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Pablo Mas

GitHub
LinkedIn

PhD candidate specialized in machine learning for drug discovery, with an emphasis on improving exploration and exploitation during lead optimization. Conducting my research within the Theoretical Chemistry Group at ENS-PSL and the Integrated Drug Discovery team at Sanofi. I am also pursuing an MBA at the Collège des Ingénieurs and teaching at ENS-PSL and Le Wagon bootcamp.

Education

Doctor of Philosophy - PhD **10/2022 — Present**
École Normale Supérieure (ENS Ulm) *Paris, France*
- Conducted research on machine learning applications in drug discovery and theoretical chemistry, in collaboration with Sanofi. Under the supervision of Pr. Rodolphe Vuilleumier (ENS) and Dr. Marc Bianciotto (Sanofi).

Master of Business Administration - MBA **01/2023 — Present**
Collège des Ingénieurs (CDI Paris) *Paris, France*
- Selective MBA program designed for top graduates from leading French Engineering Schools.

Master of Science - MSc **09/2021 — 09/2022**
BME Paris - PSL University *Paris, France*
- Relevant courses: Deep learning and neurosciences - Deep learning and neurocomputational projects - Quantification for Neuroimaging - Machine Learning for Bioimaging

Master of Science ("Diplôme d'ingénieur") - MSc **09/2018 — 09/2021**
ESPCI Paris *Paris, France*
- Biotechnology specialization (3rd year): Systems biology and neurobiology - Biochemistry and molecular biotechnology - Deep learning - Statistical learning - Advanced analytical chemistry

Bachelor of Science - BSc **09/2016 — 09/2018**
Sorbonne University *Paris, France*
- Dual bachelor's degree with majors in physics and chemistry.

Experience

Research scientist (CIFRE PhD) **10/2022 — Present**
Sanofi *Paris, France*
- Developed rational exploration and exploitation strategies for molecule prioritization during the lead optimization phase, supported by a comprehensive toolkit for medicinal chemists.
- Simulated active-learning based selection scenarios on legacy drug discovery projects.
- Developed QSAR/QSPR models in low and high data regimes.

Research intern **02/2022 — 09/2022**
Aramis Lab (INRIA & Paris Brain Institute) *Paris, France*
- Developed deep learning algorithms using graph neural networks for automated segmentation of peptide accumulation in whole-slide images, enabling improved stratification of Alzheimer's disease patients.

Research intern **04/2021 — 08/2021**
LSABM (ESPCI Paris - PSL) *Paris, France*
- Developed a LC-MS method to detect mustard gas-modified DNA traces in biological samples, in collaboration with the French Defence Procurement Agency.

Analytical scientist intern **07/2020 — 12/2020**
Adocia *Lyon, France*
- Developed and characterized (via HPLC and NMR) a protective hydrogel for islets of Langerhans (beta cells) as part of a cell therapy project aimed at creating an artificial pancreas.

Research intern **06/2018 — 08/2018**
Phenix Lab (CNRS) *Paris, France*
- Investigated water dynamics in 15th-century paintings through NMR relaxometry, X-ray, and IR spectroscopy.

Data analyst intern **05/2017 — 08/2017**
Development Alternatives Incorporated *Washington DC, USA*
- Developed data visualization dashboards and contributed to a report for the Aspen Institute : "A Global Opportunity: Get Youth Working".

Publications

Gkeka, P.; Llompart, P.; Amaning, K.; Bianciotto, M.; Filoche-Romme, B.; Foricher, Y.; **Mas, P.**; Papin, D.; Rameau, J.-P.; Schio, L.; Marcou, G.; Varnek, A.; Moussaid, M. **Harnessing Medicinal Chemical Intuition from Collective Intelligence**. 2024. https://doi.org/10.21203/rs.3.rs-4365958/v1. (under review)

Bailey, M.; Moayedpour, S.; Li, R.; Corrochano-Navarro, A.; Kötter, A.; Kogler-Anele, L.; Riahi, S.; Grebner, C.; Hessler, G.; Matter, H.; Bianciotto, M.; **Mas, P.**; Bar-Joseph, Z.; Jager, S. **Deep Batch Active Learning for Drug Discovery**. eLife 2024. https://doi.org/10.7554/elife.89679.2.

Moayedpour, S.; Corrochano-Navarro, A.; Sahneh, F.; Noroozizadeh, S.; Koetter, A.; Vymetal, J.; Kogler-Anele, L.; **Mas, P.**; Jangjou, Y.; Li, S.; Bailey, M.; Bianciotto, M.; Matter, H.; Grebner, C.; Hessler, G.; Bar-Joseph, Z.; Jager, S. **Many-Shot In-Context Learning for Molecular Inverse Design** arXiv 2024. https://doi.org/10.48550/arxiv.2407.19089.

Jimenez, G.; **Mas, P.**; Kar, A.; Peyrache, J.; Ingrassia, L.; Boluda, S.; Delatour, B.; Stimmer, L.; Racoceanu, D. **A Meta-Graph Approach for Analyzing Whole Slide Histopathological Images of Human Brain Tissue with Alzheimer's Disease Biomarkers**. Med. Imaging 2023: Digit. Comput. Pathol. 2023. https://doi.org/10.1117/12.2657475.

Conferences

EuroQSAR 2024 **09/2024**
Barcelona, Spain

CS3 - Strasbourg Summer School in Cheminformatics **06/2024**
Strasbourg, France

MLSS - Machine Learning Summer School **03/2024**
Okinawa, Japan

6th Artificial Intelligence in Chemistry Symposium **09/2023**
Cambridge, UK

GGMM - Young Modellers Conference **05/2023**
Toulouse, France

Teaching

École Normale Supérieure (ENS Ulm) **09/2023 — Present**
Elaborated and supervised data challenges for the "AI in Chemistry" graduate course, hosted on ENS's data challenge platform.
- 2023 challenge: Predicting molecule-protein interaction for drug discovery.
- 2024 challenge: ADMET property prediction for drug discovery.

Le Wagon Bootcamp **09/2021 — Present**
- Delivered machine learning as well as deep learning courses to 250+ students.
- Supervised final bootcamp projects.

Skills

Tools	Python (scikit-learn, PyTorch, Tensorflow, RDKit, deepchem...), Git, AWS, Matlab, SQL, AWS LaTeX
Communication	French (native), English (fluent - C1 level), Spanish (intermediate - B1 level)

Extracurricular activities

- Treasurer of the ESPCI Paris – PSL student's office, in charge of a 150 000€ budget.
- External Relations Officer of the ESPCI Paris – PSL sports union.
- **Sports:** Handball (15 years, two-time high-school champion of Morocco), Diving (PADI 2), Skiing, Squash.