Ismael Gómez García

Researcher & Data Scientist

Curriculum Vitae

SKILLS

Python	+++++
R	+++++
Scientific research	+++++
Data analysis & visualiz.	+++++
Machine learning	+++++
Computational geometry	++++
C/C++	++++
PDE modeling & simulation	+++
AI optimization	+++
Linux	+++
Relational databases	+++
Chemistry	++
Biomedicine	++

LANGUAGES

Spanish	**NATIVE**
English	**C1**

PUBLICATIONS

Research papers	**x12**
Conferences	**x5**
Patents	**x1**
Open source projects	**x2**

LINKS OF INTEREST

WORKING EXPERIENCE

Lecturer at CEA CAPA

Sep 2024 – Present | Part time

- University of Massachusetts Amherst, foreign program.
- Lecturer: Computer Science 110
- Lecturer: Introduction to Engineering

Senior Research Scientist at Chemotargets

May 2022 – Present

- Data Science & Machine Learning (big pharma: ACS).
- Mentoring & guidance of junior team members.

Senior Clinical Data Scientist at Savana/Capgemini

November 2020 – May 2022

- Data science & Statistics (big pharma: Pfizer, Janssen).
- Mentoring & guidance of junior team members.

PhD fellow at IMDEA materials institute

November 2015 – November 2020 | Part time

- Molecular property prediction with geometry & topology.
- C/C++ programming of chemoinformatic tools.

Data scientist at Hospital Clínico San Carlos

November 2015 – November 2020 | Part time

- Statistics & Machine Learning with R (clinical data).

Bioinformatician at AI department in UPM

November 2013 – November 2015

MSc fellow at HPCN group at UAM

July 2011 – November 2013

EDUCATION

PhD in Materials Science and Engineering — **UC3M**
2016 – 2021
Cum Laude & Outstanding thesis award.

MSc in R&D in Computing — **UAM**
2012 – 2013

Bachelor's in Computer Science — **UAM**
2006 – 2012

Bachelor's in Mathematics — **UAM**
2007 – 2011

ACADEMIC RECORD

RESEARCH PAPERS (10 PUBLISHED, 2 UNDER REVIEW):

2024 – Nature Reviews Drug Discovery (D1). Computational Drug Repurposing: Progress and Evaluation of in Silico Resources. *Major revision.*

2024 – Molecular Pharmaceutics (Q1). Refined ADME properties for drug classes. *Major revision.*

2021 – Allergy. Development and validation of the Food Allergy Severity Score. DOI: https://doi.org/10.1111/all.15165

2021 – ChemArxiv. DOI: 10.26434/chemrxiv.14706447.v1

2020 – CrystEngComm: Toward crystalline porosity estimators for porous molecules. DOI: 10.1039/C9CE01753D

2019 – Lab on a Chip: Tumor on a chip: a microfluidic model to study cell response to environmental gradients. DOI: 10.1039/C9LC00270G

2019 – Molecular Systems Design and Engineering: Computational discovery of a large-imine-cage-based porous molecular material and its application in water desalination. DOI: 10.1039/C9ME00018F

2018 – Journal of Computational and Theoretical Chemistry: Toward automated tools for characterization of molecular porosity.
DOI: 10.1021/acs.jctc.8b00764.

2018 – EBioMedicine: Organotypic microfluidic breast cancer model reveals starvation-induced spatial-temporal metabolic adaptations.
DOI: 10.1016/j.ebiom.2018.10.046

2018 – Molecular Systems Design and Engineering: In silico design and assembly of cage molecules into porous molecular materials. DOI: 10.1039/C8ME00055G

2017 – CrystEngComm: Towards stable porous crystalline phases of molecular belts. DOI: 10.1039/C7CE01679D

2017 – Crystal Growth and Design: Out-of-Oblivion Cage Molecules and Their Porous Crystalline Phases. DOI: 10.1021/acs.cgd.7b01095

ORAL PRESENTATIONS AND POSTERS IN CONFERENCES (4):

2019 – Oral presentation at EAACI Conference, Lisbon

2019 – Poster at International Conference on Multifunctional, Hybrid and Nanomaterials, Sitges

2018 – Oral presentation at FAAM Conference, Copenhagen. Winner of an EAACI travel grant.

2015 – Poster presentation at SSBSS, Taormina

PATENTS (1):

2015: Heterogeneous parallel systems for accelerating simulations based on discrete grid numerical methods. Patent code: EP2608084 (A1).

OPEN-SOURCE SOFTWARE TOOLS (2):

Molipor – http://www.nanoporousmaterials.org/programs/

Tasc – http://doi.org/10.5281/zenodo.4836276

ADDITIONAL TEACHING EXPERIENCE

CORPORATE TRAININGS:

2020-Current – Continuous mentoring and guidance of junior team members through the data science & engineering tools for business intelligence.

September 2023 – Seminar on in-house QSAR methods (Chemotargets).

January 2022 – Seminar: Geometry-based molecular discovery (Chemotargets).

October 2021 – Seminar: Applied geometric deep learning (Capgemini).

EXTERNAL SEMINARS & COURSES:

July-August 2015. Teaching at the Summer School of Science (Croatia).

June 2015. Course: Arduino for life scientists at the EVOPROG summer school (University of Warwick).

STUDENT GUIDANCE:

September 2015-June 2016. Co-direction of the final grade project (TFG): "Los orígenes del cálculo: de Arquímedes a Leibniz."

September 2014-June 2015. Co-direction of the final grade project (TFG): "Aquacore: Interfaz para el control de sistemas microfluídicos."

September 2014-June 2015. Guidance of three undergraduate students during their practicum (Grade in Computer Science).