# Cédric **Bouysset**

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

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### Education

Université Côte d'Azur Nice, France PHD IN CHEMISTRY 2018 – current

- Dissertation title: Molecular Basis of Chemosensory Perception
- Supervisors: Dr. Sébastien Fiorucci and Pr. Serge Antonczak
- Techniques: Molecular Modeling, Chemoinformatics, Machine Learning

Université de Strasbourg Strasbourg, France

MASTER DEGREE IN CHEMOINFORMATICS (WITH HONOURS) 2016 - 2018

Université de Nice Sophia Antipolis Nice France

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FIRST CYCLE OF MEDICAL STUDIES 2011 - 2013

Lycée Albert Premier Monaco SCIENTIFIC BACCALAUREATE (WITH HONOURS) 2011

### Experience \_\_\_\_

**Google Summer of Code MDAnalysis** 

RDKIT INTEROPERABILITY PROJECT DEVELOPER

Development for the Python module MDAnalysis:

BACHELOR DEGREE IN CHEMISTRY (WITH HONOURS)

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

### Institut de Science et d'Ingénierie Supramoléculaires (ISIS)

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

### Compagnie Monégasque de Banque, BNP Paribas Wealth Management, & LCL Banque et **Assurance**

SUMMER REPLACEMENT CLERK & TELLER

• Customer reception, filing, data entry for banking transactions.

Monaco

Summer 2012 - 2016

## Research Internships \_\_\_\_\_

### **Molecular and Numerical Models of Chemosensory Perceptions**

INSTITUT DE CHIMIE DE NICE, UNIVERSITÉ CÔTE D'AZUR

Development of QSAR models on gustative and olfactive properties in humans and insects

Supervisor: Sébastien Fiorucci

### **Automatic Rescoring of Docking Results by End-point Free Energy Approaches**

INSTITUT DE SCIENCE ET D'INGÉNIERIE SUPRAMOLÉCULAIRES, UNIVERSITÉ DE STRASBOURG

· Calculation of binding affinities of ligand-receptor complexes from MD simulations, using the MM/PBSA approach

• Supervisor: Marco Cecchini

#### **Molecular Modeling of Bitter Taste Receptors**

Institut de Chimie de Nice, Université Côte d'Azur

• Development of 3D models of bitter taste receptors using homology modeling

• Supervisor: Sébastien Fiorucci

Strasbourg, France

Jun. 2020 - Aug. 2020

Jul. 2017 - Aug. 2017

2013 - 2016

Strasbourg, France

Mar. - Jun. 2017

Nice, France

Feb. - Jul. 2018

Nice, France Jun. 2016

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# Peer-reviewed publications \_\_\_\_\_

