Special Issue

Applications of Large Language Models to Identify and Predict Bio-Activity of Proteins and Peptides

Message from the Guest Editor

A natural protein or peptide can be thought of as a sentence consisting of a linear chain of residues and a vocabulary of 20 standard amino acids. The order in which amino acids are arranged determines the tertiary structure of proteins in their environment, which in turn gives them specific functions, which we can understand as the meaning of protein/peptide sentences. Understanding the relationship between protein sequences, structure, and function has long been a major focus of biological research. With the development of deep learning, especially pre-trained language models, the development of machine learning models based only on sequences but that can capture the structural and functional properties of proteins has been a field that researchers around the world have been vigorously expanding. Based on the above ideas, many protein language models (PLMs) have been developed, such as UniRep, ESM1, ESM2, and ESM3. Through sequence "semantic" pre-training, PLMs learn the fundamentals of protein structure and function, enabling them to perform a wide range of protein modeling and design tasks.

Guest Editor

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As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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