

Miquel Duran-Frigola, PhD

Ersilia Open Source Initiative | <https://ersilia.io>

Email: miquel@ersilia.io

Phone: +34 680 477 789

Twitter: @mduranfrigola

ORCID ID: 0000-0002-9906-6936

Researcher ID: AAO-3505-2021

Experience

Lead Scientist & Co-Founder at Ersilia Open Source Initiative (UK) / Since Jul 2020

Development of a computational drug discovery resource endorsing open science principles and focused on low- and middle-income countries

Research Associate at IRB Barcelona (Spain) / Jan 2018 — Jun 2020

Structural Bioinformatics and Network Biology Laboratory

Invention of a computational drug discovery platform. Supervision of PhD and MSc students

Visiting Fellow at CIDRZ (Zambia) / Jul 2019 – Dec 2019

Centre for Infectious Disease Research in Zambia, Central Laboratory

Harmonization and large-scale analysis of clinical and laboratory data

Post-Doctoral Researcher at IRB Barcelona (Spain) / Feb 2016 – Dec 2017

Structural Bioinformatics and Network Biology Laboratory

Development of a drug discovery protocol for the 'omics' characterization of chemical libraries

PhD Student at IRB Barcelona (Spain) / Sept 2011 – Jan 2016

Structural Bioinformatics and Network Biology Laboratory

Network biology approaches to pharmacology and drug side effects

Visiting Researcher at Manhica Health Research Center (Mozambique) / Sep 2015 – Dec 2015

ISGlobal – Bill & Melinda Gates Foundation

Machine learning methods to determine causes of death in developing countries

Visiting Researcher at Tel Aviv University (Israel) / Apr 2014 – Jul 2014

Eytan Ruppin's Laboratory

Genome-scale metabolic modeling of cancer

Researcher for Development at Central American University (El Salvador) / Feb 2010 – Sep 2010

Chemical Engineering Department

Water analysis and improvement of environmental factors in war refugee communities

Researcher at IQS School of Engineering (Spain) / Feb 2009 – Jan 2010

Photochemistry Lab

Synthesis and photophysical characterization of porphyrin derivatives

Visiting student at MIT (USA) / Jul 2009 – Sep 2009

Harvard-MIT Health Sciences and Technology Division / Edelman's Laboratory

Photodynamic treatment against atherosclerosis

Visiting student at Superior Council of Scientific Research (Spain) / Jun 2008 – Sep 2008

Theoretical and Computational Chemistry Group

Gas-phase reactivity using quantum chemistry

Education

Pompeu Fabra University / Sep 2011 – Jan 2016

PhD in Biomedicine / Cum Laude, Extraordinary Award UPF

Pompeu Fabra University / Oct 2010 – Jun 2012

MSc in Bioinformatics for Health Sciences / First in class. Project obtained with Honors

IQS School of Engineering / Jul 2009 – Feb 2010

IQS Chemical Engineer / Project obtained with Honors

IQS School of Engineering / Sep 2003 – Jun 2009

BSc in Organic Chemistry / First in class

Scholarships and Grants

La Caixa BioMedTec Grant / To foster a spin-off of my research
EADA MAP Program / For a spin-off proposal
Lindau Nobel Laureate Meeting / Selected Young Researcher attendee
EMBO Short-term fellowship / Stay at Tel Aviv University
FEBS Short-term fellowship / Stay at Tel Aviv University
Spanish FPU fellowship / 4-year PhD funding
Catalan Agency for Development Cooperation / Selected candidate UNESCO – Ramon Llull University
Seed Fund MIT – Spain and Cambra de Comerç de Barcelona Grant / Selected candidate
Collaboration Grant AGAUR / Introduction to research at IQS School of Engineering
JAE-Intro / Introduction to research at Superior Council of Scientific Research
Francesc Castelló fellowship to academic excellence / Full tuition of my BSc in Chemistry
Caixa Manresa fellowship to access University / In recognition of high-school graduate studies

