Guillermo Ramajo Fernández

AI Research Scientist

Building machine learning systems and foundation models for computational biology and drug discovery.

Email | LinkedIn | GitHub | Google Scholar | ResearchGate | Website

Download CV (PDF)

PROFESSIONAL SUMMARY

AI Research Scientist and PhD candidate in Artificial Intelligence specializing in foundation models, self-supervised learning and machine learning systems for computational biology and drug discovery.

My research combines artificial intelligence, molecular representation learning and biological data analysis to develop models capable of extracting meaningful insights from complex scientific datasets.

I have experience designing deep learning pipelines in PyTorch, publishing international conference research, and building AI systems that bridge fundamental research with practical scientific applications.

RESEARCH AREAS

Foundation Models | Scientific AI | Drug Discovery | Computational Biology | Agentic AI | Self-Supervised Learning | Molecular Representation Learning | Deep Learning

EXPERIENCE

AI Research Scientist

Universidad CEU San Pablo · Madrid, Spain
Feb 2023 – Present

- Develop machine learning models for computational biology, molecular representation learning and drug discovery applications.
- Designed a self-supervised transfer learning framework for collision cross-section prediction using 61,863 experimentally measured molecular samples.
- Achieved a 3.20% mean relative prediction error while improving cross-dataset generalization through learned molecular representations.
- Develop PyTorch-based deep learning pipelines for training, evaluation and analysis of biomedical AI models.
- Published international conference research in machine learning for computational metabolomics and biomedical AI.

Computer Science Teacher

Comunidad de Madrid · Spain
Feb 2022 – Nov 2022

- Designed and delivered programming and computer science courses focused on software development, algorithms and computational thinking.
- Mentored students through practical programming projects and hands-on technical training.

EDUCATION

PhD in Artificial Intelligence

Universidad CEU San Pablo
2023 – 2027

Research focus: Foundation models, self-supervised learning, molecular representation learning and agentic AI systems for biomedical discovery.

Master's Degree in Artificial Intelligence

Universidad Internacional de La Rioja

Specialization in machine learning, deep learning, computer vision, natural language processing and predictive modeling.

Master's Degree in Integrative Synthetic Biology

Research conducted at Centro de Investigaciones Biológicas Margarita Salas (CSIC)

Applied molecular biology and genome engineering techniques to research projects in regenerative medicine, Alzheimer's disease and cancer immunotherapy.

SELECTED PUBLICATIONS

A Self-Supervised Transfer Learning Approach for Collision Cross-Section Prediction

IWANN 2025 · International Work-Conference on Artificial Neural Networks

Training Deep Learning Neural Networks for Predicting CCS Using the METLIN-CCS Dataset

IWBBIO 2024 · International Conference on Bioinformatics and Biomedical Engineering

SELECTED PROJECTS

Molecular Foundation Models Evaluation

Research framework exploring learned molecular representations and machine learning approaches for chemical property prediction.

AI Cloud Classification System

Computer vision application using artificial intelligence to identify cloud formations from images.

TECHNICAL SKILLS

Programming

Python · SQL · Git · Linux

Machine Learning

PyTorch · Transformers · Deep Learning · Self-Supervised Learning

Scientific Computing

RDKit · Molecular Representations · Bioinformatics

AI Systems

LLMs · Agentic AI · Retrieval-Augmented Generation

LANGUAGES

Spanish — Native
English — Professional proficiency