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A General Method For Designing Self-Assembling Protein Nanomaterials

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OTHER INFORMATION

KEYWORDS

Protein design, protein assembly, self-assembly, nanomaterial, self-assembling protein nanomaterial, drug delivery, protein cage, molecular machine

CATEGORIZED AS

- **Biotechnology**
 - Health
 - Other
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2012-648-0

SUMMARY

UCLA researchers in the Department of Chemistry & Biochemistry have developed a novel computational method for designing proteins that self-assemble to a desired symmetric architecture. This method combines symmetrical docking with interface design, and it can be used to design a wide variety of self-assembling protein nanomaterials.

BACKGROUND

Molecular self-assembly is the process by which molecules adopt a defined arrangement directed through non-covalent interactions (e.g. hydrogen bonding, metal coordination, hydrophobic forces, van der Waals forces, π - π interactions, and/or electrostatic), as well as electromagnetic interactions. Molecular self-assembly allows the construction of challenging molecular topologies, and it is a powerful approach to create shapes and patterns on the atomic scale. The functional and physical properties of proteins make them attractive as building blocks for the development of advanced functional nanomaterials.

Previous approaches have used coiled-coil and helical bundle interactions, engineered disulfide bonds, chemical crosslinks, metal-mediated interactions, templating by non-biological materials in conjunction with computational interface design, or genetic fusion of multiple protein domains or fragments that naturally self-associate as the driving force for interactions between the subunits in self-assembling structure. Designing assemblies based on non-covalent interactions is difficult and has poor precision because of the complexities of modeling protein structures and energetics.

INNOVATION

Researchers at UCLA have developed a novel computational method for designing self-assembling protein materials. Protein building blocks are docked together symmetrically to identify complementary packing arrangements, and low-energy protein-protein interfaces are designed between the building blocks in order to drive self-assembly. When tested, the designed proteins assemble to the desired oligomeric state that closely match the designed models in solution.

APPLICATIONS

- ▶ Self-assembling functional protein nanomaterials
- ▶ Biomimetic materials
- ▶ Protein cage for drug delivery
- ▶ Custom designed molecular machines

ADVANTAGES

- ▶ Self-assembling protein materials can be designed with higher accuracy at atomic level
- ▶ This method is applicable to the design of a broad range of symmetric materials

STATE OF DEVELOPMENT

This design strategy has been successfully tested with atomic level accuracy.

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Issued Patent	8,969,521	03/03/2015	2012-648

RELATED MATERIALS

- ▶ King, Neil P., William Sheffler, Michael R. Sawaya, Breanna S. Vollmar, John P. Sumida, Ingemar André, Tamir Gonen, Todd O. Yeates, and David Baker. "Computational design of self-assembling protein nanomaterials with atomic level accuracy." *Science* 336, no. 6085 (2012): 1171-1174.

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