BIOMATERIALS

Forces in Biomolecular Systems SFB 863

# Protein and RNA Structure Prediction through Co-Evolutionary Information


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Abstract:

Exploring the interrelationship of structure and function is crucial for the understanding of molecular life. Despite significant progress of experimental methods, the structural characterization of important structures for both proteins and RNA – typically preceding any detailed mechanistic exploration of their function – remains challenging. In recent years, increasingly ubiquitous availability of sequential information and advanced statistical analysis has allowed to trace the co-evolution of residues and predict partial contact maps. These contact maps can be exploited in structure prediction tools. One maximum entropy based approach is called Direct Coupling Analysis (DCA)[1] and, e.g., was found to be sufficient for the blind prediction of a protein complex [2] and its active conformation[3] later confirmed by experiment. For RNA, it is comparably simple to predict RNA secondary structure. Predicting tertiary contacts has remained – despite significant effort – an elusive task met with limited success. In contrast, our novel rnaDCA is able to extract tertiary contacts from genomic data. We further demonstrate that these tertiary contacts are sufficient to systematically improve tertiary RNA prediction quality [4]. Considering the large gap of known ncRNA sequences to experimentally resolved tertiary structures, we are convinced that this will significantly impact all structural RNA related research.



References

[1] Weigt M et al., Proc Nat Acad Sci USA (2009) 106, 67-72; F. Morcos et al., Proc Nat Acad Sci (2011) 108, E1293-E1301
[2] Schug A et al., Proc Nat Acad Sci USA (2009) 106, 22124-22129
[3] Dago A et al., Proc Nat Acad Sci USA (2012), 109: E1733-42
[4] E. De Leonardis et al. Direct-Coupling Analysis of nucleotide coevolution facilitates RNA tertiary structure prediction, (submitted)


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