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

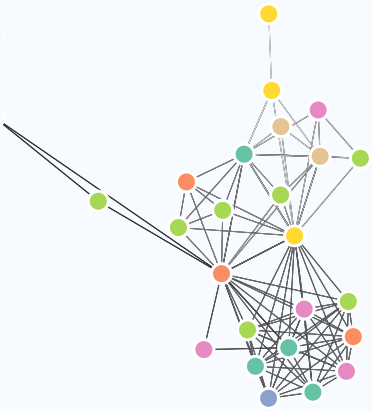
RESEARCH EXPERIENCE

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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Sergio Ruiz

PROGRAMMING SKILLS

- R
- Bash
- Python
- Web Development
- SQL
- C++

Source code available at github.com/sruizcarmona/

Last updated on May 19, 2021

2018 | 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, 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)

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 | 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-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

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

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 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