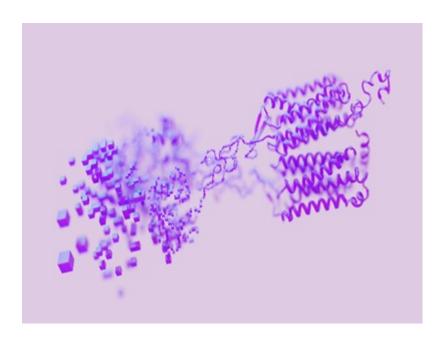


# **Deep Learning Approaches for Protein Scaffolding**

This technology uses advanced deep learning methods to design proteins with specific functional sites, offering a novel approach to protein design that is both efficient and versatile.



# **Technology ID**

BDP 8458

# **Category**

Therapeutics/Platform
Technology
Selection of Available
Technologies
Therapeutics/Other

### **Authors**

David Baker

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### What is the Problem?

Protein design is a critical aspect of synthetic biology, with applications ranging from drug development to environmental solutions. However, designing proteins that perform specific functions remains a significant challenge. Traditional methods require the specification of the fold or secondary structure of the scaffold, which can be complex and time-consuming.

# What is the Solution?

The technology leverages deep learning to scaffold functional sites in proteins without needing to pre-specify the fold or secondary structure of the scaffold. It uses two approaches: "constrained hallucination" and "inpainting". Constrained hallucination optimizes sequences such that their predicted structures contain the desired functional site. Inpainting starts from the functional site and fills in additional sequence and structure to create a viable protein scaffold in a single forward pass through a specifically trained network. These methods have been used to design candidate immunogens, receptor traps, metalloproteins, enzymes, and

protein-binding proteins.

# What is the Competitive Advantage?

The technology offers a more efficient approach to protein design by eliminating the need to pre-specify the fold or secondary structure of the scaffold. This approach for designing functional sites does not require any user inputs, other than the structure and sequence of the desired functional site. It can be applied to a wide range of protein design problems, making it a versatile tool in the field of synthetic biology.

### **Patent Information:**

# US20230416726A1

### **References**

 Wang, J., Lisanza, S., Juergens, D., Tischer, D., Watson, J. L., Castro, K. M., Ragotte, R., Saragovi, A., Milles, L. F., Baek, M., Anishchenko, I., Yang, W., Hicks, D. R., Expòsit, M., Schlichthaerle, T., Chun, J. H., Dauparas, J., Bennett, N., Wicky, B. I. M., Muenks, A., DiMaio, F., Correia, B., Ovchinnikov, S., Baker, D.(2022), https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9621694/, https://www.science.org/journal/science, 377, 387-394