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Big Data Analytics in Biology: Biomolecular Structure Prediction and Beyond by Tracing Residue Co-Evolution

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One grand challenge of life sciences in the coming years is to fully leverage experimental progress like high-throughput sequencing by taking advantage of recent advances in other disciplines, in particular in information technology. Exploring the interrelationship of structure and function is crucial for understanding life on the molecular level. Yet despite significant progress of experimental methods, the crucial structural characterization of many important proteins and non-coding RNA (ncRNA)- typically preceding any detailed mechanistic exploration of their function- remains challenging. Typically, such work has focused on proteins as "molecular workhorses"of cells, yet recent work has attributed more and more crucial functions to ncRNA as most of eukaryotic genomes does not code for proteins. Our vision is to develop the technological and algorithmic framework for mining these vast amounts of raw sequence data with the goal of predicting experimentally poorly accessible biomolecular structures by tracing residue co-evolution. Going beyond structure prediction, we can also link co-evolutionary patterns to functional questions like antibiotic drug resistance.

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