




CLAUDIA AFONSO

Lisbon, Portugal (available for immediate relocation or remote work)

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I'm a data scientist with expertise in programming, data wrangling, machine learning, and statistical analysis of large datasets. My background also includes chemistry and biomedical research, with hands-on experience in chemical and molecular biology techniques. I'm currently seeking opportunities where I can apply my technical and analytical skills to solve real-world problems in data-driven industries. My GitHub portfolio showcases projects where I've applied programming and machine learning techniques to solve problems in various contexts.

Education

MSc in Data Science Faculty of Sciences, University of Lisbon	Sep 2022 – Jul 2025 <i>Lisbon, Portugal</i>
PhD in Biomedical Sciences Faculty of Medicine, University of Lisbon	Jan 2018 – Oct 2024 <i>Lisbon, Portugal</i>
Minor in Computer Science Faculty of Sciences, University of Lisbon	Sep 2022 – Jul 2024 <i>Lisbon, Portugal</i>
MSc in Bioorganic Chemistry NOVA School of Science and Technology, NOVA University of Lisbon	Sep 2015 – Dec 2017 <i>Caparica, Portugal</i>
MSc in Neuroscience Faculty of Medicine, University of Lisbon	Sep 2014 – Jul 2017 <i>Lisbon, Portugal</i>
BSc in Chemistry with a Minor in Biology Faculty of Sciences, University of Lisbon	Sep 2011 – Jul 2014 <i>Lisbon, Portugal</i>

Experience

Research Scientist in Data Science Faculty of Sciences, University of Lisbon	Nov 2023 – Apr 2025 <i>Lisbon, Portugal</i>
<ul style="list-style-type: none">Built a computational pipeline to recommend compounds for drug discovery by leveraging molecular representations and chemical similarity methodsEfficiently processed large-scale chemical datasets (16,000+ compounds) within project timelines to generate molecular fingerprints and structure interaction data for sequential recommendationIndependently evaluated the SASRec deep learning model for chemical compound recommendation across 13 hyperparameter configurations and 5 molecular fingerprint typesIdentified and documented key limitations of a published approach to sequence-aware recommendation	
Research Scientist in Biomedical Sciences Institute of Molecular Medicine	Jan 2018 – Sep 2022 <i>Lisbon, Portugal</i>
<ul style="list-style-type: none">Developed novel chemical biology strategies for protein modification - communicated findings through 2 peer-reviewed publicationsEngineered 3 protein sequences via site-directed mutagenesis for site-selective conjugationExpressed and purified 5 proteins in E. coli using AKTA FPLC systemsPerformed bioconjugation on peptides, proteins and antibodies, characterizing the conjugates by LC-MSSystematically processed 1000+ protein samples by LC-MS, troubleshooting analytical and equipment challengesPurified protein conjugates by ultrafiltration and size-exclusion chromatography and characterized them by LC-MS, ELISA, SDS-PAGE, Western blot and circular dichroismSynthesized 2 chemical reagents and characterized them by NMR and LC-MSEstablished an ELISA assay to quantify protein acetylation levels, eliminating the need for a commercial kit	

Visiting Research Scientist in Biomedical Sciences Yusuf Hamied Department of Chemistry, University of Cambridge	Sep 2021 – Oct 2021 <i>Cambridge, United Kingdom</i>
<ul style="list-style-type: none">Assisted in bioconjugation and LC-MS characterization experiments of an antibody	

Research Intern in Biochemistry

Oct 2017 – Nov 2017

University Medicine Greifswald

Greifswald, Germany

- Evaluated the toxicity of cold atmospheric plasma on human epithelial and tumor cells using in vitro cell-based assays and RT-PCR analysis

Graduate Researcher in Bioorganic Chemistry

Sep 2016 – Sep 2017

NOVA School of Science and Technology, NOVA University of Lisbon

Caparica, Portugal

- Optimized the expression of ^{13}C and ^{15}N isotope-labelled proteins in E.coli for NMR studies
- Mapped the epitope of an anti-amyloid- β antibody using ^1H - ^{15}N HSQC NMR with 2 amyloid peptides (A β 1-40 and A β (1-42) - communicated findings in 1 peer-reviewed publication

Graduate Researcher in Neuroscience

Sep 2015 – Sep 2016

Institute of Molecular Medicine

Lisbon, Portugal

- Investigated the pharmacological effects of an adenosine A2A receptor agonist on the myelination process using cell culture, immunofluorescence and microscopy

Undergraduate Researcher in Chemistry

Mar 2014 – Jul 2014

Faculty of Sciences, University of Lisbon

Lisbon, Portugal

- Synthesized a psychoactive cathinone and conducted its characterization by NMR, FTIR and GC-MS

Core Competencies

Data Science

- Programming | Version Control | Machine Learning | Databases | Data Mining | Statistical Analysis

Chemistry

- Cheminformatics | Bioconjugation | Small Molecule & Protein Characterization | Organic Synthesis

