# SERGIO RUIZ-CARMONA

I am currently a Research Officer and Bioinformatician at the Baker Institute, under the supervision of professor Mike Inouye. My research interests are broad and involve mainly the relationship between genetic variants and their effect on protein structures.

I carried out my MSc and PhD in Barcelona in the Barril Lab, where I worked with different structure-based drug design methods with the aim to improve drug design for non-standard targets.

## 🎓 EDUCATION

**2017 | 2012**

### PhD in Biomedicine
Universitat de Barcelona                            📍 Barcelona, ES

- Virtual Screening for novel MoA: Apps. and method developments
- Development and application of **structure-based drug discovery** methods
- Awards: **Extraordinary prize** for PhD Thesis and **Ramon Margalef award** for best publication

**2012 | 2010**

### MSc in Bioinformatics for Health Sciences
Universitat Pompeu Fabra                            📍 Barcelona, ES

- Expanding Druggable Genome: PP-Interfaces as a new target class
- Study of novel rational approach to find PP interfacial binders

**2010 | 2006**

### BSc in Biotechnology
Universitat Autònoma de Barcelona                   📍 Barcelona, ES

## 💻 RESEARCH EXPERIENCE

**Today | 2019**

### Research Officer and Bioinformatician
Inouye Lab
Baker Heart and Diabetes Institute                  📍 Melbourne, AU

- I am working in a project that overlaps Structural Biology and Genomics, in collaboration with David Ascher's Lab. Mainly, I am trying to understand how rare missense variants alter protein structures and can induce different diseases
- My role also involves giving Bioinformatics support to the whole institute, where I apply different statistical and data analysis methods in a wide range of projects, mainly related with cardiovascular diseases and diabetes

View this CV online at
https://www.ruizsergio.com/cv/
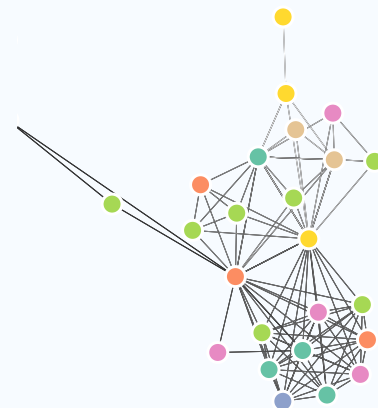
## CONTACT

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- 🔗 ruizsergio.com
- in Sergio Ruiz

## PROGRAMMING SKILLS

- R
- Bash
- Python
- Web Development
- SQL
- C++
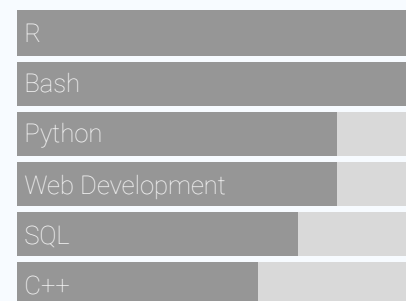
*Source code available at*
*github.com/sruizcarmona/*

*Last updated on May 19, 2021*

## Postdoctoral Researcher

2018 | 2017

Barril Lab, Universitat de Barcelona 📍 Barcelona, ES

- After finishing my PhD, I worked in exciting collaborative projects in the field of epigenetics and cancer, where I carried out multidisciplinary research and learned new experimental skills

## EMBO Short–Term Fellow

2017

Andreas Bender Lab, Unversity of Cambridge 📍 Cambridge, GB

- I spent 2 months in one of the main Pharmacogenomics groups in the world, where I used **gene-expression profiles** of different biological systems to study BRD4 and drug selectivity
- 2 months (Sep/Oct 2017) research stay. Funded by **EMBO** (also awarded **FEBS** Short-Term Fellowship)

## MuTaLig COST Action Short–Term Fellow

2017

Peter Kolb Lab, Philipps Universität Marburg 📍 Marburg, DE

- I applied the methods developed during my PhD, Dynamic Undocking, Docking and MD simulations, in order to find multipotent compounds targeting **RNAse P** of extremely pathogenic bacteria
- 1 month (Nov 2017) research stay. Funded by **MuTaLig COST Action**

## Predoctoral Researcher

2016 | 2011

Barril Lab, Universitat de Barcelona 📍 Barcelona, ES

- Master's and PhD research projects in the Xavier Barril Lab
- I applied a combination of experimental and computational techniques to study non-standard drug targets. I also developed novel structure-based computational methods to help in identifying novel drugs

I have been working in several multidisciplinary research groups around the globe. I have applied a broad range of concepts and ideas in the drug discovery field (both experimental and computational) and also in genomics and data analysis

# ⚙ SKILLS AND TRAINING

## Computational Techniques

Computer-Aided Drug Discovery (SBDD), Virtual Screening, Docking, Molecular Dynamics, Chemoinformatics, Quantum Chemistry, Bioinformatics Tools and Analysis

## Scientific Software

Bioinformatics software, pymol, openbabel, databases, molecular docking programmes and molecular modelling tools (Schrödinger, MOE)

## Programming

R, Python, Perl, C++, LaTeX, Bash, Java, MySQL, HTML and Android and Web Development

## Experimental Techniques

Biophysical Screening (SPR, DSF), Cell Growth, Protein Expression and Purification

## 📖 SELECTED PUBLICATIONS

**2021**

### Oxygen Pathway Limitations in Patients with Chronic Thromboembolic Pulmonary Hypertension

*Circulation*
Read it here

- Erin J Howden *, **Sergio Ruiz-Carmona ***, [...] Andre La Gerche, Marion Delcroix and Guido Claessen

