

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 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 | <ul style="list-style-type: none">● PhD in Biomedicine
Universitat de Barcelona<ul style="list-style-type: none">• 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 |  Barcelona, ES |
| 2012

2010 | <ul style="list-style-type: none">● MSc in Bioinformatics for Health Sciences
Universitat Pompeu Fabra<ul style="list-style-type: none">• Expanding Druggable Genome: PP-Interfaces as a new target class• Study of novel rational approach to find PP interfacial binders |  Barcelona, ES |
| 2010

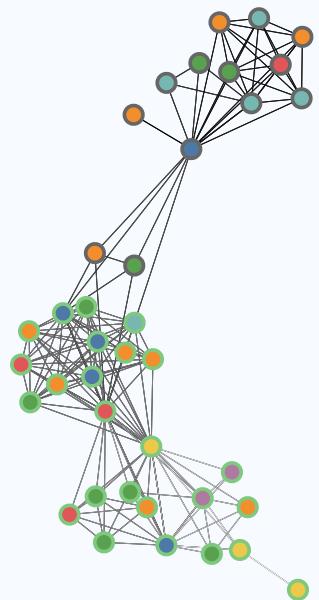
2006 | <ul style="list-style-type: none">● BSc in Biotechnology
Universitat Autònoma de Barcelona |  Barcelona, ES |

RESEARCH EXPERIENCE

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|--------------------|--|--|
| Today

2019 | <ul style="list-style-type: none">● Research Officer and Bioinformatician
Inouye Lab
Baker Heart and Diabetes Institute<ul style="list-style-type: none">• I am working in a project that overlaps Structural Biology and Genomics, 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 |  Melbourne, AUS |
| 2019

2017 | <ul style="list-style-type: none">● Postdoctoral Researcher
Barril Lab, Universitat de Barcelona<ul style="list-style-type: none">• 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 |  Barcelona, ES |

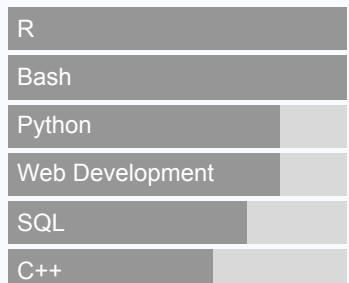


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CONTACT

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 [@RuizCSergio](#)
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PROGRAMMING



Source code in [github](#),
built with [datadrivencv](#) package

Last updated in Mar, 2022

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

- **Molecular Modeling**

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

- **Computational Tools**

Drug Discovery (Virtual screening, Molecular dynamics), Machine learning, Data visualization, Statistical analysis, REDCap, Bioinformatics and Data analysis

- **Scientific Software**

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

- **Programming**

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

- **Experimental Techniques**

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

- **Management Skills**

2021 EMBO Practical Course: Research to service: Planning and running a bioinformatics core facility; Mental Health and OHS certifications



SELECTED PUBLICATIONS

2022

- **The carbon footprint of bioinformatics**

Molecular Biology and Evolution

Read it [here](#)

- Jason G Grealey, [...] **Sergio Ruiz-Carmona**, Michael Inouye

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
- Result of a Bioinformatics Core collaboration. [Shiny app](#) developed

2021

- **Loss of the long non-coding RNA OIP5-AS1 exacerbates heart failure in a sex-specific manner**

iScience

Read it [here](#)

- Aowen Zhuang, A Calkin, [...] **Sergio Ruiz-Carmona**, [...] and Brian G Drew
- Result of a Bioinformatics Core collaboration

2019

- **An investigation of structural stability in protein-ligand complexes reveals the balance between order and disorder**

Communications Chemistry

Read it [here](#)

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

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**, Peter 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-ERBa/NCoR**

Journal of Computer-Aided Molecular Design

Read it [here](#)

- Yvonne Westermaier, **Sergio Ruiz-Carmona**, [...] Pierre Ducrot and Xavier Barril

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

- 2017 • **LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening**
Journal of chemical information and modeling
 Read it [here](#)
 - Leandro Radusky, **Sergio Ruiz-Carmona**, [...] and Marcelo A Martí
- 2016 • **Docking-undocking combination applied to the D3R Grand Challenge 2015**
Journal of Computer-Aided Molecular Design
 Read it [here](#)
 - **Sergio Ruiz-Carmona** and Xavier 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 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

III 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 | 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

Virtual Poster Presentation

📍 Lorne, AUS

2020

- Var2Prot: A new tool to unravel the 3D structural effect of genetic variants

Lorne Proteins 2020

Oral Communication

📍 Lorne, AUS

2019

- Var2Prot: A new tool to unravel the 3D structural effect of genetic variants

GIW/ABACBS 2019

Poster Presentation

📍 Sydney, AUS

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

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 Res. Conf.: New Frontiers in CADD

📍 Mount Snow (VT), USA

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

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



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

2021

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2020

SELECTED PRESS STORIES

- **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

2021

- **Shiny App development**

Related to a project we published in the Journal *Circulation*

2021

- **New tools for new medicines, The Conversation article**

Lay-summary of some of my work and opinion for The Conversation Spain

2020

- **COVID-19 daily dashboard, until Nov 2020**

Personal project to showcase COVID-19 evolution in Victoria during major lockdown in 2020

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](#)