Molecular Biology

- Bacterial & Mammalian Cell Culture | Protein Expression & Purification | Site-Directed Mutagenesis

Professional

- Project Management | Analytical Problem-Solving | Communication | Interdisciplinary Collaboration

Technical Skills

– **Programming Languages:** Python | SQL | SAS | R

– **Libraries:** RDKit | Scikit-learn | TensorFlow | Pandas | NumPy | Matplotlib | Seaborn

– **Technologies & Software:** PostgreSQL | MongoDB | PowerBI | Git | GitHub | LaTeX | MS Office | MassLynx

– **Developer Tools:** Visual Studio Code | Git

– **Laboratory:** LC-MS | Mass Spectrometry | UHPLC | HPLC | FPLC | NMR | Affinity (AC), Ion-Exchange (IEX) & Size-Exclusion (SEC) Chromatography | Ultrafiltration | SDS-PAGE | Western Blot | ELISA | PCR | RT-PCR | Immunofluorescence | Microscopy

– **Equipment:** Waters Acquity UHPLC systems coupled to QDa detectors | AKTA purification systems | Bruker NMR spectrometers

– **Languages:** Portuguese | English (C1) | German (B1) | French (A1)

Publications

- **Afonso CF**, Marques MC, António JPM, Cordeiro C, Gois PMP, Cal PMSD, Bernardes GJL. Cysteine-Assisted Click-Chemistry for Proximity-Driven, Site-Specific Acetylation of Histones. *Angewandte Chemie International Edition* 2022, 61, e202208543 (DOI: [10.1002/anie.202208543](https://doi.org/10.1002/anie.202208543))
- Laserna V, Abegg D, **Afonso CF**, Martin EM, Adibekian A, Ravn P, Corzana F, Bernardes GJL. Dichloro Butenediamides as Irreversible Site-Selective Protein Conjugation Reagent. *Angewandte Chemie International Edition* 2021, 60, 23750–23755 (DOI: [10.1002/anie.202108791](https://doi.org/10.1002/anie.202108791))
- Posado-Fernández A, **Afonso CF**, Dória G, Flores O, Cabrita EJ. Epitope Mapping by NMR of a Novel Anti-A β Antibody (STAB-MAb). *Scientific Reports* 2019, 9(1), 12241 (DOI: [10.1038/s41598-019-47626-2](https://doi.org/10.1038/s41598-019-47626-2))

Projects

Birth Plan Manager | Python |

- Developed a command-line tool in object-oriented Python to manage childbirth assistances in hospital settings

Database Performance Analysis | Python, SQLite, MongoDB |

- Created SQLite and MongoDB databases using a flights dataset
- Benchmarked query execution times to compare relational with NoSQL databases with and without indexing

Ecommerce Data Warehouse | Python, Pandas, SQL, PostgreSQL, PowerBI |

- Designed and implemented an ETL pipeline to create an ecommerce data warehouse in PostgreSQL
- Answered business questions through SQL querying and PowerBI dashboards

Machine Learning Portfolio | Python, Scikit-learn |

- Developed regression and classification machine learning models to predict critical temperatures using a chemical dataset of 21,000+ superconductors with 81 features
- Implemented the Q-learning reinforcement learning algorithm in Python

Network Fastest Path Finder | Python |

- Built a command-line tool using object-oriented Python to find the fastest path between stations in a network with a depth-first search algorithm

Certifications

SAS Certified Associate: Programming Fundamentals Using SAS 9.4 | Lisbon, Portugal **Nov 2024**

Courses

14th Lisbon Machine Learning School (LxMLS2024) | Lisbon, Portugal **Jul 2024**

The Hitchhiker's Guide to single-cell RNA-sequencing | Lisbon, Portugal **Jul 2024**

Gulbenkian Training Program in Bioinformatics – Proteomics Data Analysis | Oeiras, Portugal **Sep 2022**

Communications

II Symposium of the Portuguese Glial Network | Braga, Portugal **May 2017**

XLVII Annual Meeting of the Portuguese Society of Pharmacology | Coimbra, Portugal **Feb 2017**

Conferences

3rd European Fourier Transform Mass Spectrometry School | Lisbon, Portugal **Jul 2022**

4th European Fourier Transform Mass Spectrometry Workshop | Lisbon, Portugal **Jul 2022**

XLIV Meeting of the Portuguese Society for Immunology | Lisbon, Portugal **Jun 2018**

Scholarships and Awards

Scholarship to attend the Lisbon Machine Learning School 2024 (LxMLS2024) | Lisbon, Portugal **Jul 2024**

Research Fellowship in Data Science | Lisbon, Portugal **Nov 2023**

Research Fellowship in Biomedical Sciences | Lisbon, Portugal **Jul 2022**

FCT Doctoral Studentship | Lisbon, Portugal **Jan 2018**

IAESTE Internship | Greifswald, Germany **Oct 2017**