세미나 초록

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발표 주제	Computational design of *de novo* protein nanostructures and experimental validations
발표 내용	Protein nanostructures such as nanocages, nanofibers, and patterned layers are often found in nature or by designand involved in diverse biological functions including delivering genetic materials, activating immune systems, and causing diseases (1). Hence, there is considerable interest in designing artificial protein nanostructures capable of controlling such biological phenomena. For past decades, computational protein design approach has been focused on physics-based methods, for instance, calculating scoring functions defined by theoretical chemistry and physics (2), but recent development of AI-based approaches, such as folding prediction, sequence design and protein generative model (3,4), have dramatically expanded our capable range of protein structure design. In this talk, I will introduce an overview of computational design for *de novo* protein nanostructures using AI-based software and show several examples of designed nanostructures including virus-like nanocages. Experimentally, the designed proteins were expressed in *E. Coli.,* and the designed nanostructureswere validated by electron microscope. **References** 1. J. Zhu, N. Avakyan, A. Kakkis et al., "Protein Assembly by Design", Chem. Rev., 121, 22, 13701-13796 (2021) 2. J. K. Leman, B. D. Weitzner, S. M. Lewis et al., "Macromolecular modeling and design in Rosetta: recent methods and frameworks", Nature Methods, 17, 665-680 (2020) 3. J. Dauparas, I. Anishchenko, N. Bennett et al., "Robust deep learning-based protein sequence design using ProteinMPNN", Science, 378, 6615, 49-56 (2022) 4. J. L. Watson, D. Juergens, N. R. Bennett et al., "De novo design of protein structure and function with RFdiffusion", Nature, 620, 1089-1100 (2023)