Geometric coarse-grained models and knowledge-based potentials for biomolecular structure evaluation

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Many biological processes of therapeutic interest, such as gene regulation, involve RNA molecules and their interactions with large protein assemblies. Recent high-throughput experiments have yielded insights into mechanisms of these processes but often structural models showing important structural features and interactions are lacking. Using 3D data available for proteins and RNA, we derived knowledge-based potentials to predict protein and nucleic-acid 3D structure. In combination with appropriate geometric representations, we obtained fast and accurate all-atom and coarse-grained predictions of biomolecular structures. We will show how we can accurately build knowledge-based potentials from various all-atom and coarse-grained measures. Using this method and an encoding of multi-body contacts through arrangement of circles on a sphere, we obtained a reasonable model of protein structure [1]. We also applied this strategy to assess RNA structures and showed that it is currently one of the best performing potentials for RNA structure evaluation [2]. These results suggest that our knowledge-based models may also be suitable for the study of RNA dynamics and interactions.

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2. Bernauer J, Huang X, Sim AYL, Levitt M: Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation. *RNA* in press.