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Tutorial 2: The impact of artificial intelligence (AI) and computer simulations on biomolecular research

Monday, 15 May 2023 16:00 (1 hour)

Advances in computer science, particularly in the field of AI, is having a significant impact on biomolecular research. AI methods such as deep neural networks have shown great promise in predicting protein structures as demonstrated by the AlphaFold project [1]. Here, I will outline recent achievements as well as present a case study that benchmarks AlphaFold's performance for G protein-coupled receptors (GPCRs) - a large and diverse family of membrane proteins that are involved in many physiological processes. For this, we carried out a comprehensive structural analysis and large-scale molecular simulations for hundreds of GPCRs from AlphaFold in different activation states (active, inactive). In a second case study, I will highlight the potential of atomistic computer simulations [2] to sample the dynamics of thousands of intramolecular contacts in a prototypical GPCR linked to relevant functional signaling outcomes. All in all, this lecture will shed light on the advancements but also existing challenges of AI and computer simulations to study complex biological systems such as GPCRs.

1. Jumper J et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021;596(7873):583-589.
2. Rodríguez-Espigares I, Torrens-Fontanals M et al. GPCRmd uncovers the dynamics of the 3D-GPCRome. Nat Methods. 2020;17:777-787.

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