Yassir Boulaamane

Work permit: Spanish | **Date of birth:** 07/01/1995 | **Place of birth:** Rabat, Morocco | **Nationality:** Moroccan | **Phone:** (+212) 666589615 (Mobile) | **Email:** boulaamane.yassir@etu.uae.ac.ma | **Website:** https://yboulaamane.github.io/ | **LinkedIn:** yassir-boulaamane | **GitHub:** yboulaamane |

Address: Plaza Cívica, Campus de la UAB, 08193 , Bellaterra, Spain (Work)

ABOUT MYSELF

Ph.D. in Cheminformatics, Computational Chemistry, Molecular Modeling, and Machine Learning, with research focused on natural product-based drug discovery for neurodegenerative and infectious diseases, as well as cross-species P450 metabolism prediction. Actively seeking opportunities in computational drug discovery.

WORK EXPERIENCE

UNIVERSITAT AUTÒNOMA DE BARCELONA – BARCELONA, SPAIN

POSTDOCTORAL RESEARCHER – 01/09/2025 – CURRENT

- Molecular modelling of metabolizing Cytochromes P450 for the identification of new generation of pesticides.
- Development of predictive computational models for pesticide reactivity with cytochromes P450.
- Model deployment for predicting P450 metabolism across species, enabling multi-parameter optimization for safety, selectivity, and sustainability.

ABDELMALEK ESSAADI UNIVERSITY – TANGIER, MOROCCO

RESEARCH ASSOCIATE – 01/09/2024 – 31/07/2025

- Delivered undergraduate lectures and seminars.
- Assisted in biochemistry laboratory sessions.
- Supervised bachelor's and master's thesis students. Actively engaged in drug discovery research projects related to neurodegenerative diseases and antimicrobial resistance.

PHARMA IT – COPENHAGEN, DENMARK

PHARMA CONSULTANT – 02/05/2024 – 07/06/2025

- Configured and validated Veeva Vault Clinical and Quality applications.
- Performed dry run and regression testing to ensure compliance and functionality.
- Assisted in SOP writing for regulated processes.
- Supported CTD drafting for regulatory submissions.

FUTURE THERAPEUTICS – BERLIN, GERMANY

ASSOCIATE RESEARCHER – 01/11/2024 – 31/12/2024

- Contributed remotely to drug discovery research projects.
- Collaborated on computational drug discovery initiatives as an independent associate.

ABULCASIS INTERNATIONAL UNIVERSITY OF HEALTH SCIENCES – RABAT, MOROCCO

ADJUNCT INSTRUCTOR – 01/10/2024 – 30/11/2024

- Taught scientific methodology and supervised medical thesis writing.
- Ensured research design quality, data analysis, and academic compliance.

ANDALUSIAN CENTER FOR DEVELOPMENTAL BIOLOGY, UNIVERSITY OF PABLO DE OLAVIDE – SEVILLE, SPAIN

VISITING PHD STUDENT – 03/05/2023 – 28/07/2023

- Performed antibacterial assays (microdilution, time-kill, permeability, checkerboard).
- Conducted outer membrane protein profiling and bacterial adhesion studies.

DEPARTMENT OF ENVIRONMENTAL ENGINEERING, UNIVERSITY OF PATRAS – AGRINIO, GREECE

VISITING PHD STUDENT – 03/05/2022 – 28/10/2022

- DNA extraction and PCR amplification from insect samples.
- Applied metagenomics techniques for microbial profiling.

EDUCATION AND TRAINING

28/12/2020 – 20/07/2024 Tangier, Morocco

DOCTOR OF PHILOSOPHY (PHD) Abdelmalek Essaadi University

Website http://www.ensat.ac.ma/ |

Field of study Biochemistry, Inter-disciplinary programmes and qualifications involving natural sciences, mathematics and statistics

Final grade With Highest Honors | **Level in EQF** EQF level 8 |

Thesis Data-driven discovery of bioactive natural products: Application to neurodegenerative and infectious diseases

10/09/2018 – 22/07/2020 Rabat, Morocco

MASTER OF SCIENCE Mohammed V University in Rabat

Address Avenue Mohamed El Jazouli, Rabat, Morocco | **Website** http://fmd.um5.ac.ma/ |

Field of study Biological and related sciences not further defined | **Final grade** Good | **Level in EQF** EQF level 7 |

Thesis Insights into the Structure-Activity Relationship of Alkynyl-Coumarinyl Ethers as Selective MAO-B Inhibitors Using Molecular Docking

06/09/2012 – 27/07/2017 Rabat, Morocco

BACHELOR OF SCIENCE Mohammed V University in Rabat

Address 4 Avenue Ibn Batouta, Rabat, Morocco | **Website** http://www.fsr.ac.ma/ |

