

Daisuke Miyata, PhD

Innovation and Technology Department, Production Technology Innovation Center,
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EDUCATION

- 2018 – 2021 **Ph.D. in Pharmaceutical Sciences**
Tohoku University, Graduate School of Pharmaceutical Sciences
Thesis: Development of Theoretical Analysis Methods for Infrared Absorption Spectra and Their Application to Static and Dynamic Structural Analysis of Proteins
Supervisor: Takakazu Nakabayashi
- 2016 – 2018 **Master of Pharmaceutical Sciences**
Tohoku University, Graduate School of Pharmaceutical Sciences
Thesis: Main-Chain Structural Analysis of Polyproline by Combining Infrared Spectroscopy and Theoretical Calculations
Supervisor: Takakazu Nakabayashi
- 2012 – 2016 **Bachelor of Pharmaceutical Sciences**
Meiji Pharmaceutical University
Thesis: Lewis Acid-Catalyzed Claisen Rearrangement Using a Chromium Porphyrin Dimer
Supervisor: Masahiro Noji

Techniques: correlation analysis, Hilbert transform, non-negative matrix factorization

PROFESSIONAL EXPERIENCE

- 2023 – Present **Research Scientist**, Kureha Corporation
- Develop robotic laboratory automation systems for chemical synthesis workflows.
- Techniques: Kalman filtering, ROS2, sensor fusion; electronic circuit design
- 2021 – 2023 **Plant Engineer**, Kureha Corporation
- Designed and optimized distillation systems and operating conditions using process simulation.
 - Proposed hybrid reaction modeling algorithms for small datasets by combining physics-based and data-driven approaches.

Techniques: reaction kinetics modeling, physics-informed neural networks (PINNs), nonlinear optimization

HONORS AND AWARDS

- 2025 Excellent Oral Presentation Award, Kureha Corporation (one of 2 awardees among 21 presenters, top 10%)
- 2021 JASSO First-Type Scholarship, Doctoral Program — Full Repayment Exemption for Outstanding Academic Achievement; total amount waived: approximately USD 26,000
- 2020 Excellent Poster Presentation Award, 59th Meeting of The Pharmaceutical Society of Japan, Tohoku Branch

PUBLICATIONS

Journal Articles

- **Daisuke Miyata** and Noriyuki Yoshio, “Superstructure Optimization Methodology for Interpretable Reaction Kinetic Modeling with Limited Data”, *Comput. Chem. Eng* (Elsevier), (*in preparation*)
- Kazunori Ban, **Daisuke Miyata** (contributed equally), Yoshiteru Matsumoto, Shinya Tahara, Hiroaki Takahashi, Shin-ichi Morita and Takakazu Nakabayashi, “Visualization of the sequence of changes in the full wavenumber range by two-dimensional correlation spectroscopy”, *Chem. Phys. Lett.* (Elsevier), 833(16), 140930, 2023.
- **Daisuke Miyata**, Takakazu Nakabayashi and Shin-ichi Morita, “Automatic Determination of the Sequential Order of Dynamic Data and Its Application to Vibrational Spectroscopy”, *J. Chem. Inf. Model.* (American Chemical Society), 60(10), 5070–5079, 2020.
- Mengmeng He, **Daisuke Miyata**, Takakazu Nakabayashi and Shin-ichi Morita, “Practical Computation of FFT-based Generalized Two-dimensional Correlation Spectroscopy”, *Anal. Sci.* (The Japan Society for Analytical Chemistry), 36(7), 885–887, 2020.
- Hitomi Okabe, **Daisuke Miyata**, Takakazu Nakabayashi and Hirotsugu Hiramatsu, “Evaluation of Dihedral Angles of Peptides Using IR Bands of Two Successive Isotope Labeled Residues”, *Bull. Chem. Soc. Jpn.* (Chemical Society of Japan), 92(1), 80–86, 2019. (Selected Paper).
- **Daisuke Miyata**, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “Application of IR spectra of two successive isotope labeled residues to the evaluation of dihedral angles of polyproline II structure”, *Chem. Phys. Lett.* (Elsevier), 718, 27–31, 2019.

Review Articles

- **Daisuke Miyata**, Takakazu Nakabayashi and Shin-ichi Morita, “Recent Progress in Bio-Raman Research”, *Laser Research* (The Laser Society of Japan), 47(2), 85–88 (2019).

Patents

- **Daisuke Miyata** and Tatsuya Yaguchi, Analysis method and program for acquiring internal imaging of wellbore geometry (*in preparation*).
- **Daisuke Miyata** and Noriyuki Yoshio, Analysis method, program, and apparatus for identifying chemical reactions, Japanese Patent Application No. 2024-229019 (filed December 25, 2024; pending).

