Adnane Aouidate

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https://chemoinfo.streamlit.app/

Languages

Arabic – Native speaker
English – Fluent
French – Fluent

Awards and Fellowships

2020 : Chinese Academy of Sciences President's International Fellowship Initiative (PIFI) for postdoctoral researchers.

2015-2018: Excellence scholarship for PhD students, National Centre for Scientific and Technique Research (**cnrst**).

2014: Award for being ranked 1rst among the two year master students "Master of Molecular Chemistry and Natural Substances", Moulay Ismail University.

2012: Award for being ranked 1rst among the three year undergraduate students in Department of Chemistry, Moulay Ismail University.

References:

Pr.Pascal Bonnet (Université d'Orléans)
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Pr.Adib Ghaleb (Université Cady Ayyad)
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Summary

I'm a Computational Chemist (7+ years) with strong working background in Computer Aided Drug Discovery and Chemoinformatics approaches (QSAR, Molecular Docking, Molecular Dynamics), data analysis and Machine learning.

Experience

Assistant Professor (Computational-Chemist)– 01/2023 to present **School of Applied Sciences of Ait Melloul,** Ibn Zohr University , Agadir, Morocco.

- Web applications development for chemoinformatic tools using Streamlit & Django.
- Exploring the chemical space of BRAF inhibitors through cheminformatic analysis and artificial intelligence.
- PhD students supervision : ADMET Predictions using ML and DL-based QSAR models.
- Academic instruction: Lectures and tutorials for students.
- Research Team Leadership: Junior researcher supervision and feedback.

Postdoctoral researcher (Chemoinformatics) – 01/2021 to 12/2022 **Structural Bioinformatic & Chemoinformatic team,** ICOA , Orleans, France.

- Encoding ACE2/SARS-CoV-2 interactions as fingerprints using chemoinformatics tools like Rdkit and ODDT.
- Developement of chemoinformatics methods to dock and score protein-protein interaction inhibitors based on Tanimoto coefficient and SPLIF-score (Structural Protein Ligand Interactions Fingerprints).
- Molecular dynamics simulation of protein-ligand complexes.
- Using « Fragment-Based Drug Discovery » to generate (LIMKs) protein kinases inhibitors.

Postdoctoral researcher (Computational-Chemist) - 2019 to 2020 **CADD Center,** SIAT, Shenzhen, China.

- Automation and developing of drug discovery Artificial Intelligence based workflows to speed up the research and development (R&D) of new bioactive molecules with KNIME software.
- Generation of large (new small molecules) chemical libraries and scaffold hopping.
- Predicting molecular properties and biological activities of small molecules.
- Chemical databases curation, preparation and elimination of non-drug like molecules (including in silico ADMET/ tox assessment).

Skills

- **Structure-based drug design (SBDD):** Molecular Docking, Virtual Screening, Molecular dynamics, Homology Modeling.
- **Ligand-based drug design (LBDD):** Pharmacophore modeling, 2D and 3D QSAR (CoMFA, CoMSIA).
- **Demonstrated proficiency in working with chemical databases:** Effectively retrieving and managing relevant chemical information to support research goals.
- **Workflows and Pipelines:** Automation of cheminformatics and machine learning workflows with KNIME software.
- **Machine learning:** Research & Develop Machine learning models for drug discovery, Risk assessment and toxicology.
- **Database preparation for virtual screening:** Maintenance of in-house and vendor database molecules for virtual screening.
- ***in silico* ADMET assessment.**
- **Experience with most of the open source tools and industry standard CADD and computational chemistry software packages:** Schrödinger Suite, Gaussian09, MOE, Material Studio, Autodock, Gromacs, KNIME, DataWarrior, Rdkit, deepchem.
- **Programing skills:** Python for Data Science, Streamlit, git, jupyter notebook.
- **Operating system:** Linux and Windows.

Link to: Education and degrees

2014-2019: **PhD** in **Computer Aided Drug Design,** My Ismail University (UMI) "**New bioactive organic molecules related to the inhibition of protein kinases. using 3D-QSAR, Molecular docking and ADMET**".

Link to: Publications and Presentations