

# Ivan Ivani, PhD

<https://realivanivani.github.io/>

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I am a PhD in Computational Chemistry with a decade of experience in computational biology, molecular modeling, and advanced data analytics. Expertise in MD simulations, force-field development and deep learning systems. Proven track record in international research collaboration, delivering impactful publications and innovative solutions in bioinformatics and molecular sciences.

## EDUCATION

- **PhD in Bioinformatics (cum laude)**, *University of Barcelona, Spain* **Dec 2016**

Thesis: *"Parameterization and validation of new state-of-the-art force field for DNA simulations"*

- **MSc in Biophysics (Top 2% of the class)**, *Charles University, Czechia* **Jun 2010**

## PROFESSIONAL EXPERIENCE

### Senior Data Analyst

**Oct 2023 – Present**

*User Experience R&D – Continental – Serbia*

- Built and maintained a comprehensive data management system for optical experiments and production data, enabling global R&D collaboration.
- Developed neural network models for predicting optical characteristic of new products. Interpreted data and predicted scrap using SHAP methods.
- Developed interactive dashboards using Python and PowerBI to streamline data insights.
- Supported the expansion of data science infrastructure and optimized data workflows.

### Senior Business Analyst

**Jun 2023 – Dec 2023**

*R&D – Syngenta – Remote*

- Led a small team of software developers to design and implement advanced features for Next-Generation Sequencing (NGS) software, with a focus on Oxford Nanopore technologies.
- Streamlined the software development lifecycle, ensuring alignment with project goals and industry standards while fostering collaboration across R&D teams.
- Delivered comprehensive reports and actionable insights to senior management, enabling informed decision-making and strategic planning for NGS initiatives.

### Data Analytics and Data Management Lead

**Jul 2018 – Jun 2023**

*Protection Unit – ICRC – Geneva, Damascus, Jerusalem and Caracas*

- Managed small teams and provided training in advanced SQL and Python methodologies.
- Developed a machine learning models (LogRes, Arima) for predicting activities and improve response
- Automated dashboards integrating external data into hum. frameworks, aiding operational planning.
- Enhanced ETD request flows visualization at HQ, supporting strategic initiatives.
- Assessed and improved database quality, enabling effective data-driven decision-making.

### Research Scientist

**Jan 2010 – Jun 2017**

*Institute for Research in Biomedicine - IRB Barcelona, Spain*

- Working in the group of Prof. Modesto Orozco on large-scale DNA MD simulations, force-field parameterization, ab-initio calculation, experimental validation and software optimization.
- Applied advanced statistical methods to interpret biological data from experiments and simulations.
- My most notable work in Nature Methods: **Ivan Ivani et al. Nature methods 13, no. 1 (2016): 55-58.**
- Full list of my publications: <https://scholar.google.com/citations?user=GqCZ-0QAAAAJ&hl=en>

### Intern Scientist

**May 2015 – Aug 2015**

*Stanford University and Pfizer, USA*

- Optimized molecular dynamics simulation software in collaboration with the pharma industry.
- Integrated experimental findings into simulation parameterization for short DNA sequences.

## PROJECTS

- **Display Design Optimization Model:** Engineered a neural network-driven model to optimize display design for achieving desired optical characteristics in production units. Employed SHAP analysis to elucidate the model's decision-making process, providing critical insights into the impact of specific input parameters on output quality and facilitating targeted process improvements.
- **EHR Analysis Models:** Developed and evaluated various machine learning models for publicly available EHR data. Python implementations using scikit-learn and TensorFlow/Keras to demonstrate sepsis prediction model.
- **Fingerprint Recognition Model:** Built a machine learning pipeline to identify fingerprint patterns with augmented deformations, leveraging advanced data augmentation techniques to improve accuracy.
- **Fraud Detection in HTTPS Requests:** Developed algorithms to detect anomalies in encrypted web traffic, enhancing cybersecurity through real-time fraud detection.
- **Traffic Predictor for a Recipe Webpage:** Designed and implemented a machine learning model using Random Forest Classifiers to predict high-traffic content for a recipe website, driving content optimization strategies.
- **Force-Field Optimization Using ML:** Automated the optimization of MD Force-fields by automating QM calculations, validating it with experimental data.
- **Open-Source Events Tracking Tool:** Conceived and developed an interactive tool that processes and visualizes key humanitarian events from open-source data, facilitating timely decision-making and strategic planning.

## SKILLS AND AWARDS

### Languages

- **Fluently:** English, Spanish, Czech, Serbian (Native). **Conversational:** Russian, German.

### Tools

- **Programming & Development:** Python (*Pandas, TensorFlow, PyTorch, PySpark*), SQL, OOP Design
- **Data Visualization & Analysis:** PowerBI, Tableau, Matlab
- **Structural Biology:** MD simulations (*AMBER, Gromacs*), QM calculations (*Schrodinger*), PyMol, Biopython
- **Deep Learning:** Neural Networks, CNNs, Anomaly detection, Biomolecule modelling, Diffusion models

### Awards and honours

- EMBO fellowship, Stanford, USA
- IUBMB Young Researcher fellowship, Taipei, Taiwan
- FEBS Young Researcher fellowship, St. Petersburg, Russia
- IRB Barcelona PhD fellowship, Barcelona, Spain
- Charles University scholarship (top 5% of students), Prague, Czechia

## HOBBIES

I am a nature lover, a sportsman and a fan of climbing. I love travelling, gastronomy and discovering new things. I enjoy constructive discussions and a collaborative environment.