

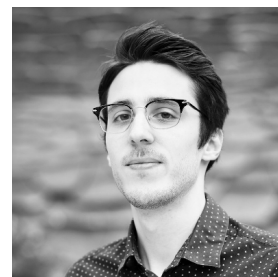
# Cédric Bouysset

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

Dec. 2019	<b>Excellence award laureate</b> , Université Côte D'Azur	<i>Nice, France</i>
Nov. 2019	<b>Best oral communication award</b> , 9 <sup>th</sup> meeting of the French Chemoinformatics Society	<i>Paris, France</i>
Sep. 2019	<b>Laureate of a GEN FOUNDATION grant</b> , awarded to students and researchers in Natural Sciences, registered UK Charity No. 1071026	<i>London, United Kingdom</i>
Jul. 2019	<b>Travel grant</b> , XXIX <sup>th</sup> ECRO Meeting	<i>Trieste, Italy</i>
Mar. 2019	<b>Best poster presentation</b> , UCA Complex Days, the Complex Systems Academy of Excellence	<i>Nice, France</i>
Dec. 2018	<b>Laureate of a GIRACT bursary</b> , 9 <sup>th</sup> European PhD in Flavor Research Bursaries for first year students	<i>Geneva, Switzerland</i>
Oct. 2018	<b>PhD Fellowship</b> , French Ministry of Higher Education and Research	<i>Nice, France</i>

### 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.

## Skills

### Computational Chemistry

<b>Chemoinformatics</b>	RDKit, ChemAxon
<b>Molecular Modeling</b>	Amber, Modeller, AutoDock, PLANTS
<b>Visualization</b>	ChimeraX, PyMOL, Blender, VMD

### Data Science

<b>Data Analysis</b>	pandas, MDAnalysis, KNIME
<b>Machine Learning</b>	scikit-Learn, KNIME, Weka

### Computer science

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

## Peer-reviewed publications

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### 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

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

## Posters

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

## Volunteer Work

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### Open source projects

300+ CONTRIBUTIONS IN 2020

[GitHub](#)

2017-2021

### 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

[PyPI](#)

2018-2021

CONTRIBUTOR

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

2020-2021

### Global Consortium for Chemosensory Research (GCCR)

[gcchemosensr.org](#)

WEB DESIGN & MAINTENANCE

2020-2021

## Teaching

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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

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**Video Games** Vocal and game server configuration and administration

**Sports** Badminton and snowboard

## Other

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**Citizenship** French

**Birth year** 1993

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