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Investigation of SHAPE mechanism with RNA 3D structure modeling PEINAN ZHAO, TRAVIS HURST, XIAOJUN XU, Department of Physics and Department of Biochemistry, University of Missouri, Columbia, MO 65211, KEVIN WEEKS, Department of Chemistry, University of North Carolina, Chapel Hill, NC 27599-3290, SHIJIE CHEN, Department of Physics and Department of Biochemistry, University of Missouri, Columbia, MO 65211, SHIJIE TEAM
— Selective 2′-hydroxyl acylation by primer extension (SHAPE) chemical probing method for RNA reflects local structural dynamics, which is intrinsically related to RNA three-dimensional structure. To gain quantitative insights into the relationship between RNA three-dimensional structure and SHAPE reactivity, we develop an algorithm to rebuild the SHAPE profile from the three-dimensional structure. The algorithm starts from RNA structures and combines nucleotide interaction strength and conformational flexibility, ligand (SHAPE reagent) accessibility and base-pairing pattern through a composite function. Comparisons between the predicted SHAPE profile and experimental SHAPE data show high correlation, suggesting the validity of the extracted analytical function. The validity of the theory supports the model for the key factors that determine SHAPE reactivity profile. Furthermore, the theory offers an effective method to select viable RNA three-dimensional structures from an ensemble of decoy structure models.

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