




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.

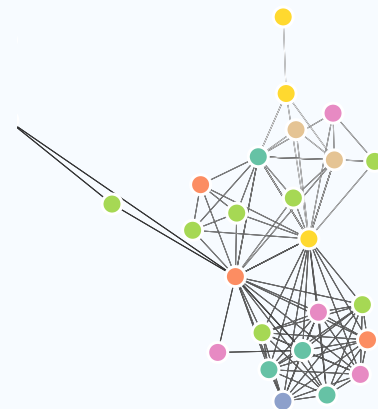
I carried out my MSc and PhD in Barcelona in the [Barril Lab](#), where I worked with different structure-based drug design methods with the aim to improve drug design for non-standard targets.

EDUCATION

- 2017
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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
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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
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2006
- **BSc in Biotechnology**
Universitat Autònoma de Barcelona  Barcelona, ES

RESEARCH EXPERIENCE

- Today
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2019
- **Research Officer and Bioinformatician**
Inouye Lab  Melbourne, AU
Baker Heart and Diabetes Institute
 - 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 disease
 - 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

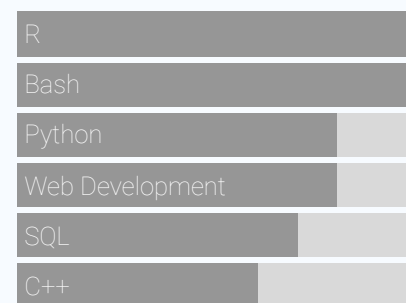


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<https://www.ruizsergio.com/cv/>

CONTACT

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PROGRAMMING SKILLS



Source code available at
github.com/sruizcarmona/,
built with [datadrivencv](#) package

Last updated on May 21, 2021

2018
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2017

● Postdoctoral Researcher

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

2017

● EMBO Short-Term Fellow

Andreas Bender Lab, University 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)

2017

● MuTaLig COST Action Short-Term Fellow

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**

2016
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2011

● Predoctoral Researcher

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-ERB α /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




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









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

- 2019
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2015
- **Associate Professor**
Faculty of Pharmacy, Universitat de Barcelona  Barcelona, ES
 - Classes in Pharmacy, Food Science and Nutrition degrees (total 400h)
 - **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
 - **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
 - **Var2Prot: A new tool to unravel the 3D structural effect of genetic variants**
[Lorne Proteins 2020](#)  Lorne, AUS
Oral Communication
 - **Var2Prot: A new tool to unravel the 3D structural effect of genetic variants**
[GIW/ABACBS 2019](#)  Sydney, AUS
Poster Presentation
 - **New approaches in SBDD: Applications to non-standard targets**
Joint Klebe & Kolb Seminars  Marburg, DE
Invited Oral Communication
 - **Virtual Screening for novel mechanisms of action: Applications and method developments**
Andreas Bender Lab Seminars  Cambridge, UK
Invited Oral Communication
 - **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
- 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
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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
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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 Computational 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](#)