

The 2024 Chemistry Nobel Prize and the New Era of AI in Chemistry and Biology

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Highlights

The 2024 Nobel Prize in Chemistry recognized the AI revolution in protein prediction and design, marking a turning point for molecular science. AlphaFold and computational design mark a new era in chemistry and biology.

Abstract

The 2024 Nobel Prize in Chemistry was awarded to David Baker, Demis Hassabis, and John M. Jumper for revolutionizing how we design and understand proteins: one half to Baker “for computational protein design,” and the other half jointly to Hassabis and Jumper “for protein structure prediction” (notably through AlphaFold), paving the way for the creation of enzymes, medicines, and materials with unprecedented precision and transformative impact on chemistry and biology.

This Nobel also highlights the central role of Artificial Intelligence in contemporary chemical and biological research. Deep learning models such as AlphaFold have demonstrated that it is possible to learn structural principles directly from data and generalize across thousands of proteins, while computational design, now increasingly driven by generative models and many-objective optimization, enables the creation of sequences and molecules with desired properties.

Equally crucial to these advances was the Critical Assessment of Protein Structure Prediction (CASP), a community-wide experiment that, since 1994, has provided a rigorous and transparent framework for objectively measuring progress in protein modeling. Through its blind prediction challenges, CASP established a shared scientific benchmark, revealing both strengths and limitations of competing methods and driving decades of continuous improvement. This benchmarking culture ultimately led to AlphaFold’s breakthrough performance at CASP14, where predicted structures reached near-experimental accuracy.

In this lecture, we will discuss the paradigm shift toward data-driven science exemplified by the 2024 Nobel Prize in Chemistry and its profound implications for the future of research in chemistry and biology. Fonte Arial 10 espaçamento simples. Insira o seu texto completo (em inglês preferencialmente, ou português), bem como tabelas, esquemas, figuras e referências nesta área. Em qualquer situação o resumo deve ser contido em **uma página**, respeitando-se as margens do template.

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