Dalron J. Robertson, M.S.

AI/ML Research Engineer | Pharm.D. Candidate

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Executive Summary

Multidisciplinary engineer-researcher combining biomedical science, machine learning, and high performance computing to build intelligent systems that accelerate scientific discovery across the life sciences.

Research & Development Projects

To view all of my development projects, visit https://dalronjrobertson.com/projects/websites

Phytochemical Bioactivity Research | Jan 2025 -May 2025 | https://bit.ly/DJR-PhytochemicalResearch

Conducted computational and experimental research on ethanol-derived Nigella sativa extracts using bioinformatics, molecular modeling, and AI-driven analysis. Presented findings at symposium; recognized by Provost for research excellence.

- **Phase 1: Literature Mining & Data Collection**
  - Leveraged Deep Research methodologies (OpenAI's LLMs) to rapidly extract and synthesize bioactivity, pharmacological, and chemical data, from PubMed, PubChem, and UniProt databases.
- **Phase 2: Compound Library & Chemical Profiling**
  - Developed a comprehensive chemical library of *Nigella sativa* phytochemicals, conducting detailed molecular descriptor calculations (Molinspiration, SwissADME), ADME/Tox assessments, and archiving structural data for computational analyses.
- **Phase 3: Target Identification & Structure Modeling**
  - Identified protein targets via SwissTargetPrediction; validated through extensive literature reviews. Generated 3D protein models using AlphaFold; developed visualizations with ChimeraX and Blender.
- **Phase 4: Virtual Screening & Molecular Docking** *(Current Phase)*
  - Performing molecular docking simulations to predict binding affinities and interaction dynamics between prioritized phytochemicals and protein targets. Evaluating the Schrödinger software suite alongside CB-Dock2 and Atomwise for comprehensive and precise ligand-target interaction modeling and analysis.
- **Performed wet-lab assays**: anti-inflammatory (protein assays), antioxidant (DPPH, H_2O_2 scavenging), phytochemical quantification (flavonoid, flavonol), and spectrophotometric analyses
- **Teaching & Mentorship:** Trained and mentored 16 undergraduate and graduate researchers on the complete computational pipeline, including software and analytical methods, significantly enhancing research productivity.

NaS Knowledge Model | Feb 2025 | https://github.com/NaS-Research/knowledge-model

Built an autonomous biomedical language model pipeline that reads 10,000+ new PubMed papers each cycle, learns from them on its own, and serves up to date, citation backed answers to scientists with zero manual data preparation or tuning required.

Key Achievements & Technical Highlights:

- Authored foundational architecture paper outlining the NaS Cortex, a domain-specific MoE language model for autonomous scientific reasoning across life sciences.
- Prototyped initial model pipeline and benchmarked autonomous update loop on Apple Silicon, defining memory, throughput, and training ceilings for distributed scaling.
- Built a monthly ingestion pipeline (PubMed E-Utilities + PDF crawl) that de-duplicates, cleans, and archives 9 k+ new papers per run in S3-versioned year / month buckets.
- Automated text normalisation, smart chunking (≤ 1 200 tokens), and embedding with SentenceTransformers → FAISS, enabling sub-second semantic search over 2 M+ vectors.
- Shipped a FastAPI retrieval-augmented generation (RAG) micro-service that runs top-k retrieval, context packing, and citation-linked answer generation in < 250 ms latency.
- One-command refresh loop ingests new literature, re-trains adapters, and publishes updates, keeping the model evergreen and hands free.

Experience

Mississippi College, Clinton, MS

Lead Graduate Researcher | Dec 2024 - Jul 2025

- Employed OpenAI LLMs to systematically extract and synthesize bioactivity data, phytochemical profiles, and pharmacological properties from extensive databases including PubMed, PubChem, and UniProt.
- Established a curated chemical library of Nigella sativa constituents, performed molecular descriptor analysis, drug-likeness screening, and prioritized lead candidates using statistical methods.
- Applied SwissTargetPrediction for precise molecular target identification and generated highly accurate 3D structural models of identified protein targets using AlphaFold.
- Created advanced visualizations for protein-ligand interactions using ChimeraX and Blender software.
- Conducted rigorous molecular docking studies utilizing CB-Dock2 and Schrödinger Suite to analyze ligand binding affinities, predict pharmacodynamic behavior, and interpret interaction dynamics through detailed visual mapping.

Scale AI, San Francisco, CA

AI Software Engineer | Sept 2023 - Jan 2025

- Collaborated with Google to enhance Gemini, developing training sets improving model accuracy and performance.
- Enhanced the Gemini-YouTube search engine for video scanning, extraction, and presentation.
- Enhanced the Google search engine by training models to deliver more accurate and relevant search results.
- Developed expertise in Side-by-Side (SxS) evaluation techniques focused on enhancing model responses, enabling real-time improvements to model training, and adjustment of training parameters.
- Conducted red teaming exercises to identify and mitigate vulnerabilities, enhancing robustness against misuse.
- Built synthesis algorithms to create real-world data to facilitate AI understanding of temporal and relational data.
- Conducted in-depth analysis of AI model outputs, assessing model performance and identifying areas for model improvement, leading to measurable increases in model precision and client satisfaction.
- Developed and implemented rigorous testing frameworks for evaluating performance of generative AI models.

Medication Management Partners, Crestwood, IL

Pharmacy Informatics & Automation, Staff Pharmacist-in-Training | Aug 2020 - Apr 2022

- Led daily standups and contributed insights in weekly leadership meetings to improve performance and workflows.
- Performed QV1/QV2 verifications, DURs, and medication reviews across 150+ LTC facilities.
- Managed robotics systems (TCGRx ATP, Parata Max, IntelliVault) to ensure accurate, compliant dispensing.
- Automated data flows and supported clinical accuracy across eMAR, Framework LTC, and DocuTrack.
- Handled claims, provider communication, and compliance with HIPAA, DEA, and state regulations

CVS Health, Chicago, IL

Staff Pharmacy Manager-in-Training | Jul 2015 - Aug 2020

Technical Skills

AI & Large Language Models: *Deepseek* | *Gemini* | *GPT* | *Grok* | *LlaMa* | *TinyLlama*

Bioinformatics & Molecular Modeling: *AlphaFold* | *ChimeraX* | *SwissTargetPrediction* | *Molinspiration* | *PubChem* | *UniProt*

DataScience & Machine Learning: *Tensorflow* | *Scikit-Learn* | *Pandas* | *NumPy*

Languages: *Javascript* | *Python* | *Pinescript* | *Java* | *C* | *C++* | *PostgreSQL* | *MySQL*

Tools & Technologies: *Git* | *AWS* | *ISOLIDE*| | *Schrödinger*| *jest* | *DocuTrack* | *Framework LTC* | *UiPath*

Web Development: *Node.js* | *React.js* | *Express.js* | *Flask* | *HTML* | *CSS* | *AJAX* | *DOM* | *jQuery*

Education

Chicago State University - *55 Credits towards Doctor of Pharmacy, Graduating May '28*

Mississippi College - *M.S., Biological Sciences*

University of Illinois Chicago - *Software Engineering Certificate*

Jackson State University - *B.S., Biology*