Cédric BOUYSSET

Cheminformatics Research Scientist

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EDUCATION:

Ph.D. in Computational Chemistry

Oct. 2018 - Sep. 2021

Université Côte d'Azur, France

Machine-Learning, Molecular Modeling, Cheminformatics, Chemosensory GPCRs

MSc in Cheminformatics

Sep. 2016 - Jun. 2018

Université de Strasbourg, France

Graduated with honours

SKILLS:

- Python, JavaScript
- RDKit, OpenEye, ChemAxon
- Numpy, pandas
- Scikit-learn, scipy
- Pydantic, mypy
- AWS
- REST, GraphQL
- GitHub Actions, Bitbucket pipelines

AWARDS:

- Best Ph.D. Thesis award, GIRACT's European PhD in Flavor Research (2022)
- Excellence award, Université Côte D'Azur (2019)
- Best oral communication, French Cheminformatics Society (2019)
- Best poster presentation, UCA Complex Days (2019)

LANGUAGES:

French (Native)
English (Proficient)
Italian (Elementary)

PROFILE:

Enthusiastic cheminformatics researcher with a passion for developing reliable and user-friendly software for drug design. Possesses a strong foundation in computational chemistry coupled with advanced skills in software development and engineering, and experience in AI-driven design. Committed to accelerating and automating drug discovery through innovative research and collaboration.

EXPERIENCE:

Cheminformatics Research Scientist

Exscientia, Oxford, UK

April 2022 - Present

- Implementing cheminformatics algorithms: filtering, scoring, clustering, compound selection, chemical space visualisation
- Maintaining critical software for our drug design platform
- Project support for cheminformatics and data science tasks

Google Summer of Code student

MDAnalysis

June 2020 - August 2020

- Developed a Python module to convert between MDAnalysis AtomGroup objects and RDKit molecules
- Designed an algorithm to infer bond orders and charges from a topology with explicit hydrogens

Technician

Institut de Science et d'Ingénierie Supramoléculaires, Strasbourg, FR

July 2017 - August 2017

- Developed computational chemistry workflows to automate structure-based virtual screening and benchmarking on local machines and clusters.

PROJECTS:

ProLIF github.com/chemosim-lab/ProLIF

Interaction fingerprint library for any molecular complex and input files

Author and maintainer since 2017

mols2grid github.com/cbouy/mols2grid

Interactive 2D molecule viewer for Jupyter notebooks

Author and maintainer since 2021

MDAnalysis github.com/MDAnalysis/mdanalysis

Python library to analyze molecular dynamics simulations

Regular contributor since 2020, Google Summer of Code mentor in 2024