**2018**

### Dynamic Undocking: A Novel Method for Structure-Based Drug Discovery

*Rational Drug Design* (Book Chapter)
Read it here

- Maciej Majewski, **Sergio Ruiz-Carmona** and Xavier Barril

**2017**

### Dynamic undocking and the quasi-bound state as tools for drug discovery

*Nature Chemistry*
Read it here

- **Sergio Ruiz-Carmona**, P Schmidtke, [...] Rod Hubbard and Xavier Barril
- **Highlighted in its issue cover**

**2017**

### Binding mode prediction and MD/MMPBSA-based free energy ranking for agonists of REV-ERBα/NCoR

*Journal of Computer-Aided Molecular Design*
Read it here

- Y Westermaier, **Sergio Ruiz-Carmona**, [...] Pierre Ducrot and X Barril

**2014**

### rDock: a fast, versatile and open source program for docking ligands to proteins and nucleic acids

*PLoS Computational Biology*
Read it here

- **Sergio Ruiz-Carmona**, Daniel Alvarez-Garcia, [...] Xavier Barril, Rod Hubbard and S David Morley

## 🏛 TEACHING EXPERIENCE

**2021**

### Introduction to R Course

Introduction to Stats Analyses Using R    📍 Melbourne, AUS

- 6h of online tutoring for Baker Heart and Diabetes Institute researchers
- Organized by Prof. Agus Salim and Dr. Gad Abraham

I collaborated with different companies (Servier, Repsol and Vernalis) where I studied physicochemical properties of both small molecules and drug targets and also developed novel methods for virtual screening

I consider myself a passionate teacher. I have always volunteered and enrolled in as many teaching opportunities as possible during the different stages of my career

**2019 | 2015** ● **Associate Professor**
Faculty of Pharmacy, Universitat de Barcelona ● Barcelona, ES

• Classes in Pharmacy, Food Science and Nutrition degrees (total 400h)

**2017** ● **Molecular Dynamics workshops**
Novel methods for Drug Discovery ● Marburg, DE

• 6h theory and hands-on workshop for Dynamic Undocking and MDmix simulations. During my research visit at Kolb's Lab

**2016** ● **Drug Discovery workshop**
Computer-aided Drug Design ● Ciudad de Mexico, MX

• Organized and imparted 30h of theory and hands-on sessions for researchers at the Instituto de Química (Chemistry Institute), at the UNAM
• With Profs. Xavier Barril and Axel Bidon-Chanal

## 🖥 SCIENTIFIC COMMUNICATIONS

**2021** ● **Characterization of the effect of disease-causing genetic variants using protein 3D structural alterations**
Lorne Proteins 2021 ● Lorne, AUS
*Virtual Poster Presentation*

**2020** ● **Var2Prot: A new tool to unravel the 3D structural effect of genetic variants**
Lorne Proteins 2020 ● Lorne, AUS
*Oral Communication*

**2019** ● **Var2Prot: A new tool to unravel the 3D structural effect of genetic variants**
GIW/ABACBS 2019 ● Sydney, AUS
*Poster Presentation*

**2017** ● **New approaches in SBDD: Applications to non-standard targets**
Joint Klebe & Kolb Seminars ● Marburg, DE
*Invited Oral Communication*

**2017** ● **Virtual Screening for novel mechanisms of action: Applications and method developments**
Andreas Bender Lab Seminars ● Cambridge, UK
*Invited Oral Communication*

**2016** ● **Dynamic Undocking and the Quasi-Bound State as Tools for Drug Discovery**
7th Joint Sheffield Conference on Chemoinformatics ● Sheffield, UK
*Oral Communication*

I have also developed rDock and Barril Lab websites, used as dissemination platforms where the different tutorials and blog entries are shared with the community

**2016** ● **Dynamic Undocking and the Quasi-Bound State as Tools for Drug Discovery**
III Symposium of Young Researchers in Medicinal Chemistry 📍 Barcelona, ES
*Oral Communication*

**2015** ● **Dynamic undocking of protein complexes: a new tool for ligand discovery**
Gordon Research Conference: New Frontiers in CADD
*Poster Presentation*
📍 Mount Snow (VT), USA

**2014** ● **rDock: A Fast, Versatile and Open Source Program for Docking Ligands to Proteins and Nucleic Acids**
8th International Workshop on New Approaches in Drug Design 📍 Marburg, DE
*Poster Presentation*

## 📈 DATA SCIENCE WRITING

**2015**
**|**
**2012**
● **rDock Docking Manuals and Tutorials**
rDock website content

- I developed and validated different tutorials for using rDock, with around 300 visits every month

**2013** ● **Small Molecule Parametrization**
Blog entry

- Blog entry about how to parametrize small molecules using Gaussian and AMBER forcefield, for Molecular Dynamic simulations
- 50 reads per month

## 🖥 SELECTED PRESS STORIES

**2021**
**|**
**2020**
● **Australasian Leadership Computing Grants**
Story about NCI Computing Grant

- Together with Mike Inouye, we were awarded a 1 year computing grant by the Australian National Compuational Infrastructure to study COVID-19 proteins and possible drug treatments

**2017** ● **Dynamic Undocking paper publication**
News about our publication and selection for cover

- Highlight from Universitat de Barcelona about our Dynamic Undocking publication in Nature Chemistry and its selection for the March 2017 printed cover