

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
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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, AUS

Baker Heart and Diabetes Institute

- 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

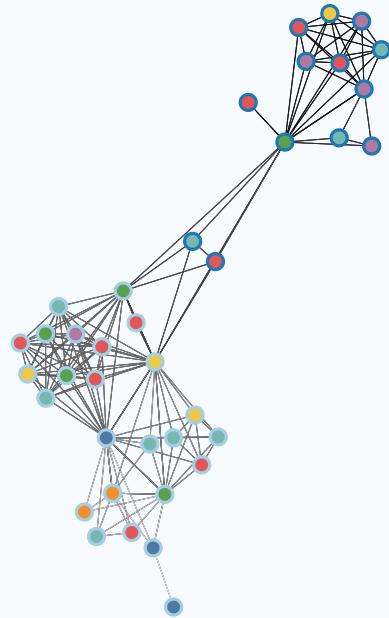
2019
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2017

● **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

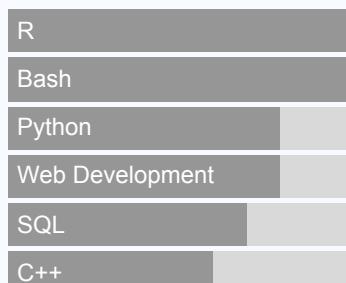


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CONTACT

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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

|
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](#)