PAVLÍNA POKORNÁ

COMPUTATIONAL STRUCTURAL BIOLOGIST

PROFESSIONAL PROFILE

Postdoctoral research associate with 7+ years of experience in computational structural biology applying molecular modeling techniques on biomolecules and their assemblies to study their structural dynamics at an atomic level.

EDUCATION

Masaryk University

April 2023 - Ph.D. Biomolecular Chemistry and Bioinformatics

Grades: thesis defense: A, state examination: B

Thesis title: "Structural dynamics of biomolecular complexes"
Thesis supervisor: Professor Jiří Šponer

The study programme focused on the structure and functions of biomolecules (proteins, nucleic acids, oligosaccharides, etc.) and their studies using both experimental (nuclear magnetic resonance, x-ray diffraction, cryo-electron microscopy, etc.), and computational (quantum chemistry, molecular mechanics and dynamics) methods.

June 2018 - Mgr. Biomolecular Chemistry

Grades: thesis defense: A, state examination: A

Thesis title: "Studies of interfaces between proteins and nucleic acids using the QM/MM method"
Thesis supervisor: Professor Jiří Šponer

Attended courses covered the fields of molecular biology, biomolecular structure, molecular modeling, bioinformatics, experimental methods in structural biology, etc.

June 2020 - Mgr. Upper Secondary School Teacher Training in Chemistry and Biology

June 2016 - Bc. Chemoinformatics and Bioinformatics

WORK EXPERIENCE

Researcher — Jan 2017 - Present

Institute of Biophysics of the Czech Academy of Sciences
Královopolská 135, 612 00 Brno
Czech Republic

Starting my employment as a master-level student, conducting research in molecular modeling using mainly molecular dynamics simulations applied to biomolecular systems.

CORE SKILLS

Molecular modeling

molecular dynamics simulations

structural biology of RNA, DNA and proteins

quantum mechanics

hybrid QM/MM methods

structural bioinformatics (alignement, structural motif search and classification, etc.)

Programming

Python

Bash + Awk

C++ and Fortran (basics)

Linux environment

Programs

Amber, Gromacs, Plumed

Turbomole, Gaussian

Pymol, VMD, Chimera, Coot

etc.

Languages

Czech (native)

English (fully proficient)

Spanish (intermediate)

ADDITIONAL EXPERIENCE

Intern — Apr 2022

Molecular and Statistical Biophysics Group, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy.

Learning enhanced-sampling simulation techniques and their application to DNA guanine-quadruplexes.

Lecturer — 2016 - 2020

Bioskop - Scientific Educational Centre of Masaryk University

Lecturing and designing science popularization courses for primary and high school students, the public, and talented high school students.

Intern — Jul - Aug 2015

Contipro a.s.

Working in a pharmaceutical company on quality assessment of nanofibres using optical methods and automating parts of the process.

Intern — Sep 2013 - Aug 2015

National Centre for Biomolecular Research, Masaryk University

Running a 2-year project on the automatization of identification and classification of tunnels in protein structures.

AWARDS

Brno PhD Talent

South Moravian Centre for International Mobility and Brno municipality

Three-year stipend awarded to 25 selected starting Ph.D. students from four universities.

Dean's prize

Faculty of Science, Masaryk University

Awarded for "Publication of outstanding results of own research", master student category.

SELECTED PEER-REVIEWED PUBLICATIONS

Pokorná,P., Krepl,M., Campagne,S., Šponer,J. (2022) Conformational Heterogeneity of RNA Stem-Loop Hairpins Bound to FUS-RNA Recognition Motif with Disordered RGG Tail Revealed by Unbiased Molecular Dynamics Simulations. J. Phys. Chem. B, 126, 9207-9221.

Krepl,M., Pokorná,P., Mlýnský,V., Stadlbauer,P., Šponer,J. (2022) Spontaneous Binding of Single-Stranded RNAs to RRM Proteins Visualised by Unbiased Atomistic Simulations With Rescaled RNA Force Field. Nucleic Acid Res., 50,12480-12496.

Pokorná,P., Krepl,M., Šponer,J. (2020) Residues Flanking the ARKme3T/S Motif Allow Binding of Diverse Targets to the HP1 Chromodomain: Insights From Molecular Dynamics Simulations. BBA - Gen. Sub., 1865, e129771.

Mráziková,K., Mlýnský,V., Kührová,P., Pokorná,P., Kruse,H., Krepl,M., Otyepka,M., Banáš,P., Šponer,J. (2020) UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. J. Chem. Theory Comput., 16, 7601-7617.

Pokorná,P., Krepl,M., Bártová,E., Šponer,J. (2019) Role of Fine Structural Dynamics in Recognition of Histone H3 by HP1γ(CSD) Dimer and Ability of Force Fields to Describe Their Interaction Network. J. Chem. Theory Comput., 15, 5659-5673.

Pokorná,P., Kruse,H., Krepl,M., Šponer,J. (2018) QM/MM Calculations on Protein-RNA Complexes: Understanding Limitations of Classical MD Simulations and Search for Reliable Cost-Effective QM Methods. J. Chem. Theory Comput., 14, 5419-5433.

Pokorná,P., Krepl,M., Kruse,H., Šponer,J. (2017) MD and QM/MM Study of the Quaternary HutP Homohexamer Complex with mRNA, L-histidine Ligand and Mg2+. J. Chem. Theory Comput., 13, 5658-5670.