JI-YOUNG YANG

+49 152 0487 5706 jiyoung.jane.yang@gmail.com Linkedin Ulm, Germany

SUMMARY

PhD candidate with expertise in advanced biological data analysis and molecular dynamics (MD) simulations, focusing on protein characterization and drug formulation development. My PhD emphasized protein-cosolute interactions using analytical chemistry and computational techniques. With a global academic and professional journey spanning South Korea and Germany, I bring interdisciplinary skills and industry-academic experience to drive innovation in pharmaceutical research and development.

EXPERIENCE

PhD Thesis

Boehringer Ingelheim

11/2020 – 07/2024 Biberach, Germany

Industrial PhD research in Analytical Development Biologicals, Early Stage Analytics Laboratory in collaboration with University Ulm

- Developed Machine Learning models for spectral deconvolution and pattern recognition in antibodies and excipients.
- Set up automated liquid handling and data analysis process with python for protein characterization studies
- Studies of antibody interactions with salt ions and cosolutes using Molecular Dynamics (MD) Simulations.
- Designed protocols for antibody stress testing, including forced degradation and enzymatic digestion.

Master Thesis & Internship

Boehringer Ingelheim

03/2020 – 10/2020 Biberach, Germany

- Developed ML model for pattern recognition of surfactant degradation profiles in drug formulations, enabling classification and clustering of degraded lipid chains from UPLC-CAD data
- Developed neural network model to predict solvation energy of electrolytes based on their atomistic properties based on conceptual Density Functional Theory principles [1,2]

Trading Specialist for pure chemicals

Samchun Pure Chemical Co. Ltd

03/2018 –09/2018 Seoul, South Korea

- Managed import/export control across Europe, the USA, Japan, and India as the primary customer contact. Optimized logistics by coordinating shipments and negotiating freight costs. Adjusted pricing strategies to align with market conditions. Ensured customs clearance and compliance with international regulations, including K-REACH.

Co-Lead National Programmes

Nucleate Germany

03/2023 - 01/2024

- Early member contributing to the development of Germany into a Core Chapter of the global nonprofit organisation *Nucleate*.
- Supported future biotech entrepreneurs by recruiting experts from biotech, intellectual property, and business development for the "Activator" mentoring program

KEY ACHIEVEMENTS

Advanced Protein Characterization and Investigation of Molecular Interaction

Applied analytical chemistry and MD simulations to uncover mechanistic insights of protein-cosolute interactions, supporting data-driven drug formulation strategies.

Application of AI-Driven Analytics

Developed ML models for spectral protein characterisation, and surfactant degradation profiling, improving formulation stability. Built neural networks for solvation energy prediction using conceptual DFT.

Automated High-Throughput Workflows

Designed Python-based liquid handling and data analysis pipelines, optimizing experimental efficiency.

EDUCATION

PhD in Analytical Chemistry

University Ulm

11/2020 - Present Ulm, Germany

MSc in Bioinformatics/Molecular Biology

University of Applied Sciences Mittweida

11/2018 - 11/2020 Mittweida, Germany

BEng in Bioengineering

Incheon National University

03/2012 - 08/2017 Incheon, South Korea

ACTIVITIES

Exchange program in Global Data Science

Boehringer Ingelheim

01/2024 - 02/2024 Ingelheim, Germany

Internal exchange program in Global Data Science team Health Care Affair & Patient Engagement for project **"AI and Data Science for Global Patent Search & Analytics"**

Exchange program in Biochemistry (German)

University Hohenheim

2016 - 2017 Stuttgart, Germany

Exchange program in Business Management (English)

University Hohenheim

2016 - 2017 Stuttgart, Germany

SKILLS

Languages

Korean (native), English (fluent C1-C2), German (fluent C1)

Programming

- Python, R, SQL : Focused on Bioinformatics, Chemometrics (RDKit, MDAnalysis), ML (Pytorch, scikit-learn) and data science
- HPC (High Performance Computing) : Bash and Slurm batch system on Linux HPC clusters
- Cluster Computing : Streamlit, Databricks, Bitbucket

Software & Tools

MS Office, Excel Visual Basic, SIMCA, Spotfire for industrial analytics

MD Simulation

Protein-Cosolutes interactions studies, small-molecule drug research in chemical sequence variants using GROMACS, NAMD, OpenMM

Lab techniques

Protein Characterization and Formulation Excipient Analysis:

- Spectroscopy: Proficient in UV/Vis, Circular Dichroism (CD), Infrared (IR), and Fluorescence spectroscopy for stability testing and structural analysis.
- Calorimetry and Light Scattering: Skilled in Differential Scanning Calorimetry (DSC), nanoDSF, and Dynamic Light Scattering (DLS) for evaluating thermal stability and aggregation.
- Chromatography: Experienced in Ultra-Performance Liquid Chromatography coupled with Charged Aerosol Detection (UPLC-CAD) for surfactant analysis in drug formulation development.

