An AI-Based Biomolecular Structure Prediction & Design Tool

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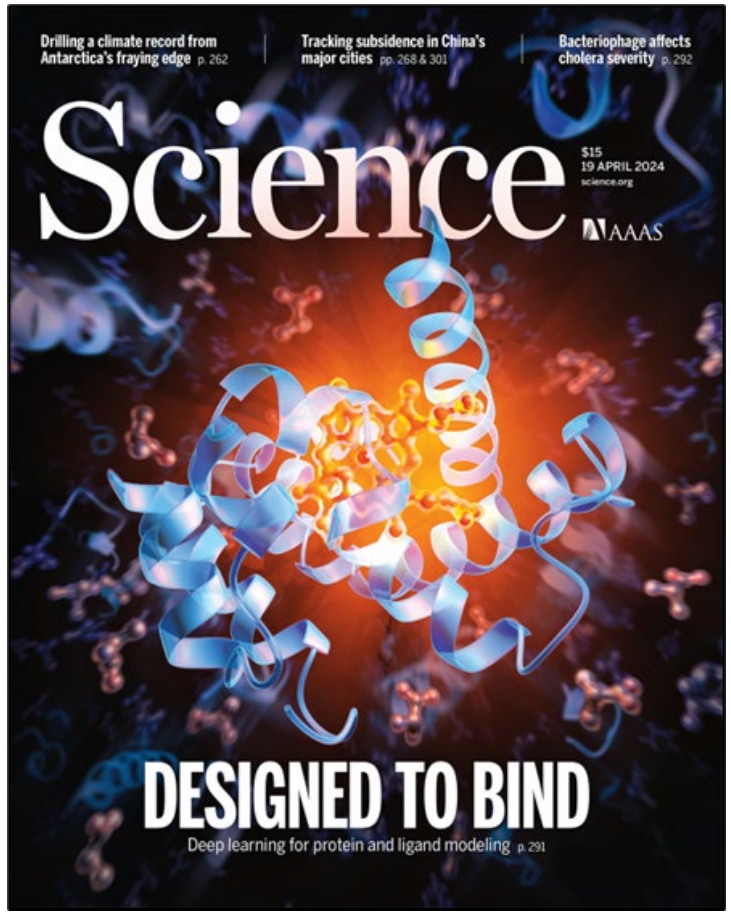
AMX



Scientific Achievement

Researchers developed a protein structure prediction & design tool, and experimentally validated its designs.

Significance and Impact

This capability could significantly impact drug design, biotechnology, and the study of biological processes.

Research Details

- Parameters including the element of each nonpolymer atom, the chemical bonds between atoms, and chirality were entered into RoseTTAFold All-Atom (RFAA).
- After input, the system was represented as a disconnected gas of amino acid residues, nucleic acid bases, and freely moving atoms, which was transformed into physically plausible structures.
- Designs were verified experimentally, in part, at the NSLS-II AMX beamline.

R. Krishna, J. Wang, W. Ahern, P. Sturmfels, P. Venkatesh, I. Kalvet, G.R. Lee, F. Morey-Burrows, I. Anishchenko, I.R. Humphreys, R. McHugh, D. Vafeados, X. Li, G.A. Sutherland, A. Hitchcock, C.N. Hunter, A. Kang, E. Brackenbrough, A.K. Bera, M. Baek, F. DiMaio, D. Baker, *Science* **6**, Vol 384, Issue 6693 (2024). DOI: 10.1126/science.adl2528

Work was performed in part at NSLS-II

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