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TECHNOLOGY VENTURES

Antibody Structure Prediction from Pre-trained Language Model (IgFold)

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Computer Electronics & Software

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Unmet Need:

Antibodies are able to bind a diverse set of antigens and have become critical therapeutics and diagnostic molecules. Antibody binding is facilitated by a set of six hypervariable loops that are diversified through genetic recombination and mutation. An accurate structural model of the hypervariable loops is essential for rational design of antibodies, but remains an expensive and time-consuming endeavor using traditional experimental methods. Even with recent advances, accurate computational prediction of these hypervariable loops remains a challenge. Therefore, there is a strong need for the development of more effective methods for structural models of hypervariable loops in antibody design.

Technology Overview:

Inventors at Johns Hopkins have developed IgFold, which is a fast method for antibody structure prediction using deep learning. IgFold consists of a pre-trained language model trained on 558 million natural antibody sequences followed by graph networks that directly predict backbone atom coordinates. IgFold predicts structures of similar or better quality than alternative methods in significantly less time. IgFold also provides accuracy estimations for each residue, which is helpful for determining whether to trust a predicted structure. As an example, IgFold predicted structures for 1.4 million paired antibody sequences, providing structural insights to 500-fold more antibodies than have experimentally determined structures.

Stage of Development:

Deployable model freely available for non-commercial use at https://github.com/Graylab/IgFold.

IgFold is available via a GitHub repository. Licensees may download it there. The completed license gives permission to use that code commercially.

References

1. Jeffrey A. Ruffolo, Lee-Shin Chu, Sai Pooja Mahajan & Jeffrey J. Gray(2023) , https://www.nature.com/articles/s41467-023-38063-x, https://www.nature.com/ncomms/, 14, 2389