INVITED SPEAKER

STRUCTURAL BIOLOGY IN A POST-ALPHAFOLD WORLD

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For many years, methods for protein structure prediction improved steadily but slowly, with the quality of predicted structures depending very much on the existence of recognisable homologues in the PDB. The sudden leap in performance by first AlphaFold in 2018 and then AlphaFold2 in 2020 took the community by surprise. The predicted structures are of high quality whether or not there are homologues in the PDB; they are not yet as good as actual experimental structures, but the confidence measures that come with the models give a reliable guide to quality. There is still a great need for experimental structure determination, but how it is done in practice is changing rapidly with the availability of good-quality models. For crystallography, molecular replacement will become even more dominant as a method for structure solution, and experimental phasing methods will be needed only rarely for protein structures. More importantly, the availability of structure information for the majority of the known proteome wil enable new science, analogous to the boost from large-scale genomics.