

ABDALLAH ABOU HAJAL

AI-Drug Discovery | Cheminformatics | Pharmaceutical Sciences (MSc) | Academic Data Analytics & AI Automation

Abu Dhabi, United Arab Emirates

Phone #: +971 56 884 9457 | Email: Abdallah.Abouhajal@gmail.com | Date of Birth: 18 June 1998 | Marital Status: Single

Personal Website: 

Linkedin Profile: 

Google Scholar: 

Scopus Profile: 

Research Output: 14 publications | 125 citations | G-scholar h-index: 7

SUMMARY

Motivated researcher with an MSc in Pharmaceutical Sciences, specializing in AI for drug discovery and cheminformatics. Since completing my degree, I have been working in academic publishing, first as a Managing Editor, and currently as a Data Analyst/AI Automation lead, where I build AI-powered automation tools to streamline editorial workflows. With first-author publications in high-impact journals (JCIM, Expert Opinion on Drug Discovery), I am now seeking a PhD to further apply machine learning and data-driven methods to drug discovery challenges.

PROFESSIONAL EXPERIENCE

Data Analyst & AI Automation Lead, Scifiniti Publishing

May 2025 – Present

- Building LLM-based AI agents to automate editorial workflows
- Developing Python-based tools to streamline publishing operations
- Creating automated dashboards for journal performance metrics
- Analyzing submission trends to identify bottlenecks and support strategic planning

Managing Editor, Scifiniti Publishing

Feb 2023 – May 2025

- Managed day-to-day operations across 5+ STEM journals
- Served as primary contact for authors, reviewers, and editors to resolve conflicts and maintain review timelines
- Contributed to improving peer review workflows and author experience

MSc Student & Research / Lab Assistant, College of Pharmacy, Al Ain University

Sep 2021 - Feb 2023

- Awarded a postgraduate scholarship (lab and research assistant duties).
- Contributed to research in drug discovery, cheminformatics, and machine learning applications.
- Delivered laboratory sessions and designed in-class activities for undergraduate students.
- Assisted in writing scientific manuscripts

EDUCATION

Master of Science in Pharmaceutical Sciences

Sep 2021 – Apr 2023

College of Pharmacy, Al Ain University – Abu Dhabi, UAE

- Graduated with Excellent (GPA: 3.94)
- Thesis: **Use of machine learning in the development of a drug discovery tool for predicting promiscuous aggregate-based inhibitors**
 - Supervised by Prof. Mohammad Ghattas (Reader in Medicinal Chemistry)
 - Co-supervised by Prof. Boulbaba Ben Amor (Reader in Artificial Intelligence & Computer Science)
- Aggregation is an important source of false positives and wasted effort in early-stage drug discovery. The project employed (1) machine learning and ensemble modeling to predict small colloiddally aggregating molecules from chemical structure, (2) large-scale data integration and feature selection to improve model performance and applicability, and (3) interpretability techniques to identify key molecular features driving aggregation. The final tool was deployed via a public web server for broad use in early-stage drug discovery.

Bachelor of Science in Pharmacy

Sep 2016 – Jun 2021

College of Pharmacy, Al Ain University – Abu Dhabi, UAE

- Graduated with Excellent (GPA: 3.83)
- Honor Student – Academic Year 2017/2018

Science Major – Secondary School Certificate

Sep 2013 – Jun 2016

Khalifa Bin Zayed High School – Abu Dhabi, UAE

- Graduated with 96.8% – Honor Student

AWARDS

First Place, BindHack Hackathon | Insilico Medicine, Masdar City

2025

Built the best-performing model for antibody-antigen binding prediction in a 6-hour AI/drug discovery competition using smart feature engineering under tight time pressure.

Three Minute Thesis (Second Place), 2nd AAU Health and Biomedical Postgraduate Symposium | Al Ain University 2024

Condensed my MSc thesis into a 3-minute talk for a general audience.

Best Quality Poster Award (First Place), 1st International Conference on Pharmacy and Biomedical Sciences | Al Ain University

2023

Presented my research on ML-based aggregation prediction as a scientific poster.

