Dr Fabien Plisson
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Professional Summary

Medicinal chemist and computational biologist with 18 years of R&D experience spanning drug discovery, AI-driven protein design, and bioinformatics. I have a proven track record in establishing and leading an independent research group, securing competitive funding, developing higher education curricula, and supervising 35+ HDR students and staff. Expertise in integrating machine learning and computational tools with experimental validation to accelerate the discovery and design of natural products and protein-based solutions for cancer, diabetes, neurodegeneration, and infectious diseases.

Core Competencies

AI & Computational Biology: Machine/deep learning (Scikit-Learn, TensorFlow, PyTorch), Statistics (R/RStudio), protein structure prediction (AlphaFold, RoseTTA series), bioinformatics, NLP for biomolecules, HPC/cloud computing (AWS, Google Colab, Hugging Face).
Drug Discovery: Peptide design, medicinal chemistry, natural product chemistry, chemoinformatics, molecular docking, QSAR modelling, high-throughput screening.
Laboratory Skills: Protein expression/purification, peptide synthesis, spectroscopy (NMR, CD, UV, IR), chromatography (RP-HPLC, UPLC), mass spectrometry.
Leadership: Research strategy, grant writing (5.6M MXN secured), team supervision, curriculum development, multidisciplinary research, and cross-sector partnerships.
Languages: English (fluent, 15+ years), Spanish (fluent, 8+ years), French (native).

Professional Experience

Founder & Lead Consultant, Ingenie Bio – Sydney, Australia | Oct 2024-present
- Providing AI/ML consulting services to academia and industry for molecular sciences applications.
- Developing predictive and generative models for property/function prediction and protein design.

Group Leader (Senior Lecturer), CINVESTAV-IPN – Irapuato, Mexico | Nov 2017-Jun 2024
- Led a computational biology research laboratory advancing AI-driven peptide drug discovery & design.
- Supervised 17 students (5 BSc, 8 MSc, 4 PhD) and mentored 18 additional HDR students.
- Secured 5.6 million MXN in grants despite Mexico's underfunded R&D system (6x less relative to GDP).
- Developed predictive and generative AI models from sequence, structure, and evolutionary data.
- Implemented bioinformatics workflows using AlphaFold and Rosetta series for protein engineering.
- Conducted high-throughput venom transcriptome analysis *via* HPC, ML, and phylogenetics.
- Designed and optimised protein expression and purification protocols for small proteins.
- Collaborated with wet-lab teams to validate bioactive peptides targeting membranes and receptors.
- Delivered courses in data science, chemical biology, chemoinformatics, and structural bioinformatics to undergraduate and postgraduate programs.

Health Data Scientist Fellow, Insight Data – Boston, USA | Sept 2016-Feb 2017
- Designed ML models to predict adverse immunogenic reactions from 450,000 vaccine reports (VAERS).
- Deployed Reac2Vac.online, a web-based predictive analytics platform for US vaccine safety.

Research Officer, The University of Queensland – Brisbane, Australia | Sept 2012-Sept 2015
- Developed novel peptide therapeutics for type 2 diabetes with Prof. David Fairlie and *Pfizer.*
- Engineered and validated GLP-1 receptor agonists with comparable potency to Exenatide (Byetta™).
- Developed PPI inhibitors for myeloid leukemia with *Protagonist Therapeutics.*
- Deployed Schrödinger Maestro for conformational search and macrocycle design.

PhD Researcher, UQ Institute for Molecular Bioscience – Brisbane, Australia | Aug 2008-Aug 2012
- Discovered novel kinase inhibitors (5 papers + **EP2662081A1**) between Prof. Robert J. Capon and Spanish company *Noscira*, using structure-based drug discovery and *in vitro* assays.
- Conducted extensive HPLC purification and structural characterisation studies (NMR, MS) of natural products from marine extracts in minute quantities (0.1-5mg).

- Pioneered predictive ML model for blood-brain permeability of small molecules.
- Participated in HTS campaigns for antimalarial discovery in collaboration with the *QIMR Berghofer* MRI.

