TANA TANDARIĆ

PhD in Chemistry

In silico research, drug R&D

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Date and place of birth: June 6th 1992, Zagreb, Croatia **Citizenship :** Croatian

PERSONAL PROFILE

Specializing in **computational biochemistry**, I explore various biological systems using **quantum chemistry (QM)**, **molecular dynamics (MD)**, **molecular docking**, and **free-energy perturbation methods (FEP).** I collaborate closely with experimentalists to improve drug design, aiming for optimised pharmacokinetics and pharmacodynamics. I'm eager to expand my skills more and contribute to drug discovery projects.

WORK EXPERIENCE

Research associate

Ruđer Bošković Institute

10/2024 – ongoing | Zagreb, Croatia

- Investigation of allosteric networks within GPCR receptors using in silico methods

Postdoctoral researcher

Uppsala University, Åqvist Group

10/2022 – 10/2024 | Uppsala, Sweden

- Using MD and FEP simulations to investigate ligand binding and selectivity within adenosine receptors
- Developed in silico protocol for allosteric sites screening within GPCRs
- Teaching assistant in the graduate course “Molecular and Statistical Mechanics“
- Mentoring master´s students

Visiting researcher

Max Perutz Labs, Žagrović Group

03/2022 – 09/2022 | Vienna, Austria

- Investigation of Phe-tRNA isomers dynamic and allosteric connection within molecule using MD simulations and relative entropy calculations (PARENT)
- Reaction mechanism of aa-tRNA isomerization (QM)

Research assistant – PhD Student

Ruđer Bošković Institute

12/2016 – 06/2022 | Zagreb, Croatia

- Reaction mechanism of inhibition of MAO B with propargylamine inhibitors established using MD, QM and EVB simulations
- Teaching assistant in the graduate course “General Chemistry with Stoichiometry“, University of Zagreb

Research volunteer

Faculty of Pharmacy and Biochemisty, University of Zagreb

2013 – 2016 | Zagreb, Croatia

- Employed NMR, organic synthesis, and QM calculations to investigate degradation of pharmaceuticals within wastewater treatment processes

Student intership

University Hospital for Tumors

02/2016 – 08/2016 | Zagreb, Croatia

- Conducting biochemical, haematological, genetic, and cytological analyses in hospital laboratory

METHODS

In silico techniques:

- MD simulations (Gromacs, Amber, Q)
- QM calculations (Gaussian, Orca)
- QM/MM calculations (Gaussian, Orca)
- FEP calculations (Q, QresFEP, QligFEP)
- EVB calculations (Q)
- Molecular docking (AutoDock Vina, Schrödinger Maestro)
- Unix operating systems
- Bash scripting
- Python 3 (numpy, pandas, seaborn, matplotlib, scipy, plotly, cufflinks, mdtraj)
- PARENT

Experimental techniques:

- NMR spectroscopy
- Cryo EM (sample preparation, freezing, data collection, and data analysis)
- Automatic hematological and biochemical analyzer
- qPCR & RT-PCR

EDUCATION

PhD

University of Zagreb

10/2016 – 02/2021

Master in Medicinal Biochemistry

University of Zagreb

09/2011 – 09/2016

VISITING PERIODS

Sorbonne Université

11/2019 – 12/2019 Paris, France

- QM/MM calculations of cyclodextrin based catalysators under the mentorship of prof. Etienne Derat

National Institute of Chemistry

10/2018 - 11/2018 Ljubljana, Slovenia

- EVB calculations of MAO enzymes under the mentorship of prof. Janez Mavri

PUBLICATIONS

21 publications 319 citations h-index: 11

Notable Journal Articles

- **Tandarić, T.**, Gutierrez de Teran, H. (**2025**) Ligand and Residue Free Energy Perturbations Solve the Dual Binding Mode Proposal for an A_{2B}AR Partial Agonist. Journal of Physical Chemistry B. 129(3), 886-899.
- Prieto-Díaz, R., Fojo-Carballo, H., Majellaro, M., **Tandarić, T.**, Azuaje, J., Brea, J., Loza, M. I., Barbazán, J., Salort, G., Chotalia, M. et al. (**2024**) Exploring Biginelli-based scaffolds as A2B adenosine receptor antagonists: Unveiling novel structure-activity relationship trends, lead compounds, and potent colorectal anticancer agents. Biomedicine & pharmacotherapy, 173, 116345, 27.
- **Tandarić, T.**, Prah, A., Stare, J., Mavri, J. & Vianello, R. (**2020**) Hydride Abstraction as the Rate-Limiting Step of the Irreversible Inhibition of Monoamine Oxidase B by Rasagiline and Selegiline: A Computational Empirical Valence Bond Study. International journal of molecular sciences, 21 (17), 6151, 13.
- **Tandarić, T.** & Vianello, R. (**2019**) Computational Insight into the Mechanism of the Irreversible Inhibition of Monoamine Oxidase Enzymes by the Antiparkinsonian Propargylamine Inhibitors Rasagiline and Selegiline. ACS Chemical Neuroscience, 10 (8), 3532-3542.

University Theses & Dissertations

- Computational Investigation of the Mechanism of the Irreversible Inhibition of the Monoamine Oxidase B Enzyme. Thesis supervisor: Robert Vianello, PhD

AWARDS & HONOURS

- **2024:** Best Poster Award (EFMC Virtual Event)
- **2022:** Award for a young scientist in the field of medicinal and pharmaceutical chemistry (Croatian Chemical Society, Selvita d.o.o.)
- **2021:** Scholarship of the Austrian Academy of Arts and Sciences (JESH - Croatia) for a stay of six months in Max Perutz labs (Vienna, Austria)
- Annual Ruđer Bošković Institute award for published scientific paper in **2019** and **2020**
- **2019:** Thiene poster award, 16th European Symposium of Organic Reactivity, Dubrovnik
- **2019:** French Government Scholarship for a one-month stay at the Sorbonne University (Paris, France)

REFERENCES

Prof. Hugo Gutierrez-de-Teran

Uppsala University, Uppsala, Sweden

hugo.gutierrez@icm.uu.se

Prof. Bojan Žagrović

Max Perutz Labs, Vienna, Austria

bojan.zagrovic@univie.ac.at

Prof. Janez Mavri

National Institute of Chemistry, Ljubljana, Slovenia

janez.mavri@ki.si

LANGUAGES

- **Native:** Croatian
- **C2:** English
- **B2:** German
- **B1:** Italian

OTHER SKILLS

- Driver's License – Croatian B
- RYS TT 200 certified Yoga teacher
- Trainee speleologist