Field of study Natural sciences, mathematics and statistics not further defined, Biological and related sciences not elsewhere classified

Level in EQF EQF level 6 | **Thesis** Health Impacts of Glyphosate Exposure

10/09/2011 – 23/06/2012 Rabat, Morocco

BACCALAUREATE Lalla Nezha High School

Address Avenue Mali, Rabat, Morocco | **Field of study** Biological and related sciences not further defined |

Level in EQF EQF level 4

LANGUAGE SKILLS

Mother tongue(s): **ARABIC**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
FRENCH	C1	C1	C1	C1	C1
ENGLISH	B2	C1	B2	B2	C1

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Proficient user

SKILLS

Molecular Docking | Bioinformatics Tools | Python | GROMACS for molecular dynamic simulation | Molecular modelling software: HyperChem, USCF Chimera, Avogadro, Autodock Vina | Virtual Screening | Experience in HPC environments and working with SLURM scheduler | Machine learning | QSAR models | Deep Neural Networks (CNNs, GANs) | Basic microbiology methods

CONFERENCES & SEMINARS

20/12/2024 – 21/12/2024 Tangier, Morocco
International Bioinformatics Conference 2024

- Participated as an organizing committee member.
- Led an oral communication entitled: "Computational screening of natural products as tryptophan 2,3-dioxygenase inhibitors: Insights from machine learning QSAR, molecular docking, ADMET, and molecular dynamics simulations."

Link https://sites.google.com/view/ibc2024

30/10/2024 – 31/10/2024 Casablanca, Morocco
International eHealth Forum 2024

- Presented a poster entitled: "Antibiotic discovery with artificial intelligence for the treatment of Acinetobacter baumannii infections."
- Best poster award.

Link https://www.iehealthf.ma/#/CallForAbstracts?lang=en

06/10/2023 – 07/10/2023 Tangier, Morocco
International Bioinformatics Conference 2023

- Participated as an organizing committee member.
- Led an oral communication entitled: "Enhanced accuracy in predicting drug blood-brain barrier permeability with a Machine Learning Ensemble model."

Link https://sites.google.com/view/ibc2023/home

08/10/2022 – 09/10/2022 Tangier, Morocco
International Bioinformatics Conference 2022

- Participated as an organizing committee member.
- Led an oral communication entitled: "QSAR and molecular modeling studies for the discovery of natural products as multi-target-directed drugs for Parkinson's disease."

Link https://sites.google.com/view/ibc2022/home

27/12/2021 – 28/12/2021 Tangier, Morocco
International Bioinformatics Conference 2021

- Participated as an organizing committee member.
- Led an oral communication entitled: "Computational studies of African Natural Products Databases to identify natural dual-target-directed antiparkinsonian drugs."
- Presented a poster entitled: "Machine Learning model to predict potential Monoamine Oxidase B inhibitors from Cannabis Compound Database."
- Best poster award.

Link https://sites.google.com/view/ibc2021

23/06/2021 – 24/06/2021
1st International Applied Bioinformatics Conference

- Led a virtual communication entitled: "Docking-based virtual screening and ADME evaluation of caffeine-based phytochemicals as inhibitors of Monoamine Oxidase B."

Link https://iabconference.com/

HONOURS AND AWARDS

31/10/2024
Best ePoster Award – International eHealth Forum 2024

Link https://www.iehealthf.ma/#/CallForAbstracts?lang=en

03/05/2023

Erasmus+ International Mobility for Studies – University of Pablo de Olavide

03/05/2022

Erasmus+ International Mobility for Studies – University of Patras

PUBLICATIONS

2025

Computational screening of natural products as tryptophan 2,3-dioxygenase inhibitors: Insights from CNN-based QSAR, molecular docking, ADMET, and molecular dynamics simulations

Boulaamane, Y., Bolivar Avila, S., Hurtado, J. R., Touati, I., Sadoq, B.-E., Al-Mutairi, A. A., Irfan, A., Al-Hussain, S. A., Maurady, A., & Zaki, M. E. A. (2025). Computational screening of natural products as tryptophan 2,3-dioxygenase inhibitors: Insights from CNN-based QSAR, molecular docking, ADMET, and molecular dynamics simulations. Computers in Biology and Medicine, 191, 110199.

2025

Metal and Metal Oxide Nanoparticles: Computational Analysis of Their Interactions and Antibacterial Activities Against Pseudomonas aeruginosa

Sadoq, BE., Mujwar, S., Sadoq, M. et al. Metal and Metal Oxide Nanoparticles: Computational Analysis of Their Interactions and Antibacterial Activities Against Pseudomonas aeruginosa. BioNanoSci. 15, 60 (2025).

