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【901】Using physics to interpret co-evolutionary data for proteins: protein structure and protein-protein interaction reconstruction

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In order to preserve the structure, and thus the function, of proteins and protein complexes, evolution must mutate amino-acids carefully, trying to introduce concerted changes (e.g. positive/negative charge contact turns into negative/positive charge contact). The simultaneous analysis of the sequences of the same protein from a multitude of organisms highlights where these correlated mutations (co-evolution) has taken place, and this information can be used, in principle, to discover which contacts are important and to consequently predict the structure of as protein and of protein complexes.
Remarkably, this intuitive goal has been hampered for a long time by the inability of algorithms to disentangle between direct and indirect correlations. In 2009 a new algorithm, based on the mapping of the space of sequences on the configurations of magnetic systems, has resolved the problem, and has ushered a new era, where sequence analysis can complement both experimental techniques and other computational approaches.
In this presentation, I will present the state of the art and some applications that have allowed us to propose new protein complexes and the structure of some complexes whose structure has not yet been determined experimentally.

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