PASSIONS & RESEARCH INTEREST

Innovative Drug Discovery and Development

Driven by a deep interest in understanding complex drug behaviors and optimizing drug discovery and development through advanced computational methods and data-driven approaches. This involves applying machine learning, predictive modeling, and molecular simulations to improve drug efficacy, stability, and safety in pharmaceutical research and development.

CONFRERENCES & AWARDS

Poster Presentation

Discover BMB

03/2023 Seattle, USA

Abstract 203 ***ASBMB*** (Americal Society for Biochemistry and Molecular Biology)

Oral Presentation

DPG Frühjahrstagung

03/2023 Dresden,Germany

Biophysics Chapter 17 Protein Structure and Dynamics *17.8 Talk*

DPG (Deutsche Physikalische Gesellschaft) Spring Conference

Engagement Individual Award

BI OPEN Global Data Science Challenge

06/2021

Boehringer Ingelheim OPEN global data science challenge for Lung Acoustic Signal Detection

REFERENCES

Prof. Dr. Boris Mizaikoff

Universität Ulm

Institute Director and Chair of Institute Analytical Chemistry and Biochemistry

boris.mizaikoff@uni-ulm.de

PD. Dr. Jens Smiatek

Boehringer Ingelheim GmbH & Co. KG

Digital Lead, Development NCE,

jens.smiatek@boehringer-ingelheim.com

Dr. Oliver Burkert

Boehringer Ingelheim GmbH & Co. KG

Lab Head of Early Stage, Analytical Development Biologicals

oliver.burkert@boehringer-ingelheim.com

PUBLICATIONS

Peer-reviewed published full articles

1. An Expression for the Diffusion Interaction Parameter for Pharmaceutical Formulations: Insights from Kirkwood-Buff Theory. Ji Young Yang, Jens Smiatek, Phys. Chem. Chem. Phys., 2025,
2. Multidomain Protein–Urea Interactions: Differences in Binding Behavior Lead to Different Destabilization Tendencies for Monoclonal Antibodies. Ji Young Yang, Oliver Burkert, Boris Mizaikoff, Jens Smiatek, J. Phys. Chem. B 2024, 128, 42, 10408–10416
3. Impact of Urea on Monoclonal Antibodies: Multiple Destabilization and Aggregation Effects for Therapeutic Immunoglobulin G Proteins Ji Young Yang, Oliver Burkert, Boris Mizaikoff, Jens Smiatek, ACS Omega 2024, 9, 5, 5517–5522
4. Combination of Explainable Machine Learning and Conceptual Density Functional Theory: Applications for the Study of Key Solvation Mechanisms I-Ting Ho, Milena Matysik, Liliana Montano Herrera, Jiyoung Yang, Ralph Joachim Guderlei, Michael Laussegger, Bernhard Schrantz, Regine Hammer, Ramón Alain Miranda-Quintana and Jens Smiatek, Phys. Chem. Chem. Phys., 2022,24, 28314-28324
5. Artificial neural networks for the prediction of solvation energies based on experimental and computational data. Jiyoung Yang, Matthias J. Knape, Oliver Burkert, Virginia Mazzini, Alexander Jung, Vincent S. J. Craig, Ramón Alain Miranda-Quintana, Erich Bluhmki and Jens Smiatek. Phys. Chem. Chem. Phys., 2020,22, 24359-24364

Under Review

1. Role of L-Arginine on multi-domain protein IgG conformational multi-states change and aggregation during thermal denaturation. Ji Young Yang, Oliver Burkert, Boris Mizaikoff, Jens Smiatek
2. Computational Simulations of Antibodies in Solution: Study of Physicochemical Properties and Interactions with Co-Solutes. Ji Young Yang, Boris Mizaikoff, Jens Smiatek [Invited Review] Applied Physics Review, AIP Publishing