2024

Dendrobium nobile alkaloids modulate calcium dysregulation and neuroinflammation in Alzheimer's disease: A bioinformatic analysis

Touati, I., Boulaamane, Y., Britel, M. R., & Maurady, A. (2024). Dendrobium nobile L. alkaloids modulate calcium dysregulation and neuroinflammation in Alzheimer's disease: a bioinformatic analysis. Pharmacological Research-Modern Chinese Medicine, 100495.

2024

Antibiotic discovery with artificial intelligence for the treatment of Acinetobacter baumannii infections

Boulaamane, Y., Molina Panadero, I., Hmadcha, A., Atalaya Rey, C., Baammi, S., El Allali, A., ... & Smani, Y. (2024). Antibiotic discovery with artificial intelligence for the treatment of Acinetobacter baumannii infections. *Msystems*, e00325-24.

2024

In silico Discovery of Dual Ligands Targeting MAO-B and AA2AR from African Natural Products Using Pharmacophore Modelling, Molecular Docking, and Molecular Dynamics Simulations

Boulaamane, Y., Touati, I., Qamar, I., Ahmad, I., Patel, H., Chandra, A., ... & Maurady, A. (2024). In silico Discovery of Dual Ligands Targeting MAO-B and AA2AR from African Natural Products Using Pharmacophore Modelling, Molecular Docking, and Molecular Dynamics Simulations. Chemistry Africa, 1-23.

2024

Computational exploration of acefylline derivatives as MAO-B inhibitors for Parkinson's disease: insights from molecular docking, DFT, ADMET, and molecular dynamics approaches

Irfan, A., Ali, Y., Boulaamane, Y., Javed, S., Hameed, H., Zahoor, A. F., ... & Zaki, M. E. (2024). Computational exploration of acefylline derivatives as MAO-B inhibitors for Parkinson's disease: insights from molecular docking, DFT, ADMET, and molecular dynamics approaches. *Frontiers in Chemistry, 12*, 1449165.

2024

Computational Investigation of Phytochemicals from Aloysia citriodora as Drug Targets for Parkinson's Disease-Associated Proteins

Y. Boulaamane, M. Khedraoui, S. Chtita, I. Touati, B.-E. Sadoq, M. R. Britel, A. Maurady, Computational Investigation of Phytochemicals from Aloysia citriodora as Drug Targets for Parkinson's Disease-Associated Proteins. ChemistrySelect 2024, 9, e202403473.

2023

Chemical library design, QSAR modeling and molecular dynamics simulations of naturally occurring coumarins as dual inhibitors of MAO-B and AChE

Boulaamane, Y., Kandpal, P., Chandra, A., Britel, M. R., & Maurady, A. (2023). Chemical library design, QSAR modeling and molecular dynamics simulations of naturally occurring coumarins as dual inhibitors of MAO-B and AChE. *Journal of Biomolecular Structure and Dynamics*, 1-18.

Journal of Biomolecular Structure and Dynamics

2023

Probing the molecular mechanisms of α-synuclein inhibitors unveils promising natural candidates through machine-learning QSAR, pharmacophore modeling, and molecular dynamics simulations

Boulaamane, Y., Jangid, K., Britel, M. R., & Maurady, A. (2023). Probing the molecular mechanisms of α-synuclein inhibitors unveils promising natural candidates through machine-learning QSAR, pharmacophore modeling, and molecular dynamics simulations. Molecular Diversity, 1-17.

Molecular Diversity

2023

Exploring natural products as multi-target-directed drugs for Parkinson’s disease: an in-silico approach integrating QSAR, pharmacophore modeling, and molecular dynamics simulations

Boulaamane, Y., Touati, I., Goyal, N., Chandra, A., Kori, L., Ibrahim, M. A., ... & Maurady, A. (2023). Exploring natural products as multi-target-directed drugs for Parkinson’s disease: an in-silico approach integrating QSAR, pharmacophore modeling, and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, 1-18.

Journal of Biomolecular Structure and Dynamics

2023

Identification of novel dual acting ligands targeting the adenosine A2A and serotonin 5-HT1A receptors

Touati, I., Abdalla, M., Boulaamane, Y., Al-Hoshani, N., Alouffi, A., Britel, M. R., & Maurady, A. (2023). Identification of novel dual acting ligands targeting the adenosine A2A and serotonin 5-HT1A receptors. Journal of Biomolecular Structure and Dynamics.

