

Google DeepMind and Isomorphic Labs release AlphaFold 3 for molecular interactions

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AlphaFold 3 predicts the structure and interactions of all of life's molecules

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Introducing AlphaFold 3, a new AI model developed by Google DeepMind and Isomorphic Labs. By accurately predicting the structure of proteins, DNA, RNA, ligands and more, and how they interact, we hope it will transform our understanding of the biological world and drug discovery.

Google DeepMind AlphaFold team

Isomorphic Labs

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In this article

Update November 11, 2024: As of November 2024, we have released AlphaFold 3 model code and weights for academic use to help advance research. Learn more about AlphaFold tools . Original post: Inside every plant, animal and human cell are billions of molecular machines. They're made up of proteins, DNA and other molecules, but no single piece works on its own. Only by seeing how they interact together, across millions of types of combinations, can we start to truly understand life's processes. In a paper published in Nature , we introduce AlphaFold 3, a revolutionary model that can predict the structure and interactions of all life's molecules with unprecedented accuracy. For the interactions of proteins with other molecule types we see at least a 50% improvement compared with existing prediction methods, and for some important categories of interaction we have doubled prediction accuracy. We hope AlphaFold 3 will help transform our understanding of the biological world and drug discovery. Scientists can access the majority of its capabilities, for free, through our newly launched AlphaFold Server , an easy-to-use research tool. To build on AlphaFold 3's potential for drug design, Isomorphic Labs is already collaborating with pharmaceutical companies to apply it to real-world drug design challenges and, ultimately, develop new life-changing treatments for patients. Our new model builds on the foundations of AlphaFold 2, which in 2020 made a fundamental breakthrough in protein structure prediction . So far, millions of researchers globally have used AlphaFold 2 to make discoveries in areas including malaria

vaccines, cancer treatments and enzyme design. AlphaFold has been cited more than 20,000 times and its scientific impact recognized through many prizes, most recently the Breakthrough Prize in Life Sciences . AlphaFold 3 takes us beyond proteins to a broad spectrum of biomolecules. This leap could unlock more transformative science, from developing biorenewable materials and more resilient crops, to accelerating drug design and genomics research.

7PNM - Spike protein of a common cold virus (Coronavirus OC43): AlphaFold 3's structural prediction for a spike protein (blue) of a cold virus as it interacts with antibodies (turquoise) and simple sugars (yellow), accurately matches the true structure (gray). The animation shows the protein interacting with an antibody, then a sugar. Advancing our knowledge of such immune-system processes helps better understand coronaviruses, including COVID-19, raising possibilities for improved treatments.

How AlphaFold 3 reveals life's molecules Given an input list of molecules, AlphaFold 3 generates their joint 3D structure, revealing how they all fit together. It models large biomolecules such as proteins, DNA and RNA, as well as small molecules, also known as ligands — a category encompassing many drugs. Furthermore, AlphaFold 3 can model chemical modifications to these molecules which control the healthy functioning of cells, that when disrupted can lead to disease. AlphaFold 3's capabilities come from its next-generation architecture and training that now covers all of life's molecules. At the core of the model is an improved version of our Evoformer module — a deep learning architecture that underpinned AlphaFold 2's incredible performance. After processing the inputs, AlphaFold 3 assembles its predictions using a diffusion network, akin to those found in AI image generators. The diffusion process starts with a cloud of atoms, and over many steps converges on its final, most accurate molecular structure. AlphaFold 3's predictions of molecular interactions surpass the accuracy of all existing systems. As a single model that computes entire molecular complexes in a holistic way, it's uniquely able to unify scientific insights.

7R6R - DNA binding protein: AlphaFold 3's prediction for a molecular complex featuring a protein (blue) bound to a double helix of DNA (pink) is a near-perfect match to the true molecular structure discovered through painstaking experiments (gray).

