

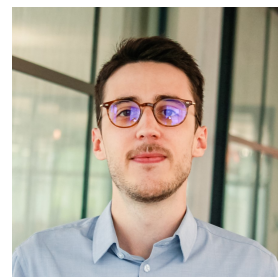
Cédric Bouysset

PHD IN CHEMISTRY · COMPUTATIONAL CHEMIST

Cheminformatics · Molecular Modeling · Machine Learning

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Experience

Academic

PhD in Chemistry

Institut de Chimie de Nice

UNIVERSITÉ CÔTE D'AZUR, FRANCE

2018 – 2021

- Molecular Basis of Chemosensory Perception
- Supervised by Dr. Sébastien FIORUCCI & Pr. Serge ANTONCZAK
- Expertise: Chemoinformatics, Molecular Modeling, Machine Learning, Programming, Chemosensory GPCRs

Internship

Institut de Chimie de Nice

UNIVERSITÉ CÔTE D'AZUR, FRANCE

Feb. – Jul. 2018

- Development of QSAR models to predict olfactory and gustatory properties of molecules in humans and insects
- Supervised by S. FIORUCCI

Internship

Institut de Science et d'Ingénierie Supramoléculaires

UNIVERSITÉ DE STRASBOURG, FRANCE

Mar. – Jun. 2017

- Automation of MD simulations from docking results
- Calculation of binding affinities to myosin using the MM/PBSA approach
- Supervised by M. CECCHINI

Internship

Institut de Chimie de Nice

UNIVERSITÉ CÔTE D'AZUR, FRANCE

Jun. 2016

- Homology Modeling of Bitter Taste Receptors
- Supervised by S. FIORUCCI

Education

Master degree in chemoinformatics

France

UNIVERSITÉ DE STRASBOURG

2016 – 2018

With Honours

Proficiency in computational chemistry: ligand-based and structure-based virtual screening, molecular modeling, chemical database

Bachelor degree in chemistry

France

UNIVERSITÉ DE NICE SOPHIA ANTIPOLIS

2013 – 2016

With Honours

First cycle of medical studies

France

UNIVERSITÉ DE NICE SOPHIA ANTIPOLIS

2011 – 2013

Honours & Awards

Feb. 2022 **Best PhD Thesis award**, 12th edition of GIRACT's European PhD in Flavor Research Awards

Geneva, Switzerland

Dec. 2019 **Excellence award laureate**, Université Côte D'Azur

Nice, France

Nov. 2019 **Best oral communication award**, 9th meeting of the French Chemoinformatics Society

Paris, France

Sep. 2019 **Laureate of a GEN FOUNDATION grant**, awarded to students and researchers in Natural Sciences, registered UK Charity No. 1071026

London, United Kingdom

Jul. 2019 **Travel grant**, XXIXth ECRO Meeting

Trieste, Italy

Mar. 2019 **Best poster presentation**, UCA Complex Days, the Complex Systems Academy of Excellence

Nice, France

Dec. 2018 **Laureate of a GIRACT bursary**, 9th European PhD in Flavor Research Bursaries for first year students

Geneva, Switzerland

Oct. 2018 **PhD Fellowship**, French Ministry of Higher Education and Research

Nice, France

Professional

Cheminformatics Research Scientist

Exscientia

OXFORD, UK

April 2022 – current

Google Summer of Code participant

MDAnalysis

REMOTE WORK

Jun. 2020 – Aug. 2020

Developer in charge of the interoperability project between MDAnalysis and RDKit python modules:

- Conversion between MDAnalysis atom groups and RDKit molecules.
- Leverage RDKit functionalities (SMARTS queries, molecular descriptors calculations... etc.) directly from MDAnalysis.

Technician

Institut de Science et d'Ingénierie Supramoléculaires

STRASBOURG, FRANCE

Jul. 2017 – Aug. 2017

- Development of computational chemistry workflows for structure-based virtual screening.

Summer Replacement Clerk & Teller

Various banks

MONACO

Summer 2012 – 2016

- Compagnie Monégasque de Banque, BNP Paribas Wealth Management, & LCL Banque et Assurance
- Customer reception, filing, data entry for banking transactions.

Skills

Chemoinformatics

RDKit, OpenEye, ChemAxon

Molecular Modeling

Amber, Modeller, AutoDock, PLANTS

Visualization

ChimeraX, PyMOL, Blender, VMD

Data Analysis

pandas, MDAnalysis, KNIME

Machine Learning

scikit-Learn, KNIME, Weka

Programming

Python, JavaScript, GraphQL, Bash, C, PHP

Web-Frontend

Bootstrap, Sphinx, Jekyll, Streamlit

Web-Backend

Django, Celery

Database

PostgreSQL, SQLite

Software Engineering

Git, GitHub Actions, Bitbucket

Peer-reviewed publications

First-author publications:

- 5 FUNCTIONAL MOLECULAR SWITCHES OF MAMMALIAN G PROTEIN-COUPLED BITTER-TASTE RECEPTORS 2021
Topin J., Bouysset C., Pacalon J., Kim Y., Rhyu M., Fiorucci S. & Golebiowski J. Cell. Mol. Life Sci.
- 4 PROLIF: A LIBRARY TO ENCODE MOLECULAR INTERACTIONS AS FINGERPRINTS 2021
Bouysset C. & Fiorucci S. J. Cheminformatics
- 3 REVERSE CHEMICAL ECOLOGY IN A MOTH: MACHINE LEARNING ON ODORANT RECEPTORS IDENTIFIES NEW BEHAVIORALLY ACTIVE AGONISTS 2021
Caballero-Vidal G., Bouysset C., Gévar J., Mbouzid H., Nara C., Delaroche J., Golebiowski J., Montagné N., Fiorucci S. & Jacquín-Joly E. Cell. Mol. Life Sci.
- 2 NOVEL SCAFFOLD OF NATURAL COMPOUND ELICITING SWEET TASTE REVEALED BY MACHINE LEARNING 2020
Bouysset C., Belloir C., Antonczak S., Briand L. & Fiorucci S. Food Chem.
- 1 MACHINE LEARNING DECODES CHEMICAL FEATURES TO IDENTIFY NOVEL AGONISTS OF A MOTH ODORANT RECEPTOR 2020
Caballero-Vidal G., Bouysset C., Grunig H., Fiorucci S., Montagné N., Golebiowski J. & Jacquín-Joly E. Sci. Rep.

