlphaFold 2 algorithm developed by DeepMind from Google. This algorithm allows NovaFold AI to accurately predict the three-dimensional structure of proteins that were impossible to predict accurately using previous algorithms.

Works within the Protean 3D interface of Lasergene

The Protean 3D application acts as the interface for both NovaFold AI and our original NovaFold application, which is based on I-TASSER, the top-performing server for six CASP Challenges in a row (CASP7-CASP12). This provides you with the flexibility to quickly obtain and compare results from two highly accurate protein structure prediction methods. Both applications let you set up and initiate one or many predictions in just a few mouse clicks.

Handles even the most difficult folding problems

NovaFold AI is the first commercial software that can accurately predict even the most challenging protein structures:

- Membrane-bound proteins
- Fusion proteins
- Cytosolic domains (CDs)
- Extra-cellular regions
- G-protein-couple receptors (GPCRs)

NovaFold AI can also model multiple domains and their interactions with linkers, also known as multidomain protein structure prediction.
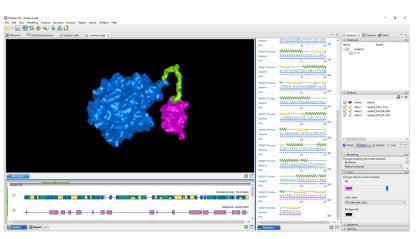

Figure 1. Protean 3D showing a completed NovaFold AI prediction of two CASP 14 targets (5W9F in pink; 6D2V in blue) modeled with a linker. The green portion of the structure is the linker GGGGSGGGGSGGGGS.

NovaFold AI uses the world's most accurate protein structure prediction algorithm

AlphaFold 2, the algorithm used in NovaFold AI, was the top-ranked protein structure prediction method in CASP 13 and CASP14. In CASP14 (2020), AlphaFold 2 averaged over 2.6x the accuracy of the second-place algorithm (Figure 2).

AlphaFold2 is also extremely fast and typically finishes structure predictions in a few hours or less.

To learn more about the AlphaFold2 algorithm, see Jumper, J., Evans, R., Pritzel, A. et al. Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589 (2021). https://doi.org/10.1038/s41586-021-03819-2.

CASP14 Group Performance

#1-ranked group, AlphaFold 2 = 2.65

#2-ranked group = 1.00

Group Ranking for Regular Targets

Average Z-Score

Figure 2. In the CASP14 Challenge, AlphaFold 2 achieved an average Z-score of 2.65 over 92 "regular" targets. The closest competitor achieved only 1.00 for the same number of targets (Graph created from the table at https://predictioncenter.org/casp14/zscores_final.cgi).
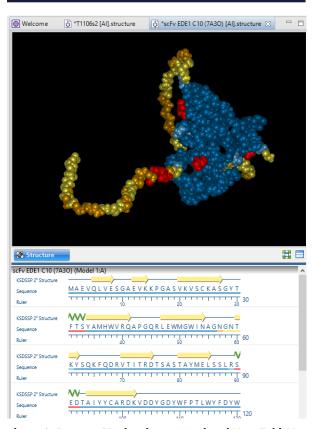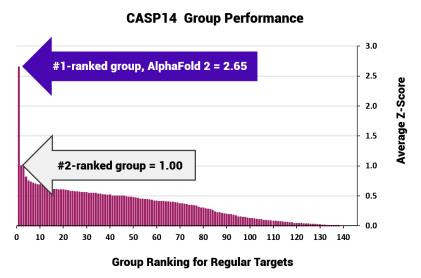

Figure 3. Protean 3D showing a completed NovaFold AI prediction for an scFv fusion protein from the anti-ZIKV (Zika virus) EDE1 monoclonal antibody C10.

We're here to help

We've designed NovaFold AI and Protean 3D to be fast and easy to use, but we know that computational biology can be challenging. That's why DNASTAR has dedicated staff to assist you in learning and using this workflow. To get started with NovaFold AI, simply contact us and request a free one-on-one webinar with one of our protein software experts.

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