

SERGIO RUIZ-CARMONA

I work as a [Clinical Data Analyst](#), uncovering insights to drive informed decision-making. Proficient in extracting EMR records using SQL, I specialize in analyzing and visualizing data using R and Power BI. With a deep understanding of clinical data and a research background, I bring a unique perspective to optimizing healthcare outcomes.

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
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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

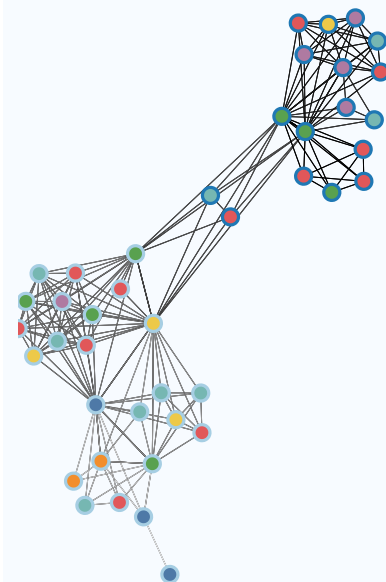
2010
|
2006

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

RESEARCH EXPERIENCE

Today
|
2022

- **Clinical Data Analyst**
Centre for Health Analytics Melbourne, AUS
Royal Children's Hospital
 - I work as a Clinical Data Analyst, uncovering insights to drive informed decision-making. Proficient in extracting Epic EMR records using SQL, I specialize in analyzing and visualizing data using R and Power BI.
 - With a deep understanding of clinical data and a research background, I bring a unique perspective to optimizing healthcare outcomes.

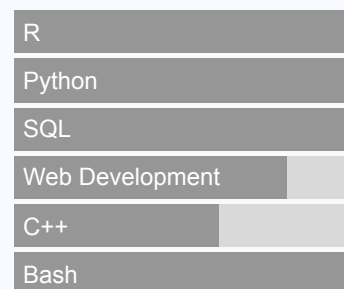


View this CV [online](#)

CONTACT

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</> PROGRAMMING



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

Last updated in Mar, 2024

2022
|
2019

● Research Officer and Bioinformatician

Inouye Lab
Baker Heart and Diabetes Institute

📍 Melbourne, AUS

- 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

2022
|
2019

● Senior Research Officer and Bioinformatician

Inouye Lab
Baker Heart and Diabetes Institute

📍 Melbourne, AUS

- 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
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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

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

● **Certifications**

Certified Health Informatician Australasia (CHIA), UX/UI Design (RMIT), Dataviz with R (IBM), Machine Learning (IBM)



SELECTED PUBLICATIONS

- 2022 ● **The carbon footprint of bioinformatics**
Molecular Biology and Evolution
Read it [here](#)
- Jason G Grealey, [...] **Sergio Ruiz-Carmona**, Michael Inouye
- 2022 ● **Computational Design of Inhibitors Targeting the Catalytic β Subunit of Escherichia coli FOF1-ATP Synthase**
Antibiotics
Read it [here](#)
- Luis Pablo Avila-Barrientos, [...] **Sergio Ruiz-Carmona**, [...] and Enrique García-Hernández
- 2022 ● **Development of an Automatic Pipeline for Participation in the CELPP Challenge**
International Journal of Molecular Sciences
Read it [here](#)
- Marina Miñarro-Lleonar, **Sergio Ruiz-Carmona**, [...] and Xavier Barril
- 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

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 ● **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-ERB α /NCoR**
Journal of Computer-Aided Molecular Design
 Read it [here](#)

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

- 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 Marti

- 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



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](#)  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
- 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

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

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

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 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](#)