Department of Chemistry
香港城市大學
City University of Hong Kong

Special Departmental Seminar

By

Prof. Naoki Sugimoto

Distinguished Professor

Frontier Institute for Biomolecular Engineering Research (FIBER)
Konan University
Kobe, Japan

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

Date: **8 January 2025 (Wednesday)**

Time: **10:30am – 11:30am**
Venue: **YEUNG-Y4302 (Yellow Zone, 4th Floor)**
Yeung Kin Man Academic Building
City University of Hong Kong
Tat Chee Avenue, Kowloon Tong

For abstract, please refer to the attached sheet.

Contact: Prof. KWOK Chun Kit (3442-6858, ckkwok42@cityu.edu.hk)

~ All Are Welcome ~

Abstract

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 versality 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

1. H. Tateishi-Karimata, K. Kawauchi, S. Takahashi, and N. Sugimoto, Development of a Pseudocellular System to Quantify Specific Interactions Determining the G-Quadruplex Function in Cells, ***J. Am. Chem. Soc.,*** **146**, 12, 8005–8015 (2024)
2. D. Banerjee, H. Tateishi-Karimata, M. Toplishek, T. Ohyama, S. Ghosh, S. Takahashi, M. Trajkovski, J. Plavec, and N. Sugimoto, In-Cell Stability Prediction of RNA/DNA Hybrid Duplexes for Designing Oligonucleotides Aimed at Therapeutics, ***J. Am. Chem. Soc.,*** **145**, 43, 23503-23518 (2023)
3. S. Ghosh, S. Takahashi, D. Banerjee, T. Ohyama, T. Endoh, H. Tateishi-Karimata, and N. Sugimoto Nearest-neighbor parameters for the prediction of RNA duplex stability in diverse in vitro and cellular-like crowding conditions, ***Nucleic Acids Res.*** **51**, 4101-4111 (2023)
4. Y. Zhang, H. Tateishi-Karimata, T. Endoh, Q. Jin, K. Li, X. Fan, Y. Ma, L. Gao, H. Lu, Z. Wang, AE. Cho, X. Yao, C. Liu, N. Sugimoto, S. Guo, X. Fu, Q. Shen, G. Xu, LR. Herrera-Estrella, and X. Fan, High-temperature adaptation of an OsNRT2.3 allele is thermoregulated by small RNAs, ***Sci. Adv.***, **8**, eadc9785 (2022)
5. K. T. McQuaid, S. Takahashi, L. Baumgaertner, D. J. Cardin, N. G. Paterson, J. P. Hall, N. Sugimoto, and C. J. Cardin, Ruthenium Polypyridyl Complex Bound to a Unimolecular Chair-Form G-Quadruplex, ***J. Am. Chem. Soc.***, **144**, 5956-5964 (2022)
6. S. Takahashi, A. Kotar, H. Tateishi-Karimata, S. Bhowmik, Z.-F. Wang, T.-C. Chang, S, Sato, S. Takenaka, J. Plavec, and N. Sugimoto, Chemical Modulation of DNA Replication along G-Quadruplex Based on Topology-Dependent Ligand Binding, ***J. Am. Chem. Soc.***, **143**, 16458-16469 (2021)
7. S. Ghosh, S. Takahashi, T. Ohyama, T. Endoh, H. Tateishi-Karimata, and N. Sugimoto, Nearest-neighbor parameters for predicting DNA duplex stability in diverse molecular crowding conditions, ***Proc. Natl. Acad. Sci. USA.***, **117**, 25, 14194-14201 (2020)
8. S. Takahashi, K. T. Kim, P. Podbevšek, J. Plavec, B. H. Kim, and N. Sugimoto, Recovery of the formation and function of oxidized G-quadruplexes by a pyrene-modified guanine-tract, ***J. Am. Chem. Soc.***, **140**, 5774–5783 (2018)
9. H. Tateishi-Karimata, K. Kawauchi, and N. Sugimoto, Destabilization of DNA G-quadruplexes by chemical environment changes during tumor progression facilitates transcription, ***J. Am. Chem. Soc.***, **140**, 642-651 (2018)
10. A. B. Rode, T. Endoh, and N. Sugimoto, Crowding shifts the FMN recognition mechanism of riboswitch aptamer from conformational selection to induced Fit, ***Angew. Chem. Int. Ed.***, **57**, 6868-6872 (2018)
11. N. Sugimoto ed., **"Handbook of Chemical Biology of Nucleic Acids"** *SPRINGER NATURE,* 2023, Vols 1, 2, and 3.

Acknowledgements : The author is grateful to the colleagues named in the cited papers 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), JSPS Core-to-Core Program (JPJSCCA20220005), The Hirao Taro Foundation of Konan Gakuen for Academic Research, and The Chubei Itoh Foundation.

Biography

Naoki Sugimoto is received Ph.D. in 1985 from Kyoto University, Japan. After postdoctoral work at University of Rochester, NY in USA, he joined Konan University, Kobe, Japan in 1988 and was a full professor from 1994 to 2024. From 2003 to 2024, he was also a director of Frontier Institute for Biomolecular Engineering Research (FIBER) at Konan University and now is a Distinguished Professor of Konan University. He was a first chairman of Forum on Biomolecular Chemistry (FBC) from 1998 to 2001, and a chairman of Division of Biofunctional Chemistry of the Chemical Society of Japan (CSJ) from 2011 to 2013. He was a president of the Japan Society of Nucleic Acids Chemistry (JSNAC) from 2017 to 2020. He is a member of the Editorial Board of *Nucleic Acids Research* and *Scientific Reports*, and so on. He received the Dr. Masao Horiba's Award in 2004, Distinguised Scientist Award from ICA (International Copper Association), New York, USA in 2005, Hyogo Science Award from Hyogo Prefecture, Japan in 2006, the CSJ Award for Creative Work in 2007, the Honorable Speaker for Applied Chemistry Lecture Series from the Chinese Academy of Sciences in 2011, Contribution Award from the Japan Society of Coordination Chemistry (JSCC) in 2014, The Imbach-Townsend Award from IS3NA (International Society for Nucleosides, Nucleotides, and Nucleic Acids), San Diego, USA in 2018, The Chemical Society of Japan Award (Top Award) in 2020, Ikehara Award (Top Award) from JSNAC (The Japan Society of Nucleic Acids Chemistry), and so on. His research interests focus on Biophysical Chemistry, Biomaterials, Bio-nano engineering, Molecular design, Biofunctional Chemistry, and Biotechnology. He has published more than 500 scientific papers, reviews, and books.