

Brandon Moore, PhD

Applied AI leader scaling teams, platforms, and molecular design impact

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Professional Experience

1910 Genetics

Boston, MA

HEAD OF AI RESEARCH & MACHINE LEARNING ENGINEERING

2022 — Present

- Set/executed AI roadmap and \$400K annual compute budget for designing small molecules and macrocyclic peptides
- Built high performing 8-person computational team from the ground up and guided 4 direct reports through promotions
- Established cross-functional integration via weekly stakeholder meetings as well as 1-on-1 mentorship of biologists and medicinal chemists on the independent use of computational simulation and AI tools (LLMs, generative models, etc.)
- Pioneered external mentorship by serving as graduate thesis advisor to a Johns Hopkins bioinformatics student
- Publications central to customer conversations: AI models that predict BBB penetration of bRo5 small molecules (JCIM) and that predict the cell membrane permeability of macrocyclic peptides (featured article, J Med Chem)

AI RESEARCH SCIENTIST I — III

2019 — 2022

- Created algorithms to design/optimize small molecules (COVID-specific work featured in Science and J Infect Dis)
- Instituted source control, MLOps, and established company-wide engineering best practices on AWS and Azure
- Ran weekly multi-team journal clubs on drug design topics: AI, cheminformatics, biological assays, medicinal chemistry

Livingstone Laboratory

Harvard Medical School

RESEARCH ASSISTANT

2011 — 2012

- Trained monkeys (*Macaca mulatta*) in a symbolic addition task and analyzed their task performance errors to better understand symbol valuation during addition (published in PNAS, featured on IFLScience)

Sinha Laboratory

MIT

RESEARCH ASSISTANT

2007 — 2011

- Collected and analyzed MEG and EEG data on the high level correlates of human face perception
- Mentored students on topics of statistical analysis and computer programming

Selected Publications

Baker C, Acquah FA, Chivukula LG, Wu L, ..., **Moore B**, Asher JO. (2026) *PEGASUS: Unlocking Polarity in Cell-Permeable Cyclic Peptides Using AI Models Built on Massively Parallel Biological Assays*. J Med Chem, 69:5175-5198.

Collins JW, Abedi M, Ramirez D, Philippe-Venec L, **Moore B**, Asher JO. (2025) *CANDID-CNS: AI Unlocks Stereochemistry and Beyond Rule of 5 to Predict CNS Penetration of Small Molecules*. JCIM, 65:12918-12928.

Education

Vanderbilt University

Nashville, TN

PHD, NEUROSCIENCE

2019

- Advisors: Jon Kaas, Vivien Casagrande
- Dissertation: Explorations of pulvinar circuitry in the northern greater galago (*Otolemur garnettii*)

Tufts University School of Medicine

Boston, MA

MPH, EPIDEMIOLOGY AND BIostatISTICS

2012

- Thesis: Assessment and recommendations concerning AANE's Life Management Assistance Program

Massachusetts Institute of Technology

Cambridge, MA

BS, BRAIN AND COGNITIVE SCIENCES

2009

Skills

Coding C, Common Lisp, Java, Perl, PHP, **Python**, R, SQL

Libraries Keras, OpenCV, Pandas, Pillow, PyTorch, RD-Kit, SciKit-Learn, SciPy, SpaCy, Transformers

Applications Adobe Suite, Claude Code, ChemDraw, Docker, Git, $\text{\LaTeX}$, MATLAB, MOE, OpenEye, PyMol, Slurm, Vina

Laboratory Primate & rodent neurosurgery, Electrophysiology, MEG/EEG, Electron Microscopy