

Ibrahim Maattallaoui

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Brief Biography

Ibrahim Maattallaoui is a PhD student in Computational Medicinal Chemistry. His research focuses on Computer-Aided Drug Design (CADD) and Artificial Intelligence applied to drug discovery, particularly the discovery and optimization.

More broadly, his research interests include medicinal chemistry, cheminformatics, molecular modeling, molecular dynamics simulations, molecular machine learning, explainable AI, generative approaches for molecular design, structure-based drug discovery, virtual screening, drug repurposing, ADMET prediction, and computational optimization of bioactive compounds. His overall objective is to contribute to the development of data-driven, interpretable, and experimentally testable computational strategies for modern drug discovery.

Selected Publication:

Maattallaoui, I., Sakho, M., Maatallaoui, A., Barraón-Catalán, E., & El Aouad, N. (2025). *Development of QSAR Models and Web Applications for Predicting hDHFR Inhibitor Bioactivity Using Machine Learning.* *Molecules*, 30(23), 4618. DOI : 10.3390/molecules30234618

Conference Contributions :

Oral Presentation — 5th International Congress of Therapeutic Innovation

Moroccan Society of Pharmacology and Therapeutics (SMPT), Tangier, Morocco, 19–21 June 2026.
Computer-Aided Drug Design: Integrated Computational Work for the Discovery of Novel Human Dihydrofolate Reductase Inhibitors.

Best Poster Award — PHYTOVALO

Dakar, Senegal, 7–11 April 2025, *Activation of PKC δ by Diterpenes from Euphorbia resinifera.*

Oral Presentation — 3rd Annual Research Day

Faculty of Medicine and Pharmacy of Tangier, Morocco, 2025, *Machine Learning-Based QSAR Modeling for Lipxygenase Inhibitors.*

Poster Presentation — 9th International Research School

Ibn Zohr University, Agadir, Morocco, 2023, *In Silico Study of Diterpenes from Euphorbia resinifera.*