Cédric **Bouysset**
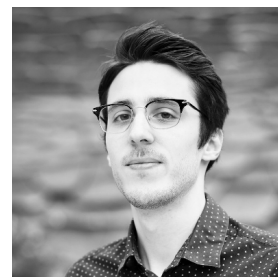
PhD in Chemistry · Computational chemist

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

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.

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*

Skills

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

Honours & Awards

Date	Award	Location
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*

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. & 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*

350 CONTRIBUTIONS IN 2021   *2017-2022*

Python modules   *PyPI*

AUTHOR & MAINTAINER OF 2 PACKAGES   *2018-2022*

- 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)