

# Anja Conev

 AnjaConev |  ac121@rice.edu |  Google Scholar

## RESEARCH INTEREST

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I am excited to **apply artificial intelligence and machine learning** (ML) to the problems in the field of **computational structural biology** with the goal of aiding drug discovery. This field is exciting and vibrant especially with the recent advances in protein structure prediction such as AlphaFold2. In particular, the computational problems I explored include: design of ML-driven molecular scoring functions, search approaches in molecular docking, analysis and visualization of the data generated by **biomolecular and macromolecular simulations**.

## EDUCATION

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- 2019 - present    PhD in Computer Science (GPA: 4.0/4.0)  
advisor: Dr. Lydia Kavvaki  
**Rice University**  
Houston, TX
- 2014 - 2019      B.S. in Electrical Engineering and Computer Technology (GPA: 9.1/10)  
**University of Belgrade,**  
Belgrade, Serbia

## PUBLICATIONS

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- Conev, Anja, Romanos Fasoulis, et al. (2024). “HLAEquity: Examining biases in pan-allele peptide-HLA binding predictors”. In: *iScience* 27.1, p. 108613. ISSN: 2589-0042. DOI: <https://doi.org/10.1016/j.isci.2023.108613>. URL: <https://www.sciencedirect.com/science/article/pii/S2589004223026901>.
- Conev, Anja, Mauricio Menegatti Rigo, et al. (2023). “EnGens: a computational framework for generation and analysis of representative protein conformational ensembles”. In: *Briefings in Bioinformatics* 24.4, bbad242. DOI: [10.1093/bib/bbad242](https://doi.org/10.1093/bib/bbad242).
- Conev, Anja, Didier Devaurs, et al. (June 2022). “3pHLA-score improves structure-based peptide-HLA binding affinity prediction”. In: *Scientific Reports* 12.1. Featured in the collection: “Top 100 in Chemistry - 2022” <https://www.nature.com/collections/jigiddbdcf>. DOI: [10.1038/s41598-022-14526-x](https://doi.org/10.1038/s41598-022-14526-x). URL: <https://doi.org/10.1038/s41598-022-14526-x>.
- Rigo, Mauricio Menegatti et al. (July 2022). “SARS-Arena: Sequence and Structure-Guided Selection of Conserved Peptides from SARS-related Coronaviruses for Novel Vaccine Development”. In: *Frontiers in Immunology* 13. DOI: [10.3389/fimmu.2022.931155](https://doi.org/10.3389/fimmu.2022.931155). URL: <https://doi.org/10.3389/fimmu.2022.931155>.
- Antunes, Dinler A. et al. (Nov. 2020). “HLA-Arena: A Customizable Environment for the Structural Modeling and Analysis of Peptide-HLA Complexes for Cancer Immunotherapy”. In: *JCO Clinical Cancer Informatics* 4, pp. 623–636. DOI: [10.1200/cci.19.00123](https://doi.org/10.1200/cci.19.00123). URL: <https://doi.org/10.1200/cci.19.00123>.
- Conev, Anja, Eleni E. Litsa, et al. (Dec. 2020). “Machine Learning-Guided Three-Dimensional Printing of Tissue Engineering Scaffolds”. In: *Tissue Engineering Part A* 26.23-24, pp. 1359–1368. DOI: [10.1089/ten.tea.2020.0191](https://doi.org/10.1089/ten.tea.2020.0191). URL: <https://doi.org/10.1089/ten.tea.2020.0191>.

Sajkunic, Sanja and Anja Conev (2013a). “Stage and Sex Structure of Red-Backed Shrike (*Lanius colurio* Linnaeus, 1758) Nesting Groups on the Territory of Petnica village”. In: *Petnica Science Center Students’ Projects* 72, pp. 250–253. URL: <https://esveske.github.io/pdf/2013/BI01306.pdf>.

– (2013b). “The Effect of Lead on Fitness Components in *D. subobscura*”. In: *Petnica Science Center Students’ Projects* 72, pp. 223–231. URL: <https://esveske.github.io/pdf/2013/BI01306.pdf>.

## TRAINING

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**ITN Trainee Workshop 2023** Sept 2023  
*Data for the Common Good, University of Chicago, Chicago, IL*

**MolSSI Software Fellow Bootcamp 2023** July 2023  
*MolSSI Institute, Virginia Tech, Blacksburg, VA*

**Computer Science Student Advancement Program** July - Oct 2018  
*Kavraki Lab, Rice University, Houston, Texas*

**Summer school of machine learning** July 2017  
*Petnica Science Center and Microsoft Development Center, Serbia*

**Experimental Chemistry, Biology and Biomedicine research camps** 2011 - 2013  
*Petnica Science Center, Serbia*

## CONFERENCES

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**ITCR 2023** Sept 2023  
*Data for the Common Good, University of Chicago, Chicago, IL*

– Research presentation *PROTEAN-CR: A proteomics toolkit for ensemble analysis in cancer research*

