## "To <u>B</u> or not to <u>B</u>" in Nucleic Acids Chemistry

Naoki Sugimoto<sup>1,2</sup>

<sup>1</sup> Frontier Institute for Biomolecular Engineering Research (FIBER), Konan University, <sup>2</sup> Graduate School of Frontiers of Innovative Research in Science and Technology (FIRST), Konan University, 7-1-20 Minatojima-minamimachi, Kobe, 650-0047, Japan E-mail: sugimoto@konan-u.ac.jp

In this presentation, I will provide an overview of the basic concepts, methods, and applications of predicting the stabilities of nucleic acid structures. We 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 structures. Finally, studies of intracellular analysis and prediction are discussed for the application of NN parameters

**Acknowledgements**: The author is grateful to the colleagues named in the cited following references from my laboratory, institute (FIBER), and others. This work was supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) and the Japan Society for the Promotion of Science (JSPS) (Grant No. JP17H06351, 18KK0164, 19H00928, and 20K21258), especially for Grant-in-Aid for Scientific Research (S) (22H04975) and JSPS Core-to-Core Program (JPJSCCA20220005), The Hirao Taro Foundation of Konan Gakuen for Academic Research, and The Chubei Itoh Foundation.

## **Recent References from Our Research Group**

*Nucleic Acids Res.* **2023**, *51*, in press; *Sci. Adv.* **2022**, *8*, eadc9785; *Chem. Commun.* **2022**, *58*, 12459–12462; *J. Am. Chem. Soc.* **2022**, *144*, 5956-5964; *Anal. Chem.* **2022**, *94*, 7400-7407; *Chem. Commun.* **2022**, *58*, 5952-5955, *Sci. Rep.*, **2022**, *12*,1149; *J. Am. Chem. Soc.* **2021**, *143*, 16458–16469; *Bull. Chem. Soc. Jpn.* **2021**, *94*, 1970-1998; *ACS Chem .Biol.* **2021**, *16*, 1147–1151;*RSC Adv.* **2021**, *11*, 37205-37217; *Nucleic Acids Res.* **2021**, *49*, 7839–7855; *Topics Curr. Chem.* **2021**, *379*, 17; *Nucleic Acids Res.* **2021**, *49*, 8449–8461; *Acc. Chem.Res.* **2021**, *54*, 2110-2120; *Chem. Soc. Rev.* **2020**, *49*, 8439–8468; *Chem. Commun.* **2020**, *56*, 2379–2390; *RSC Adv.* **2020**, *10*, 33052–33058; *Biochemistry.* **2020**, *59*, 2640–2649; *Proc. Natl. Acad. Sci. U.S.A.* **2020**, *117*, 14194–14201; *Anal. Chem.* **2020**, *92*, 7955–7963; *Biochemistry.* **2020**, *59*, 1972–1980; *Ncleic Acids Res.* **2020**, *48*, 3975–3986; *Biochem. Biophys. Res. Commun.* **2020**, *55*, 177–183; *Chem. Commun.* **2020**, *56*, 2379–2390; *Sci. Rep.* **2020**, *10*, 2504 and **Sugimoto**, **N.** "Chemistry and Biology of Non-Canonical Nucleic Acids" *WILEY.* **2021**, *1–*288.



Naoki Sugimoto. Kyoto University (BS, 1979; MS, 1982; Ph.D. 1985, Prof. Jiro Osugi), University of Rochester, USA (Postdoc, 1985-1988, Prof. Douglas H. Turner), Konan University (Assistant Prof., 1988-1991; Associate Prof. 1991-1994; Full Prof. 1994-present). Director of FIBER, Konan University (2003-present). [Field of research] Nucleic Acids Chemistry, which is the Field of Dreams.