TECHNICAL & RESEARCH SKILLS

Programming & Data Analysis

- Python (proficient)
- Classical ML: Pandas, NumPy, Matplotlib, scikit-learn, TensorFlow AutoGluon, CatBoost, LightGBM.
- LLM & Agentic AI: LLM API integration (Ollama, Anthropic, OpenAI), Microsoft Agent Framework, agentic workflow design.
- SPSS (basic proficiency)

Cheminformatics & Drug Discovery

- RDKit, MolVS, SHAP, programmatic MD simulation setup and trajectory analysis
- Machine learning & Chemical Language Models for Early-Stage Drug Discovery

Research & Professional Skills

- Full research lifecycle: hypothesis design → modeling → manuscript preparation
- Data-driven problem solving and strategic planning
- Project lead, workflow automation, and attention to detail.
- Cross-disciplinary communication and team collaboration

RESEARCH INTERESTS

- AI in drug discovery | Cheminformatics | Agentic AI & LLM applications in drug discovery | Predictive modeling | Explainable AI (XAI) | Chemical language models (CLMs) | Software development

LANGUAGES

- **English** (IELTS Academic 7.5 — L8.0, R8.5, W6.5, S7.5) | **Arabic** (Native)

PUBLICATIONS

1. **Abou Hajal A***, Al Meslamani AZ, Computational approaches to adverse outcome pathway networks: advances in construction, quantification, and regulatory decision support. *Computational Toxicology*. 2026;100429 ***Corresponding author**
2. **Abou Hajal A***, Bustanji L, Bryce RA, Ghattas MA. An introduction to GitHub and its significance for AI-Driven drug discovery. *Expert Opinion on Drug Discovery*. 2026;2641511. ***Corresponding author**
3. **Abou Hajal A***, Sakkal M. Introducing AutoML framework for drug–drug interaction prediction: Application of AutoGluon. *Toxicology Mechanisms and Methods*. 2026;1–11. ***Corresponding author**
4. Sakkal M, **Abou Hajal A***. Large language models in drug delivery: A review of the current landscape and future perspectives. *J Pharm Sci*. 2025;115(2):104147. ***Corresponding author**
5. Sakkal M, **Abou Hajal A***. Machine learning predictions of tumor progression: How reliable are we? *Computers in Biology and Medicine*. 2025;191:110156. ***Corresponding author**
6. Al Meslamani AZ, **Abou Hajal A**. Language models for drug–drug interactions: current applications, pitfalls, and future directions. *Expert Opinion on Drug Metabolism and Toxicology*. 2025;21(9):1083–1102.
7. **Abou Hajal A**, Bryce RA, Amor BB, Atatreh N, Ghattas MA. Boosting the accuracy and chemical space coverage of the detection of small colloidal aggregating molecules using the BAD Molecule Filter. *Journal of Chemical Information and Modeling*. 2024;64(13):4991–5005.
8. **Abou Hajal A**, Al Meslamani AZ. Insights into artificial intelligence utilisation in drug discovery. *Journal of Medical Economics*. 2024;27(1):304–308.
9. **Abou Hajal A**, Al Meslamani AZ. Overcoming barriers to machine learning applications in toxicity prediction. *Expert Opinion on Drug Metabolism and Toxicology*. 2024;20(7):549–553.
10. Elnour AA, **Abou Hajal A**, Goaddar R, Elsharkawy N, Mousa S, et al. Exploring the pharmacy students' perspectives on off-campus online learning experiences amid COVID-19 crises: A cross-sectional survey. *Saudi Pharmaceutical Journal*. 2023;31(7):1339–1350.
11. Kharaba Z, AlAhmad MM, Elnour AA, **Abou Hajal A**, Abumweis S, et al. Are we ready yet for digital transformation? Virtual versus on-campus OSCE as assessment tools in pharmacy education. A randomized controlled head-to-head comparative assessment. *Saudi Pharmaceutical Journal*. 2023;31(3):359–369.
12. Al Mazrouei N, Elnour AA, **Abou Hajal A**, Sadeq A, Khalid AK, et al. A cross-sectional survey on the experience of people with allergic rhinitis amidst COVID-19 pandemic: The impact of the facemask: A pilot study. *Pharmacy Practice*. 2023;21(3):18.
13. Elnour AA, Raja NS, **Abou Hajal A**, et al. Protocol for systematic review and meta-analysis of randomized controlled trials, cost-benefit analysis and interrupted time-series interventions on pharmacist's prescribing. *Pharmacy Practice*. 2022;20(3):2713.

PUBLICATIONS

14. Hudaib MM, **Abu Hajal AF**, Sakkal MM. Chemical composition of the volatile oil from aerial parts of *Rosmarinus officinalis* L. growing in UAE. *Journal of Essential Oil Bearing Plants*. 2022;25(2):282–289

MANUSCRIPTS UNDER REVISION & ONGOING PROJECTS

1. Chemical Language Models for Early-Stage Drug Discovery: Applications, Pitfalls, and Future Directions
(Under review in Journal of Computer-Aided Molecular Design)
2. Computational Flagging of Assay Interference in Drug Discovery: A Review of Rule-Based, Machine Learning, Graph Neural Networks, and Chemical Language Models **(Submitted to Journal of Chemical Information and Modeling)**