AI-powered Protein Modelling and Design

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The field of computational protein design (CPD) is currently experiencing an unprecedented phase of development, significantly impacting biotechnology. Our advanced CPD technologies leverage a unique combination of automated reasoning and machine/deep learning algorithms, along with molecular modeling and simulation methods, to enable the rational design of tailored proteins. The original automated reasoning capacities provide accuracy and computational efficiency, while also offering the ability to integrate design requirements together with physics-based models and/or learning-based models from various sources of protein data (including, sequence, structure, biochemical/biophysical data). This comprehensive approach provides effective means to efficiently address design challenges and pursue complex design objectives, which can be indirectly learned through machine/deep learning. The synergy between these AI algorithms and molecular simulations empowers us to consider multiple molecular and conformational states crucial for protein function. In this presentation, I will focus on our latest advances in CPD, highlighting their capabilities, with an emphasis on their application in the field of enzyme, molecular assembly and protein binder engineering for biotechnologies and health.

KEYWORDS:. AI; protein design; molecular modelling; machine/deep learning; automated reasoning