

“To *B* or not to *B*” in Nucleic Acids Chemistry

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Nucleic acids (DNA and RNA) are genetic materials in living organisms and formed by a sequence of nucleobases. The stability of nucleic acids structures cannot be determined from only the sequence composition, as this property critically depends on the surrounding environment of the solution. The intracellular condition is greatly different from that of the diluted buffer typically used for standard experiments and is not constant in each local area of the cell. Thus, to make excellent nanomaterials with nucleic acids working in cells, stability predictions should reflect the situation under intracellular conditions and are required importantly. In this lecture, I will provide an overview of the basic concepts, methods, and applications of predicting the stabilities of nucleic acid structures.¹⁻¹¹ I explain the theory of the most successful prediction method based on a nearest-neighbor (NN) model. To improve the versatility of prediction, corrections for various solution conditions considered hydration have been investigated. I also describe advances in the prediction of non-canonical structures of G-quadruplexes and i-motifs. Finally, studies of intracellular analysis and stability prediction are discussed for the application of NN parameters for human health and diseases.

Selected important papers published in recent several years

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11. N. Sugimoto ed., “Handbook of Chemical Biology of Nucleic Acids” SPRINGER NATURE, 2023, Vols 1, 2, and 3.

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