



**SZKOŁA DOKTORSKA  
BioMedChem**

Uniwersytetu Łódzkiego  
i Instytutów Polskiej  
Akademii Nauk w Łodzi



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20 maja, 2024

## ZAPROSZENIE

W imieniu Dyrekcji Centrum Badań Molekularnych i Makromolekularnych i Prezesa Łódzkiego Oddziału Polskiej Akademii Nauk oraz w imieniu Dyrektora Szkoły Doktorskiej BioMedChem Uniwersytetu Łódzkiego i Instytutów Polskiej Akademii Nauk w Łodzi mamy zaszczyt zaprosić na serię wykładów, które wygłosi

### Profesor Naoki SUGIMOTO

a Distinguished Professor of Konan University, Kobe, Japan,  
Director of Frontier Institute for Biomolecular Engineering Research (FIBER)

#### Plan wykładów:

**4 czerwca godz. 11.00 – 12.00**

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

Wykład dla naukowców środowiska łódzkiego (UŁ, PŁ, UMED, IBM PAN, CBMiM PAN)

**5 czerwca godz. 9.00-10.30**

##### **Basic Physical Chemistry of Nucleic Acids**

Wykład dla doktorantów Szkół Doktorskich i młodszych pracowników naukowych środowiska łódzkiego

**6 czerwca godz. 9.00-10.30**

##### **Applied Physical Chemistry of Nucleic Acids**

Wykład dla doktorantów Szkół Doktorskich i młodszych pracowników naukowych środowiska łódzkiego

*Wszystkie wykłady będą odbywały się w Centrum Badań Molekularnych i Makromolekularnych  
Polskiej Akademii Nauk (CBMiM PAN), ul. Sienkiewicz 112, Budynek A, sala 08/09,*

*Jest możliwość parkowania samochodu na terenie Instytutu (ograniczona ilość) lub na  
sąsiednich ulicach*

## **Streszczenie wykładu**

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

**Naoki Sugimoto**

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

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. 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.

**Keywords:** Nucleic acids, stability prediction, nearest-neighbor (NN) parameters, G-quadruplex, i-motifs.

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## 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) [Selected as a Supplementary Cover]
- (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)

## CV



### **Naoki Sugimoto**

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

### **Biography**

Naoki Sugimoto 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, Distinguished 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, 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, with more than 9 000 citations, h=47.