**ACM-BCB 2023** Sept 2023  
*ACM-BCB, Houston, TX*

– Rapid-fire presentation *HLAequity: examining biases in pan-allele peptide-HLA binding predictors*

*Recent poster presentations:*

- **CECAM-PsiK**, June 2023  
*Freie Universitat, Berlin, Germany*
- **CRA-WP Grad Cohort for Women**, April 2023  
*San Francisco, SF, US*
- **27th SCSB Annual Symposium**, April 2023  
*Galveston, TX, US*
- **27th SCSB Annual Symposium**, April 2023  
*Galveston, TX, US*
- **ITCR 2022**, September 2022  
*St Louis, WA, US*

## AWARDS AND FELLOWSHIPS

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**Ken Kennedy-HPE Cray Fellowship** 2023-2024  
*Ken Kennedy Institute 2023/24*

**MolSSI Software Fellowship** 2023-2024  
*MolSSI 2023/24*

A 12-month Fellowship from the [MolSSI](#) institute for pursuing the development of software infrastructure, middleware, and frameworks that benefit the broader field of computational molecular sciences, including biomolecular and macromolecular simulation, quantum chemistry, and materials science.

**ITN travel award** Sep 2022  
*ITCR 2022*

Travel award to visit the NCI Informatics Technology for Cancer Research (ITCR) conference and participate in a training workshop.

**Rice Datathon 2022 - Second Place in the Bill.com Challenge** Jan 2022  
*Rice Datathon 2022*

For our work titled *Insight into Connection* on link prediction task with a graph neural network approach.

**Poster Presentation Session: Potential Impact Award** Oct 2020  
*2020 Ken Kennedy Institute Data Science Conference*

For the poster titled: "Combining Structure and Sequence Data to Predict Peptide-HLA Binding Affinity"

**"Dositeja" scholarship for studying abroad** 2019-2021  
*Ministry of Youth and Sport, Republic of Serbia*

"Dositeja" is a scholarship awarded by the Fund for Young Talents of the Republic of Serbia to talented and successful students.

## OPEN-SOURCE PROJECTS

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### **HLAEquity**

In our work on HLAEquity we examine allele biases in pan-allele machine learning peptide-HLA binding affinity predictors. We provide an interactive platform for visualizing and assessing dataset and algorithmic bias using a population coverage metric.

### **EnGens**

EnGens is a computational framework for generation and analysis of representative protein conformational ensembles. EnGens performs dimensionality reduction and clustering of the structural datasets to identify representatives from each cluster into a subset of a representative ensemble that can be used for downstream tasks.

### **SARS-Arena**

This work emerged as our response to the SARS-Cov-2 pandemic. Leveraging the resources we previously developed, we tuned our antigen prediction pipelines to fit the purpose of SARS-Cov-2 related antigen discovery.

### **3pHLA-score**

In this work we explored the use of ML models for training a system-specific scoring function for the purpose of scoring the binding energy of peptide ligands to HLA protein receptors. The main contribution includes the novel per-peptide-position training protocol as a proof of concept.

## HLA-Arena

HLA-Arena provides an interactive pipeline for structural computational modeling and analysis of the human leukocyte antigen (HLA) protein and its interaction with the peptide ligands (antigens).

## TEACHING/MENTORSHIP

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### Teaching assistant at Rice University

2020-2021

*Computer Science Department, Rice University*

Experience running recitation sessions, constructing quiz questions, grading, running office hours, writing blogs for the final project.

- COMP 600 (Graduate Seminar in Computer Science) - Spring 2024
- COMP 557 (Artificial Intelligence) - Fall 2021
- COMP 540 (Statistical Machine Learning) - Spring 2021
- COMP 557 (Artificial Intelligence) - Fall 2020

### Co-mentoring interning students at KavrakiLab

2021-2022

*KavrakiLab, Computer Science Department, Rice University*

Experience guiding students who joined KavrakiLab and worked on projects in the field of structural computational biology and applied machine learning.

- Jaila Lewis (University of Houston) - Summer 2022
- Aleksandar Gavric (University of Belgrade) - Summer 2021
- Davyd Fridman (Rice University) - Summer 2021
- Nonso Chukwurah (Rice University) - Spring 2021

### Student demonstrator at University of Belgrade

2018

*School of Electrical Engineering, University of Belgrade*

## PROFESSIONAL EXPERIENCE

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### Junior full stack web developer Nov 2018 - Jun 2019

*eFront, Belgrade*

### Web development Internship Feb - Apr 2018

*Pamet.doo, Belgrade*

### Student reviewer 2017

*KAPK, Serbia*

### Programming internship Oct - Dec 2016

*MikroElektronika, Belgrade*

## SKILLS AND HOBBIES

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Programming skills Python, R, C, C++, Java

Operating systems Linux, Windows

Communication skill good communication skills gained through my experience with collaborative interdisciplinary research as well as past experiences as a television presenter and organizer, and in a youth theater group

Organizational skills good communication skills gained through the experience in mentorship, teaching and collaborative projects

Hobbies guitar, drama, yoga, [creative writing](#)