Honors and Awards

Extraordinary Award for my PhD / Pompeu Fabra University
Best Poster Presentation / 2nd IRB Barcelona PhD Student Symposium
Extraordinary Award Proves d'Accés a la Universitat / Exam to access University
Proves Cangur Award / National Mathematics competition
Fem Matemàtiques Award / National Mathematics competition
2nd Award Good Practices in University Cooperation for Development / Team recognition

Publications / * first (co-) author, **corresponding author. Sorted by year of publication

Bertoni, Duran-Frigola** et al. Bioactivity descriptors for uncharacterized compounds. Nat Commun, 2021 (in press)

Pry et al. Cervical cancer screening outcomes in Zambia, 2010–19: a cohort study, Lancet Global Health, 2021

Pauls et al. Identification and drug-induced reversion of molecular signatures of Alzheimer's disease onset and progression in AppNL-GF, AppNL-F and 3xTg-AD mouse models, BioRxiv, 2021

Douglass et al. A Community Challenge for Pancancer Drug Mechanism of Action Inference from Perturbational Profile Data. BioRxiv, 2020

Duran-Frigola** et al. Bioactivity profile similarities to extend the universe of COVID-19 drugs. J Chem Inf Mod, 2020

Duran-Frigola** et al. Extending the small molecule similarity principle to all levels of biology with the Chemical Checker. Nat Biotechnol, 2020

Pry et al. Patient-reported reasons for declining same-day antiretroviral therapy initiation in routine HIV care settings in Lusaka, Zambia: results from a mixed-effects regression analysis, JAIDS Soc, 2020

Moncunill et al. Antigen-stimulated PBMC transcriptional protective signatures for malaria immunization. Sci Transl Med, 2020

Mateo et al. Personalized cancer therapy prioritization based on driver alteration co-occurrence patterns. Genome Med, 2020

Luck et al. A reference map of the human binary protein interactome. Nature, 2019

Duran-Frigola** et al. Formatting biological big data for modern machine learning in drug discovery. WIREs Comput Mol Sci, 2019

Fernandez-Torras, Duran-Frigola**, Aloy. Encircling the regions of the pharmacogenomics landscape that determine drug response. Genome Med, 2019

Persi, Duran-Frigola* et al. Systems analysis of intracellular pH vulnerabilities for cancer therapy. Nat Commun, 2018

Mateo et al. Exploring the OncoGenomic landscape of cancer. Genome Med, 2018

Juan-Blanco, Duran-Frigola, Aloy. Rationalizing drug response in cancer cell lines. J Mol Biol, 2018

Duran-Frigola*, Mateo, Aloy. Drug repositioning beyond the low-hanging fruits. Curr Opin Syst Biol, 2018

Duran-Frigola* et al. Detecting similar binding pockets to enable systems polypharmacology. Plos Comput Biol, 2017

Mateo et al. A PanorOmic view of personal cancer genomes. Nucl Acid Res, 2017

Sfriso, Duran-Frigola* et al. Residues coevolution guides the systematic identification of alternative functional conformations in proteins. Structure, 2016

Yang et al. Widespread expansion of protein interaction capabilities by alternative splicing. Cell, 2015

Jung et al. Isolation of human colon stem cells using surface expression of PTK7. Stem Cell Rep, 2015

Oberhardt et al. Systems-wide prediction of enzyme promiscuity reveals a new underground alternative route for pyridoxal 5'-phosphate production in E. coli. Plos Comput Biol, 2015

Jaeger, Duran-Frigola*, Aloy. Drug sensitivity in cancer cell lines is not tissue-specific. Mol Cancer, 2015

Arroyo et al. Systematic Identification of Molecular Links between Core and Candidate Genes in Breast Cancer. J Mol Biol, 2015

Duran-Frigola*, Rossell, Aloy. A chemo-centric view of human health and disease. Nat Commun, 2014

Juan-Blanco, Duran-Frigola, Aloy. IntSide: a web server for the chemical and biological examination of drug side effects. Bioinformatics, 2014

Arroyo, et al. Charting molecular links between driver and susceptibility genes in colorectal cancer. Biochem Biophys Res Commun, 2014

