Diego E. Kleiman

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Education

University of Illinois at Urbana-Champaign (UIUC)   **Urbana, IL, USA**
Ph.D. in Biophysics and Quantitative Biology, GPA: 4.0/4.0   *Expected 2025*
Concentration: Computational Science and Engineering

New York University in Abu Dhabi (NYUAD)   **Abu Dhabi, UAE**
Bachelor of Science, Physics + CS (minor), GPA: 3.9/4.0   *May 2020*
Honors: *Magna Cum Laude*, NYU Founders' Day Award, Member of Phi Beta Kappa

Escuela Normal Juan Pascual Pringles   **San Luis, Argentina**
Secondary School Diploma, GPA: 9.8/10   *November 2014*
Honors: *Valedictorian*

Publications

- **Kleiman, D. E.**, & Shukla, D. (2022). Multiagent Reinforcement Learning-Based Adaptive Sampling for Conformational Dynamics of Proteins. *Journal of chemical theory and computation.* `https://doi.org/10.1021/acs.jctc.2c00683`
- He, W., Naleem, N., **Kleiman, D. E.**, & Kirmizialtin, S. (2022). Refining the RNA Force Field with Small-Angle X-ray Scattering of Helix–Junction–Helix RNA. *The journal of physical chemistry letters*, 13(15), 3400-3408. `https://doi.org/10.1021/acs.jpclett.2c00359`
- Zhao, C., **Kleiman, D. E.**, & Shukla, D. (2021). Intriguing Role of Water in Plant Hormone Perception. *bioRxiv.* `https://doi.org/10.1101/2021.10.04.462894`

Academic Conferences & Symposia

Oral Sessions
- Multi-agent Reinforcement Learning Based Adaptive Sampling of Conformational Free Energy Landscapes of Proteins. **American Chemical Society Fall 2022 Meeting**. Chicago, IL, USA. August 21-25, 2022.

Poster Sessions
- Optimization of Hydration Sites in Plant Hormone Receptors for Agrochemical Design. **66th Annual Meeting of the Biophysical Society**. San Francisco, CA, USA. February 19-23, 2022.
- Exploring the Ion-Mediated RNA Interactions of a Helix-Junction-Helix RNA Model Through Well-Tempered Metadynamics Simulations. **64th Annual Meeting of the Biophysical Society**. San Diego, CA, USA. February 16, 2020.
- Manta Rover: an Automated System for Coral Reef Remediation. **New York University 2018 Undergraduate Research Session**. New York, NY, USA. August 3, 2018.
- E. coLAMP: A portable device for rapid detection of Shiga toxin-producing Escherichia coli. **International Genetically Engineered Machine (iGEM) Competition**. Boston, MA, USA. November 9-13, 2017.

Awards & Recognition

New York University Tandon School of Engineering   **New York, NY, USA**
Undergraduate Summer Research Program Fellowship   *June 2018*

6th Annual UAE Undergraduate Research Competition   **Abu Dhabi, UAE**
Finalist   *April 2018*

International Genetically Engineered Machine (iGEM) Competition   **Boston, MA, USA**
Gold Medal   *November 2017*

International Biology Olympiad   **Bali, Indonesia**
Representative of Argentina (second best in country). Bronze Medal (position 105/238).   *July 2014*

Teaching

University of Illinois at Urbana-Champaign (UIUC)   **Urbana, IL**
BIOP–401: Introduction to Biophysics   *Fall 2022*
Teaching Assistant (confirmed appointment)

Short Courses & MOOCs

International School for Advanced Studies (SISSA)   **Trieste, Italy**
Summer School   *June 2019*
Classical Molecular Dynamics for Material Science, Nanotechnology, and Biophysics

Coursera   **Remote**
Online Coursework   *2018*
Deep Learning Specialization by deeplearning.ai

Software Skills

Programming languages
Python, C/C++, Matlab, Mathematica.

Operative systems
Unix, macOS, Windows.

Numerical computing
NumPy, SciPy.

Molecular dynamics and bioinformatics
OpenMM, GROMACS, VMD, BioPython.

Data visualization
Matplotlib, Seaborn, gnuplot, xmgrace.

Web development
HTML, CSS, Flask.

Machine learning
Scikit-Learn, TensorFlow, Keras, OpenCV.

Database development
MongoDB, SQL, Pandas.

Data mining
Beautiful soup, Pyppeteer.

General
MS Office 365, Google Docs, Prezi, VLEs.

Other Work in Education & Outreach

University of Illinois at Urbana-Champaign   **Urbana, IL**
WYSE Camp Counselor, STEM outreach for underrepresented students in engineering   *July 2021*

International Biology Olympiad Group Challenge   **Nagasaki, Japan (remote position)**
Group Project Facilitator, team received Award of Excellence   *July–October 2020*

Addictest.com   **Rabat, Morocco (remote position)**
SAT Tutor   *June–July 2020*

Academic Enrichment Program at NYUAD   **Abu Dhabi, UAE**
Mathematics Tutor   *November 2019–February 2020*

Preparation Course for Medical School Admission Test at UNCuyo   **Mendoza, Argentina**
Official Physics and Biology Tutor   *June 2015–January 2016*

Leadership & Community Engagement

The Anchorage Society: Student-Run LGBTQ+ Organization at NYUAD   **Abu Dhabi, UAE**
Treasurer   *August 2019–May 2020*

Languages

English fluent. **Spanish**: native fluency. **French**: fluent (written), intermediate (oral).