Other publications:

- 4 MDANALYSIS 2.0 AND BEYOND: FAST AND INTEROPERABLE, COMMUNITY DRIVEN SIMULATION ANALYSIS 2022
Naughton F. B., Alibay I., Barnoud J., Barreto-Ojeda E., Beckstein O. Bouysset C., Cohen O., Gowers R. J., MacDermott-Opeskin H., Matta M., Melo M. N., Reddy T., Wang L., Zhuang Y. Biophys. J.
- 3 RECENT SMELL LOSS IS THE BEST PREDICTOR OF COVID-19 AMONG INDIVIDUALS WITH RECENT RESPIRATORY SYMPTOMS 2021
Gerkin R. C. and 128 colleagues Chem. Senses
- 2 MORE THAN SMELL—COVID-19 IS ASSOCIATED WITH SEVERE IMPAIRMENT OF SMELL, TASTE, AND CHEMESTHESIS 2020
Parma V. and 121 colleagues Chem. Senses
- 1 METAL IONS ACTIVATE THE HUMAN TASTE RECEPTOR TAS2R7 2019
Wang Y., Soohoo A. L., Lei W., Christensen C., Margolskee R. F., Bouysset C., Golebiowski J., Zhao H., Fiorucci S. & Jiang P. Chem. Senses

Seminars & Conference Talks

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| Oct. 2021 | 10th RDKit UGM , “Interactive visualization and filtering of small molecule datasets with mols2grid” | <i>Virtual Conference</i> |
| Oct. 2020 | 9th RDKit UGM , “From RDKit to the Universe and back” | <i>Virtual Conference</i> |
| Nov. 2019 | 9th Meeting of the French Chemoinformatics Society (SFCi) , “Decoding sweet taste from chemical structures” | <i>Paris, France</i> |
| Apr. 2019 | International Perfume Museum (MIP) & Collège de l'Archet , “How our brain perceives odors and flavors” | <i>Nice, France</i> |
| Apr. 2019 | 21st Group of Graphism and Molecular Modeling (GGMM) Conference , “Numerical model of structure-taste relationships” | <i>Nice, France</i> |

Posters

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| Oct. 2022 | 11th RDKit UGM , “Encoding molecular interactions as fingerprints with ProLIF” | <i>Berlin, Germany</i> |
| Sep. 2021 | European Chemoreception Research Organization (ECRO) XXXIst Meeting , “Functional Molecular Switches of Mammalian G Protein-Coupled Bitter-Taste Receptors” | <i>Cascais, Portugal</i> |
| May 2021 | 16th Weurman Flavour Research Symposium , “Bitter-Taste Receptors: From Sequence to Structure” | <i>Virtual Conference</i> |
| Aug. 2020 | International Symposium on Olfaction and Taste (ISOT) , “Bitter-Taste Receptors: From Sequence to Structure” | <i>Virtual Conference</i> |
| Nov. 2019 | GDR-O3 Annual Meeting , “Molecular insights into the structure-function relationships of bitter taste receptors” | <i>Toulouse, France</i> |
| Sep. 2019 | European Chemoreception Research Organization (ECRO) XXIXth Meeting , “Molecular insights into the structure-function relationships of bitter taste receptors” | <i>Trieste, Italy</i> |
| Apr. 2019 | 26th PACA Chemistry Day , “Modeling taste perception from chemical structures” | <i>Nice, France</i> |
| Mar. 2019 | 2nd UCA Complex Days Meeting , “Modeling taste perception from chemical structures” | <i>Nice, France</i> |

Volunteer Work

Open source projects

350 CONTRIBUTIONS IN 2021

[GitHub](#)

2017-2022

Python modules

AUTHOR & MAINTAINER OF 2 PACKAGES

- [mols2grid](#): Interactive chemical viewer of small molecule libraries
- [ProLIF](#): Interaction fingerprint library for complexes made of ligand, protein, DNA or RNA molecules extracted from MD trajectories, docked complexes or experimental structures

CONTRIBUTOR

2020-2022

- [MDAnalysis](#): Library for the analysis of molecular dynamics trajectories

Global Consortium for Chemosensory Research (GCCR)

[gcchemosensr.org](#)

WEB DESIGN & MAINTENANCE

2020-2022

Teaching

2019 – 2021 **Chemical senses**, Lectures and practicals

First year bachelor students

2018 – 2020 **Molecular structure and representation**, Exercise sessions

First year bachelor students

2018 – 2019 **Microscopic structure of matter**, Practicals

First year bachelor students

2019 – 2020 **Chemistry of solutions**, Exercise sessions

Second year bachelor students

2019 – 2021 **Molecular structure and macroscopic properties**, Exercises and practicals

Second year bachelor students

Activities

Video Games Vocal and game server configuration and administration

Sports Badminton and snowboard

Other

Citizenship French

Birth year 1993

Languages French (native), English (fluent), Italian (elementary)