Invited Lectures

- **Daisuke Miyata**, “Practical Data Science: The Role of Data Scientists in Chemical Companies”, Data Science Practical Exercise B (MEXT-certified Mathematics, Data Science and AI Education Program), Fukushima University, January 2026.

Presentations

- **Daisuke Miyata** and Noriyuki Yoshio, “A Superstructure Optimization Approach for Interpretable Reaction Kinetic Modeling with Small Datasets” (Oral Presentation), 2025 AIChE Annual Meeting, Boston, November 2025.

Non-refereed Conference Presentations

- **Daisuke Miyata**, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “Development of Protein Structural Analysis Methods Based on Theoretical Analysis of Infrared Absorption Spectra”, The 59th Tohoku Branch Meeting of the Pharmaceutical Society of Japan, November 2020. (Poster Presentation)
- **Daisuke Miyata**, Takakazu Nakabayashi and Shinichi Morita, “Automatic determination of the sequential order of signal changes and its application to vibrational bands of protein H-D exchange process”, The 57th Annual Meeting of the Biophysical Society of Japan, Miyazaki, September 2019. (Poster Presentation)
- **Daisuke Miyata**, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “Development of a Peptide Dihedral Angle Analysis Method Using Infrared Spectroscopy: Fundamentals and Application to Polyproline”, The 58th Molecular Science Young Researchers Summer School, University of Tsukuba, June 2019. (Poster Presentation)
- **Daisuke Miyata**, Hirotsugu Hiramatsu and Takakazu Nakabayashi, A Novel Protein Structural Analysis Method Using Infrared Spectroscopy and Theoretical Calculations, The 58th Molecular Science Young Researchers Summer School, Shizuoka, August 2018. (Poster Presentation)
- **Daisuke Miyata**, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “A Novel Protein Structural Analysis Method Combining Infrared Spectroscopy and Theoretical Calculations”, Bio. Phys. Chem. Research Workshop – Exploring the Intersection of Biology, Physics, and Chemistry –, Tokyo University of Agriculture and Technology, April 2018. (Oral Presentation)
- **Daisuke Miyata**, Hitomi Okabe, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “Main-Chain Structural Analysis of Polyproline Using Infrared Absorption Spectroscopy with Two Successive $^{13}\text{C}=^{18}\text{O}$ Isotope Labels”, The 11th Molecular Science Symposium, Sendai, September 2017. (Poster Presentation)
- **Daisuke Miyata**, Hitomi Okabe, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “Establishment of a Structural Analysis Method for Peptide Dihedral Angles Using Infrared Absorption Spectra of Two Successive $^{13}\text{C}=^{18}\text{O}$ Isotope Labels”, New Frontiers in Chemical Reaction Pathway Exploration 2017, Sendai, September 2017. (Poster Presentation)
- **Daisuke Miyata**, Hitomi Okabe, Hirotsugu Hiramatsu and Takakazu Nakabayashi, “A New Method of

Evaluating the Dihedral Angle of Peptide Using IR Absorption Spectroscopy”, Tohoku University’s Chemistry Summer School 2017, Sendai, August 2017. (Poster Presentation)

TEACHING EXPERIENCE

- 2024 – 2026 Mentor, Kureha Corporation
- 2018 – 2021 Research Assistant, Tohoku University
Supervised undergraduate students conducting infrared spectroscopy experiments as part of research training
- 2016 – 2018 Teaching Assistant, Tohoku University
Supported undergraduate laboratory courses in infrared spectroscopy

ACADEMIC SERVICE AND COMMUNITY ACTIVITIES

- 2019 Executive Committee Member (Head of Section IV), The 59th Molecular Science Young Researchers Summer School, Aug. 19–23, Kyoto University, Japan (Invited lecture by Dr. Kunihiro Ishii, RIKEN).
- 2018 Organizing Committee Member (Planning and Moderator), Research Workshop: Bio. Phys. Chem. –Exploring the Triple Interface of Biology, Physics, and Chemistry–, December.
- 2018 Organizing Committee Member (Planning and Moderator), Research Workshop: Bio. Phys. Chem. – Exploring the Triple Interface of Biology, Physics, and Chemistry, September.
- 2017 Student Organizer, Tohoku University’s Chemistry Summer School 2017.

LANGUAGES

- English: CEFR C1 (TOEFL: 5.0/6.0)
- Japanese: Native

MEMBERSHIPS

- 2024 – Present The Robotics Society of Japan
- 2023 – Present The Japanese Society for Artificial Intelligence
- 2023 – Present The Society of Instrument and Control Engineers

EXTRACURRICULAR ACTIVITIES

- Atsumi Peninsula Ultra Nature Run 73 km, April 2025 — 11:29:01
- Tobishima Ultra Marathon 100 km, December 2024 — 15:29:01
- Suwa Eight Peaks Middle Triathlon (Half Ironman), June 2025 — 6:18:34