Rosàs et al. Modifications of microvascular EC surface modulate phototoxicity of a porphycene anti-ICAM-1 immunoconjugate. Langmuir, 2013

Duran-Frigola*, Mosca, Aloy. Structural systems pharmacology: the role of 3D structures in next-generation drug development. Chem Biol, 2013

Duran-Frigola*, Aloy. Analysis of chemical and biological features yields mechanistic insights into drug side effects. Chem Biol, 2013

Duran-Frigola*, Aloy. Recycling side effects into clinical markers for drug repositioning. Genome Med, 2012

Duran-Frigola* et al. Dual fluorescence in 9-amino-2,7,12,17-tetraphenylporphycene. Phys Chem Chem Phys, 2011

Participation in Congresses and Seminars / A selection is listed

Illuminating the Druggable Genome, Heidelberg, Feb 2020

IeDEA conference, Johannesburg, Oct 2019

Systems Biology: Networks, Cold Spring Harbor Laboratory, USA, 2019, 2015 and 2013

CSH Workshop, Vienna, Oct 2016

Resources and Techniques in Computational Drug Discovery, Tangier, May 2016

Lindau Nobel Laureate Meeting, Lindau, June-July 2015 / Selected attendee

IV IMPPC Annual Conference, Barcelona, Apr 2015

Bayesian Methods in Biostatistics and Bioinformatics, Barcelona, Dec 2012

Chemical Biology, Heidelberg, Sept 2012

ICREA Conference on Network Medicine, Barcelona, Nov 2011

Skills & Others

Languages: English (full proficiency), French (basic), Portuguese (basic), Spanish, Catalan

Programming: Python, R, Matlab, Bash, SQL, TensorFlow

Teaching: Supervision of 5 undergraduate students, 4 MSc students and 1 PhD thesis

Fields of research: Network analysis, structural bioinformatics, machine (deep) learning, chemoinformatics, biostatistics, constraint-based modeling, drug discovery

Short-term visits

Ben Raphael's Laboratory, Princeton University, 19 Mar - 5 Apr 2017 / Network-based algorithms

ChEMBL Laboratory, EBI-Hinxton, UK, 2016 / Database management

Certified courses

MalariaX: Defeating Malaria from Genes to the Globe, Harvard-X / Completed Jan 2019

Societies

Catalan Society of Biology, since 2019

Catalan Society of Chemistry, since 2021

Consultancies

Data visualisation for ISGlobal

Medical informatics for CIDRZ

Computational pharmacology for Janssen, Almirall, Anaxomics, Omnia & Nostrum

Capacity building for University of Bern

Editorial Board: Frontiers in Drug Discovery

Reviewer: European Journal of Pharmacology, Bioinformatics, Plos Computational Biology, Plos One, MDPI Molecules, Scientific Data, BMC Bioinformatics, Scientific Reports, eLife

Fiction Writing

Publications

Més o menys jo (Bridge, 2nd Ed., Catalan and Spanish). Crítica Serra d'Or Award / Nov 2014

Can Prat (Short story in Risc, Rata, Anthology of Contemporary Writers, Catalan and Spanish) / Mar 2017

La concavitat de l'horitzó, Cinc indicis... (Short stories in 24 contes al dia, Godall, Catalan) / Apr 2018

Education

Barcelona School of Management, Pompeu Fabra University / Oct 2016 – Sep 2017

Master's in Creative Writing / Project obtained with Honors

Open University of Catalonia / Since Sep 2020

BSc in Humanities

Ateneu Barcelonès Literature School / Jan 2011 – Jun 2013

Creative Writing School / Narrative, novel, playwriting, African novels

Honors and Awards

Can Serrat Writer's Grant 2019 / Writer in residence in Can Serrat International Art Residence

Montserrat Roig Fellowship 2018 / Writer in residence in Joan Miró Foundation

Talent Scholarship 2017 / Tuition Master's in Creative Writing

2nd Prize Joaquim Ruyra 2014 / To my fiction book

Crítica Serra d'Or Award 2015 / Prestigious recognition to my fiction book