### First-author publications:

First	t-author	publications:	
5		NAL MOLECULAR SWITCHES OF MAMMALIAN G PROTEIN-COUPLED BITTER-TASTE RECEPTORS Bouysset C., Pacalon J., Kim Y., Rhyu M., Fiorucci S. & Golebiowski, J.	Under review
4	PROLIF: A LIBRARY TO ENCODE MOLECULAR INTERACTIONS AS FINGERPRINTS  Bouysset C. & Fiorucci S.		Accepted Journal of Cheminformatics
3	REVERSE CHEMICAL ECOLOGY IN A MOTH: MACHINE LEARNING ON ODORANT RECEPTORS IDENTIFIES NEW BEHAVIORALLY ACTIVE AGONISTS  Caballero-Vidal G., Bouysset C., Gévar J., Mbouzid H., Nara C., Delaroche J., Golebiowski J., Montagné N., Fiorucci S. & Jacquin-Joly E.		2021 CMLS
2	Novel Scaffold of Natural Compound Eliciting Sweet Taste Revealed by Machine Learning Bouysset C., Belloir C., Antonczak S., Briand L. & Fiorucci S.		2020 Food Chemistry
1	MACHINI RECEPTO	E LEARNING DECODES CHEMICAL FEATURES TO IDENTIFY NOVEL AGONISTS OF A MOTH ODORANT  OR	2020
	Caballero	Vidal G., Bouysset C., Grunig H., Fiorucci S., Montagné N., Golebiowski J. & Jacquin-Joly E.	Scientific Reports
Othe	er publi	cations:	
3	RECENT	2021	
	Gerkin R.	C. and 128 colleagues	Chemical Senses
2		IAN SMELL—COVID-19 IS ASSOCIATED WITH SEVERE IMPAIRMENT OF SMELL, TASTE, AND CHEMESTHESIS and 121 colleagues	2020 Chemical Senses
1 Sel	Wang Y.,	ons Activate the Human Taste Receptor TAS2R7 Soohoo A. L., Lei W., Christensen C., Margolskee R. F., Bouysset C., Golebiowski J., Zhao H., Fiorucci S. & Jiang P.  rs & Conference Talks	2020 Chemical Senses
	ct. 2021	10 <sup>th</sup> RDKit UGM, "Interactive visualization and filtering of small molecule datasets with mols2grid"	Virtual Conference
00	ct. 2020	9 <sup>th</sup> RDKit UGM, "From RDKit to the Universe and back"	Virtual Conference
No	ov. 2019	<b>9<sup>th</sup> Meeting of the French Chemoinformatics Society (SFCi)</b> , "Decoding sweet taste from chemical structures"	Paris, France
Ар	or. 2019	International Perfume Museum (MIP) & Collège de l'Archet, "How our brain perceives odors and flavors"	Nice, France
Ap	or. 2019	21st Group of Graphism and Molecular Modeling (GGMM) Conference, "Numerical model of structure-taste relationships"	Nice, France
Po	sters		
Ma	ay 2021	<b>16<sup>th</sup> Weurman Flavour Research Symposium,</b> "Bitter-Taste Receptors: From Sequence to Structure"	Virtual Conference
Au	ıg. 2020	International Symposium on Olfaction and Taste (ISOT), "Bitter-Taste Receptors: From Sequence to Structure"	Virtual Conference
No	ov. 2019	<b>GDR-03 Annual Meeting,</b> "Molecular insights into the structure-function relationships of bitter taste receptors"	Toulouse, France
	ep. 2019	<b>European Chemoreception Research Organization (ECRO) XXIX</b> <sup>th</sup> <b>Meeting,</b> "Molecular insights into the structure-function relationships of bitter taste receptors"	Trieste, Italy
Ap	or. 2019	26 <sup>th</sup> PACA Chemistry Day, "Modeling taste perception from chemical structures"	Nice, France

Nice, France

Mar. 2019 **2<sup>nd</sup> UCA Complex Days Meeting,** "Modeling taste perception from chemical structures"

### **Honours & Awards**

Dec. 2019	Excellence award laureate, Université Côte D'Azur	Nice, France
Nov. 2019	<b>Best oral communication award</b> , 9 <sup>th</sup> meeting of the French Chemoinformatics Society	Paris, France
Sep. 2019	Laureate of a GEN FOUNDATION grant, awarded to students and researchers in Natural	London, United Kingdom
3ep. 2019	Sciences, registered UK Charity No. 1071026	
Jul. 2019	Travel grant, XXIX <sup>th</sup> 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	Geneva, Switzerland
Dec. 2016	students	
Oct. 2018	PhD Fellowship, French Ministry of Higher Education and Research	Nice, France

# **Community Service**

Open source projects GitHub

300+ CONTRIBUTIONS IN 2020 2017-2021

Python modulesPyPI2 PACKAGES2018-2021

• mols2grid: Interactive chemical viewer of small molecule libraries

• ProLIF: Interaction fingerprint library for MD or docking simulations of ligand, protein, DNA or RNA complexes

### **Global Consortium for Chemosensory Research (GCCR)**

Website

Web design & Maintenance 2020-2021

### Skills\_\_\_\_\_

**Chemoinformatics** RDKit, ChemAxon

Molecular ModelingAmber, Modeller, AutoDock Vina, PLANTSMolecular VisualizationChimeraX, PyMOL, Blender, VMD, 3Dmol.jsData AnalysisJupyter-notebook, pandas, MDAnalysis, KNIME

**Programming** Python, JavaScript, Bash, C, PHP

Machine Learning Scikit-Learn, KNIME, Weka

**Web-Frontend** HTML5, CSS, Bootstrap, Sphinx, Streamlit

Web-BackendDjango, CeleryDatabasePostgreSQL, SQLiteSoftware EngineeringGit, GitHub Actions, Docker

# 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 (27 years old)

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