

# Dr. Noelia Ferruz

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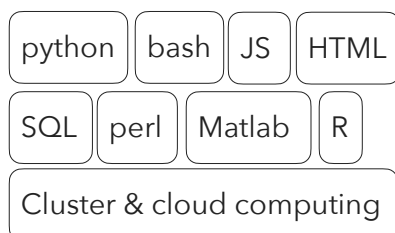
**Publications** ➡ [Google Scholar profile](#)

**Linkedin** ➡ <https://www.linkedin.com/in/noeliaferruz>



*Incoming Ramon y Cajal group leader with focus on computational protein design*

## PROGRAMMING



## STRENGTHS



Driven

Motivator & leader  
Communication



Statistical analysis  
Structural biology  
Machine learning

## LANGUAGES



## PASSIONATE ABOUT

Data analysis

Programming

Maths

Machine learning

Competitive running

Travelling

Challenges - big or small.

## RESEARCH EXPERIENCE

### BEATRIU DE PINÓS FELLOW

University of Girona, Spain

From Apr. 2022 (current position)

- Implementation of language and diffusion models for controlled de novo protein sequence generation

### POSTDOC RESEARCHER

University of Bayreuth, Germany

Dec. 2016 - Mar. 2022 (now Associate)

Apr. 2021- Nov. 2021: Parental leave

- Analysis of large databases to find evolutionarily related protein fragments via **hidden Markov models (HMMs)**.
- Analysis of protein relationships using **network analysis**.
- **Front and backend** implementation of several web servers: [proteintools.uni-bayreuth.de](http://proteintools.uni-bayreuth.de), [fuzzle.uni-bayreuth.de](http://fuzzle.uni-bayreuth.de), & [fuzzle.uni-bayreuth.de/2.0](http://fuzzle.uni-bayreuth.de/2.0).
- Software development of [ProtLego](#), a tool for protein design.

### POSTDOCTORAL FELLOW

Pfizer at Boston, USA

Mar. 2016 - Oct. 2016

- Establishing the use of Acellera's software for its application as a standard tool in Pfizer's preclinical programs.
- Generation of multi-microsecond MD data on **GPU clusters**.
- Predictive analysis of large amounts of MD and biological data by **statistical methods** to provide human-interpretable conclusions.

### PROJECT MANAGER

Acellera Labs at Barcelona, Spain

Feb. 2014 - Feb. 2016: part-time

- Analysis of large amounts of data and communication of results by reports, presentations and scientific publications.
- Management of several research projects that led to first-author publications.
- Main collaborators: **Janssen Pharmaceuticals, Boehringer Ingelheim, and Pfizer**.

## EDUCATION

### **PhD COMP. BIOPHYSICS**

UPF, PRBB, Barcelona

Sep. 2012 - Mar. 2016

Thesis: 'Understanding Ligand-Receptor Recognition by Means of High-Throughput Molecular Dynamics. A Perspective for Drug Discovery' - CUM LAUDE

Defense: March 4, 2016

Supervisor: Gianni De Fabritiis

### **MSc. BIOINFORMATICS**

UPF, PRBB, Barcelona

Sep. 11 - June 2013

Thesis: 'Quantitative characterisation of binding kinetics, energetics and poses in fragment based drug design'

Supervisor: Gianni De Fabritiis

### **ERASMUS MUNDUS**

University of Cambridge

Sep. 2010 - June 2011

Thesis: 'Study of the conformational regulation of kinase domains'

Supervisor: Peter J. Bond

### **BSc & MSc CHEMISTRY**

University of Zaragoza

Feb. 2006 - Sep. 2011

## OTHER MERITS

### **PROFESSIONAL ATHLETE**

Personal bests:



800m: 2:15

1500m: 4:40:85

3000m: 10:20:42

10k: 37:35

1/2 marathon: 1:30:36

## TEACHING SUMMARY

**BIOMEDICAL PROGRAMMING.** Elite Bayern. July, 2017-2020 (64h).

**PROTEIN MODELING.** University of Bayreuth. Feb, 2017/18 (32h).

**ELEMENTS OF MATHEMATICS.** Univ. Pompeu Fabra 2014 (30h).

**INTRODUCTION TO PYTHON.** Univ. Pompeu Fabra 2013 (30h).

## GRANTS & CONTRACTS SUMMARY

**RAMON Y CAJAL 2021.** RYC2021-034367-I.

**NHR RRZE CLUSTER:** Awarded 100,000 GPU-hours.

**PROJECT 'GENERACIÓN DE CONOCIMIENTO 2021'.**

PID2021-124718NA-I00 (Awarded 20,500 €).