Leading drug discovery at Isomorphic Labs AlphaFold 3 creates capabilities for drug design with predictions for molecules commonly used in drugs, such as ligands and antibodies, that bind to proteins to change how they interact in human health and disease. AlphaFold 3 achieves unprecedented accuracy in predicting drug-like interactions, including the binding of proteins with ligands and antibodies with their target proteins. AlphaFold 3 is 50% more accurate than the best traditional methods on the PoseBusters benchmark without needing the input of any structural information, making AlphaFold 3 the first AI system to surpass physics-based tools for biomolecular structure prediction. The ability to predict antibody-protein binding is critical to understanding aspects of the human immune response and the design of new antibodies — a growing class of therapeutics. Using AlphaFold 3 in combination with a complementary suite of in-house AI models, Isomorphic Labs is working on drug design for internal projects as well as with pharmaceutical partners. Isomorphic Labs is using AlphaFold 3 to accelerate and improve the success of drug design — by helping understand how to approach new disease targets, and developing novel ways to pursue existing ones that were previously out of reach.

AlphaFold Server: A free and easy-to-use research tool

8AW3 - RNA modifying protein: AlphaFold 3's prediction for a molecular complex featuring a protein (blue), a strand of RNA (purple), and two ions (yellow) closely matches the true structure (gray). This complex is involved with the creation of other proteins — a cellular process fundamental to life and health.

Google DeepMind's newly launched AlphaFold Server is the most accurate tool in the world for predicting how proteins interact with other molecules throughout the cell. It is a free platform that scientists around the world can use for non-commercial research. With just a few clicks, biologists can harness the power of AlphaFold 3 to model structures composed of proteins, DNA, RNA and a selection of ligands, ions and chemical modifications. AlphaFold Server helps scientists make novel hypotheses to test in the lab, speeding up workflows and enabling further innovation. Our platform gives researchers an accessible way to generate predictions, regardless of their access to computational resources or their expertise in machine learning. Experimental protein-structure prediction can take about the length of a PhD and cost hundreds of thousands of dollars. Our previous model, AlphaFold 2, has been used to predict hundreds of millions of structures, which would have taken hundreds of millions of researcher-years at the current rate of experimental structural biology.

Sharing the power of AlphaFold 3 responsibly With each AlphaFold release, we've sought to understand the broad

impact of the technology , working together with the research and safety community. We take a science-led approach and have conducted extensive assessments to mitigate potential risks and share the widespread benefits to biology and humanity. Building on the external consultations we carried out for AlphaFold 2, we've now engaged with more than 50 domain experts, in addition to specialist third parties, across biosecurity, research and industry, to understand the capabilities of successive AlphaFold models and any potential risks. We also participated in community-wide forums and discussions ahead of AlphaFold 3's launch. AlphaFold Server reflects our ongoing commitment to share the benefits of AlphaFold, including our free database of 200 million protein structures. We'll also be expanding our free AlphaFold education online course with EMBL-EBI and partnerships with organizations in the Global South to equip scientists with the tools they need to accelerate adoption and research, including on underfunded areas such as neglected diseases and food security. We'll continue to work with the scientific community and policy makers to develop and deploy AI technologies responsibly.

Opening up the future of AI-powered cell biology

7BBV - Enzyme: AlphaFold 3's prediction for a molecular complex featuring an enzyme protein (blue), an ion (yellow sphere) and simple sugars (yellow), along with the true structure (gray). This enzyme is found in a soil-borne fungus (*Verticillium dahliae*) that damages a wide range of plants. Insights into how this enzyme interacts with plant cells could help researchers develop healthier, more resilient crops.

AlphaFold 3 brings the biological world into high definition. It allows scientists to see cellular systems in all their complexity, across structures, interactions and modifications. This new window on the molecules of life reveals how they're all connected and helps understand how those connections affect biological functions — such as the actions of drugs, the production of hormones and the health-preserving process of DNA repair. The impacts of AlphaFold 3 and our free AlphaFold Server will be realized through how they empower scientists to accelerate discovery across open questions in biology and new lines of research. We're just beginning to tap into AlphaFold 3's potential and can't wait to see what the future holds.

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