Research Engineer, PIERRE FABRE and CNRS – Toulouse, France | Mar 2007-May 2008
- Synthesised 100+ analogues from scarce natural products (5-10mg scale) and sensitive conditions.
- Co-invented patented synthetic process (**FR2941697A1),** reducing multi-step chemical synthesis.

EDUCATION & TRAINING

2012 **Ph.D. Organic Chemistry**, The University of Queensland (UQ) – Australia
2007 **MSc Chemical Engineering**, ENSCM, Grande École – Montpellier, France
2007 **MSc Biomolecular Engineering**, ENSCM, Grande École – Montpellier, France

SELECTED PUBLICATIONS & PATENTS

26 peer-reviewed publications in *Springer Nature Scientific Reports, Chemical Science, Angewandte Chemie, ChemBioChem, Digital Discovery*, *Microbial Genomics* and others.

- Aguilera-Puga, M.d.C. & Plisson, F.* Structure-aware machine learning strategies for antimicrobial peptide discovery. *Scientific Reports* 2024, 14, 11995. [DOI] [Research Square] [Github]
- Saldívar-González, F. I.; Aldas-Bulos, V. D.; Medina-Franco, J. L. & Plisson, F.*. Natural Product Drug Discovery in the Artificial Intelligence Era. *Chemical Science* 2022, 13, 1526-1546. [DOI]
- Plisson, F.*; Ramírez-Sánchez, O. & Martínez-Hernández, C. Machine learning-guided discovery and design of non-hemolytic peptides. *Scientific Reports* 2020 10, 16581. [DOI] [Github]

1 patent: Derguini, F.; Plisson, F.; Massiot, G. Preparation of tagitinin C and F derivatives as anti-cancer agents. Patent application FR 2941697 A1 20100806 (2010) [Europe PMC] [Google Patents].

GRANTS & AWARDS

Lead CI/PI on 5.6 million MXN in grants from CONAHCYT, FOSEC SEP, and CGSTIC (2017-2024).
Roche & Mexican Health Foundation - Rosenkranz Medical Research Prize in Biotechnology (2021).
Forum for Health Research from Guanajuato State Award (2018).
Mexican Research Council Early-Career Research Fellowship (2017-2022).
IMB Research PhD Scholarship & UQ International Tuition Research Award (2008-2012).

SELECTED PRESENTATIONS & SERVICES

- ▷ *Scientific outreach:* 65+ seminars at universities and conferences across the Americas, Europe, Asia, and Australia (2017-2025), 15 conference proceedings and two podcasts.
- ▷ *Panel discussions:* Symposium on Bioinformatics and Engineered Intelligence (Adelaide, 2025), Hit ID Symposium (Melbourne, 2025), Health Data Science (online, 2021), Allbiotech Summit (Mexico, 2018)
- ▷ *Workshop organiser/speaker:* BIRS-CMO Computational Biology (Oaxaca, 2023), RIIAA (Mexico City, 2021/2022), CABANA Chemoinformatics (Mexico, 2019) & Bioinformatics (Colombia, 2019)
- ▷ *Peer-reviewer*: 60+ manuscripts for Nature, RSC, ACS, Oxford, BMC journals.
- ▷ *Grant reviewer*: Mexican Research Council, Canada NFRF, UK Rosetree Trust, European Commission.
- ▷ *External PhD examiner*: University of Queensland (2021), Tecnológico de Monterrey (2021), University of Guanajuato (2018).

CONTINUOUS LEARNING

2024 mRNAs as Medicines (Moderna)
2024 Machine learning in production - MLOps (deeplearning.ai)
2024 Open Source Models with Hugging Face (deeplearning.ai)
2023 How Diffusion Models Work (OpenAI & deeplearning.ai)
2022 Deep Learning for Molecules and Materials (A.D. White, dmol.pub)
2022 STAT 453: Introduction to Deep Learning (S. Raschka, sebastianraschka.com)
2021 MIT 6.S191: Introduction to Deep Learning (introtodeeplearning.com)
2020 Sequence models (Deep Learning Specialisation) (A. Ng, deeplearning.ai)
2019 Neural Networks and Deep Learning (A. Ng, deeplearning.ai)
2013 Data Analysis, Johns Hopkins Bloomberg School of Public Health (J. Leek)