**BEATRIU DE PINÓS.** Universitat de Girona. (Awarded 132,000 €).

**EDUCATIONAL TENURE-TRACK POSITION.** University of Groningen, GBB. (Rejected in favour of Beatriu de Pinós).

**MARIA ZAMBRANO 2021.** University of Zaragoza. (Rejected in favour of Beatriu de Pinós).

**DFG SACHBEIHILFE.** Co-organisation of an international conference. 2021. (Awarded 24,000 €).

**WIN-UBT GRANT.** Conference organisation. (Awarded 8,100 €).

**FUTURE AND EMERGENT TECHNOLOGIES (FET) OPEN HORIZON 2020 'pre-ART'.** Prof. Birte Höcker 2017-2021.

**EUROPEAN RESEARCH COUNCIL PROJECT 'PROTLEGO'.** Prof. Birte Höcker 2015-2020.

**UNIVERSITY BAYREUTH TRAVEL GRANT.** 2017/2018/2019. (Awarded between 500- 1,500 € each time).

**NVIDIA GPU GRANT.** 2017. (Awarded a GTX TITAN Xp).

**FI-AGAUR THESIS DEFENCE AID.** 2016. (Awarded 3,000 €).

**FI-AGAUR.** Competitive PhD Fellowship. February 2013. (Awarded 46,500 €).

## SUPERVISION SUMMARY

- 03/2020 - 08/2020. University Bayreuth. MSc Student
- 08/2019 - 09/2019. University Bayreuth. MSc student.
- 03/2019 - 08/2019. University Bayreuth. BSc student.
- 03/2019 - 08/2019. University Bayreuth. MSc student.
- 09/2015 - 07/2016. University Pompeu Fabra. MSc student.

## ORGANISATION OF CONFERENCES

- Co-organisation of the international conference APFED-22: 'Advances in protein Folding, Engineering, and Design'. <https://apfed22.uni-bayreuth.de/> Bayreuth, Germany.
- Support organising 'PreArt Workshop'. 18/19th September, Bayreuth, Germany. <https://www.pre-art.uzh.ch/workshops/>

## LIST OF PUBLICATIONS.

<sup>†</sup>equal contribution, <sup>\*</sup>corresponding author. 13/16 are first-author publications.

### Articles published by outlets with scientific quality assurance:

1. **Ferruz, N.<sup>\*</sup>**, Schmidt, S. Höcker, B. ProtGPT2 is a deep unsupervised language model model for protein design. *Nat Commun* **13**, 4348 (2022).
2. **Ferruz, N.<sup>\*</sup>**, Höcker, B. Controllable protein design with language models. *Nat Mach Intell* **4**, 521–532 (2022).
3. **Ferruz, N.**, Höcker, B. Dreaming ideal protein structures. *Nat. Biotechnol.* **40**, 171–172 (2022).
4. **Ferruz, N.<sup>\*</sup>**, Schmidt, S. & Höcker, B. ProteinTools: a toolkit to analyze protein structures. *Nucleic Acids Res.* **49**, W559–W566 (2021).
5. **Ferruz, N.**, Noske, J. & Höcker, B. Protlego: A Python package for the analysis and design of chimeric proteins. *Bioinformatics* (2021) doi:10.1093/bioinformatics/btab253.
6. **Ferruz, N.<sup>\*</sup>**, Michel, F., Lobos, F., Schmidt, S. & Höcker, B. Fuzzle 2.0: Ligand Binding in Natural Protein Building Blocks. *Front. Mol. Biosci.* **8**, 805 (2021).
7. Kröger, P.<sup>†</sup>, Shanmugaratnam, S.<sup>†</sup>, **Ferruz, N.**, Schweimer, K. & Höcker, B. A comprehensive binding study illustrates ligand recognition in the periplasmic binding protein PotF. *Structure* (2021) doi:10.1016/j.str.2020.12.005.
8. **Ferruz, N. et al.** Identification and Analysis of Natural Building Blocks for Evolution-Guided Fragment-Based Protein Design. *J. Mol. Biol.* (2020) doi:10.1016/j.jmb.2020.04.013.
9. Lechner, H.<sup>†</sup>, **Ferruz, N.<sup>†</sup>** & Höcker, B. Strategies for designing non-natural enzymes and binders. *Current Opinion in Chemical Biology* vol. 47 67–76 (2018).
10. **Ferruz, N. et al.** Dopamine D3 receptor antagonist reveals a cryptic pocket in aminergic GPCRs. *Sci. Rep.* **8**, 1–10 (2018).
11. **Ferruz, N.**, Tresadern, G., Pineda-Lucena, A. & De Fabritiis, G. Multibody cofactor and substrate molecular recognition in the myo-inositol monophosphatase enzyme. *Sci. Rep.* **6**, 1–10 (2016).
12. **Ferruz, N.** & De Fabritiis, G. Binding Kinetics in Drug Discovery. *Mol. Inform.* **35**, 216–226 (2016).
13. **Ferruz, N.**, Harvey, M. J., Mestres, J. & De Fabritiis, G. Insights from Fragment Hit Binding Assays by Molecular Simulations. *J. Chem. Inf. Model.* **55**, 2200–2205 (2015).
14. Arena, S. et al. Emergence of multiple EGFR extracellular mutations during cetuximab treatment in colorectal cancer. *Clin. Cancer Res.* **21**, 2157–2166 (2015).
15. Lauro, G.<sup>†</sup> **Ferruz, N.<sup>†</sup>** et al. Reranking docking poses using molecular simulations and approximate free energy methods. *J. Chem. Inf. Model.* **54**, 2185–2189 (2014).
16. Buch, I., **Ferruz, N.** & De Fabritiis, G. Computational modeling of an epidermal growth factor receptor single-mutation resistance to cetuximab in colorectal cancer treatment. *J. Chem. Inf. Model.* **53**, 3123–3126 (2013).