Cédric **Bouysset**
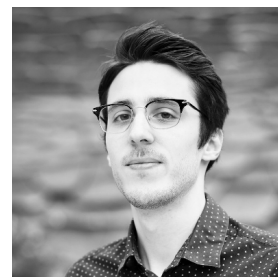
PhD Student · Teaching Assistant

Institut de Chimie de Nice, Université Côte d'Azur, Nice, FR

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Experience

Academic

PhD in Chemistry   *Institut de Chimie de Nice*
UNIVERSITÉ CÔTE D'AZUR, FRANCE   *2018 – current*
- 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

Professional

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.

Education

Master degree in chemoinformatics   *France*
UNIVERSITÉ DE STRASBOURG   *2016 – 2018*
With Honours

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*

Skills

Computational Chemistry

Chemoinformatics	RDKit, ChemAxon
Molecular Modeling	Amber, Modeller, AutoDock, PLANTS
Visualization	ChimeraX, PyMOL, Blender, VMD

Data Science

Data Analysis	pandas, MDAnalysis, KNIME
Machine Learning	scikit-Learn, KNIME, Weka

Computer science

Programming	Python, JavaScript, Bash, C, PHP
Web-Frontend	Bootstrap, Sphinx, Jekyll, Streamlit
Web-Backend	Django, Celery
Database	PostgreSQL, SQLite
Software Engineering	Git, GitHub Actions

Honours & Awards

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*

Peer-reviewed publications

First-author publications:

5   FUNCTIONAL MOLECULAR SWITCHES OF MAMMALIAN G PROTEIN-COUPLED BITTER-TASTE RECEPTORS   *Accepted*
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. & Jacquin-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. & Jacquin-Joly E.   *Sci. Rep.*

Other publications:

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

Oct. 2021   **10th RDKit UGM**, "Interactive visualization and filtering of small molecule datasets with mols2grid"   *Virtual Conference*

Oct. 2020   **9th RDKit UGM**, "From RDKit to the Universe and back"   *Virtual Conference*

Nov. 2019   **9th Meeting of the French Chemoinformatics Society (SFCi)**, "Decoding sweet taste from chemical structures"   *Paris, France*

Apr. 2019   **International Perfume Museum (MIP) & Collège de l'Archet**, "How our brain perceives odors and flavors"   *Nice, France*

Apr. 2019   **21st Group of Graphism and Molecular Modeling (GGMM) Conference**, "Numerical model of structure-taste relationships"   *Nice, France*

Posters

Sep. 2021   **European Chemoreception Research Organization (ECRO) XXXIst Meeting**, "Functional Molecular Switches of Mammalian G Protein-Coupled Bitter-Taste Receptors"   *Cascais, Portugal*

May 2021   **16th Weurman Flavour Research Symposium**, "Bitter-Taste Receptors: From Sequence to Structure"   *Virtual Conference*

Aug. 2020   **International Symposium on Olfaction and Taste (ISOT)**, "Bitter-Taste Receptors: From Sequence to Structure"   *Virtual Conference*

Nov. 2019   **GDR-O3 Annual Meeting**, "Molecular insights into the structure-function relationships of bitter taste receptors"   *Toulouse, France*

Sep. 2019   **European Chemoreception Research Organization (ECRO) XXIXth Meeting**, "Molecular insights into the structure-function relationships of bitter taste receptors"   *Trieste, Italy*

Apr. 2019   **26th PACA Chemistry Day**, "Modeling taste perception from chemical structures"   *Nice, France*

Mar. 2019   **2nd UCA Complex Days Meeting**, "Modeling taste perception from chemical structures"   *Nice, France*

Volunteer Work

Open source projects *GitHub*

300+ CONTRIBUTIONS IN 2020 *2017-2021*

Python modules *PyPI*

AUTHOR & MAINTAINER OF 2 PACKAGES *2018-2021*

- mols2grid: Interactive chemical viewer of small molecule libraries
- ProLIF: Interaction fingerprint library for MD or docking simulations of ligand, protein, DNA or RNA complexes

CONTRIBUTOR *2020-2021*

- MDAnalysis

Global Consortium for Chemosensory Research (GCCR) *gcchemosensr.org*

WEB DESIGN & MAINTENANCE *2020-2021*

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, competitive training
Sports	Badminton and snowboard

Other

Citizenship	French
Birth year	1993
Languages	French (native), English (fluent), Italian (elementary)