"To B or not to B" in Nucleic Acids Chemistry

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In this lecture, I will provide an overview of the basic concepts, methods, and recent applications of predicting the stabilities and functions of nucleic acid structures. I explain the theory of the most successful prediction method based on a nearest-neighbor (NN) model. To improve the versality of prediction, corrections for various solution conditions considered hydration have been investigated. I also describe advances in the prediction of non-canonical nucleic acids 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.

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Selected publications from our group in recent several years:

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5. Takahashi, S., Ghosh, S., Trajkovski, M., Ohyama, T., Plavec, J., Sugimoto, N. Twisting tetraplex DNA: A strand dynamics to regulate i-motif function in diverse molecular crowding environments. ***Nucleic Acids Res.***, 53, gkaf500 (2025).
6. Liu, L., Takahashi, S., Ghosh, S., Endoh, T., Yoshinaga, N., Numata, K., Sugimoto, N. Predictability of environment-dependent formation of G-quadruplex DNAs in human mitochondria. ***Comm. Chem.***, 8, 135 (2025).
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