Journal of Biomolecular Structure and Dynamics

2023

Insights into the Structure-Activity Relationship of Alkynyl-Coumarinyl Ethers as Selective MAO-B Inhibitors Using Molecular Docking

Yassir Boulaamane, Mohammed Reda Britel, and Amal Maurady

2022

Structural exploration of selected C6 and C7-substituted coumarin isomers as selective MAO-B inhibitors

Boulaamane, Y., Ahmad, I., Patel, H., Das, N., Britel, M. R., & Maurady, A. (2023). Structural exploration of selected C6 and C7-substituted coumarin isomers as selective MAO-B inhibitors. *Journal of Biomolecular Structure and Dynamics*, *41*(6), 2326-2340.

Journal of Biomolecular Structure and Dynamics

2022

In silico studies of natural product-like caffeine derivatives as potential MAO-B inhibitors/AA2AR antagonists for the treatment of Parkinson's disease

Boulaamane, Y., Ibrahim, M. A., Britel, M. R., & Maurady, A. (2022). In silico studies of natural product-like caffeine derivatives as potential MAO-B inhibitors/AA2AR antagonists for the treatment of Parkinson's disease. *Journal of Integrative Bioinformatics*, *19*(4), 20210027.

Journal of Integrative Bioinformatics

2022

β-amino carbonyl derivatives: Synthesis, Molecular Docking, ADMET, Molecular Dynamic and Herbicidal studies.

Bhandari, S., Agrwal, A., Kasana, V., Tandon, S., Boulaamane, Y., & Maurady, A. (2022). β-amino carbonyl derivatives: Synthesis, Molecular Docking, ADMET, Molecular Dynamic and Herbicidal studies. ChemistrySelect, 7(48), e202201572.

Chemistry Select

RECOMMENDATIONS

George Tsiamis Associate Professor

Hereby, I certify that Yassir Boulaamane visited my Lab of Systems Microbiology and Applied Genomics at the Department of Environmental Engineering, University of Patras from the 5th of May 2022 until the 04th of November 2022 under my supervision.

During his visit Yassir Boulaamane worked on the characterization of the bacteriome from *Aedes aegyptii* using New Generation
Sequencing technologies. In order to accomplish this, he used advanced molecular techniques in order to prepare NGS Illumina
libraries and state of the art bioinformatic tools for the data analyses.

He is a conscientious, highly motivated, and very organized worker, is quick to learn and takes an interest in results obtained, giving pride in the quality of his work. Yassir is an amiable and approachable person who works well both unsupervised and within a team, and he is also responsible and trustworthy.

Email gtsiamis1@gmail.com

Younes Smani Professor

To whom it may concern, CABD Univ. Pablo de Olavide/CSIC Carretera de Utrera km. 1 41013, Seville, Spain www.cabd.es It is a great pleasure to write this reference letter in support of Dr. Yassir Boulaamane's application. After joining my lab for a three-month internship in 2023, Yassir became actively involved in our ongoing studies on drug development for the treatment of bacterial infections. During this time, he honed his expertise in microbiological techniques (such as microdilution and time-kill assays), cell culture (including the isolation and cultivation of human epithelial cells), and bacterial adhesion assays on host cells. Yassir demonstrated an impressive ability to learn quickly and efficiently acquire fundamental knowledge. He conducted various experiments independently and obtained highly promising data, which were published in the journal mSystems (DOI: 10.1128/msystems.00325-24). Yassir also wrote his own project proposals, manuscripts, and posters. He is the first and corresponding author on several articles and a collaborator on others. Additionally, he actively participated in numerous conferences, presenting both oral and poster communications. I must emphasize that Yassir Boulaamane exhibited exceptional skills in working independently while also excelling in collaboration with other lab members. He demonstrated leadership and successfully coordinated the assigned tasks. Beyond his scientific abilities, Yassir is a very pleasant and easygoing individual who maintained excellent relationships with everyone in the lab. I am confident that he will excel in carrying out any proposed project and make significant contributions to your institution.

Email ysma@upo.es | **Phone** (+34) 954349051

Pankaj Mishra, PhD Doctor

I am writing to support Yassir Boulaamane in his application for a postdoctoral position. I have known him for the past few years, first through our community and later as an attendee of a machine learning course I taught, which focused on applications to small molecules. During this time, I have seen his enthusiasm for learning and his commitment to making the most of available resources. In the course, Yassir Boulaamane was a diligent and engaged participant. He approached the material with curiosity and worked hard to understand the concepts, often taking the initiative to ask

insightful questions. While we did not collaborate on any research projects, he demonstrated a strong capacity for learning and a genuine interest in advancing his knowledge in the field. Based on my experience with him, I believe Yassir Boulaamane would be a valuable addition to your research group. He is motivated and hardworking, and I expect he will approach new challenges with the same dedication I observed in my interactions with him.

Email pankaj@futuretx.ai

HOBBIES AND INTERESTS

Hiking

Photography

Blogging

Travelling