BENJAMIN J. SHIELDS

Researcher, Drug Discovery

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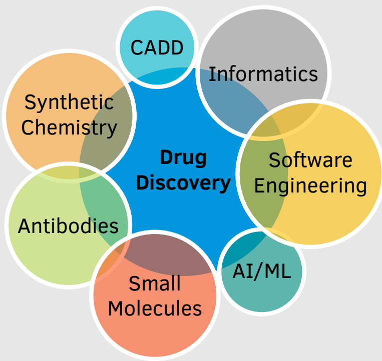
b-shields

Expertise



Skills & Expertise

Drug Discovery: Target ID • Hit ID • Hit-to-lead Opt • Lead Opt • ADMET • (Neuro)PK • Omics

Modalities / Areas: Small Molecule • Antibody • TPD • PPI • Immunology • Oncology • Neurodegeneration

CADD: Virtual Screening • Docking • MD • FEP • DFT • Cheminformatics • Bioinformatics

AI/ML: Supervised • Clustering • MCP • Knowledge Graphs • Bayesian Optimization • Generative Design • Deep Learning

Engineering: HPC • Cloud • CI • CD

Education

Ph.D., Chemistry
Princeton University

M.A., Chemistry (distinction)
Princeton University

B.S., Chemistry (highest honors)
University of North Carolina Asheville

B.A., Applied Math (highest honors)
University of North Carolina Asheville

Relevant Experience

2024 - Present — **Senior Staff Engineer / Project Leader** — Drug Discovery, SandboxAQ

- **Drug Discovery & Development**: Leading milestone-based drug discovery and diagnostics contracts with academic, biotech, and major pharmaceutical company collaborators. Acted as project leader and/or contributor on 10+ small molecule and antibody projects from business development to exectuion. Every contract milestone was delivered successfully and on schedule. Efforts impacted target ID, hit ID, hit-to-lead, and lead optimization.
- **Software Development**: Designed, built, and maintained cloud native core cheminformatics, machine learning, and antibody design software platforms used to support every drug discovery client engagement and research project.
- **Leadership**: Managed a team of engineers extending and maintaining software platforms and supporting client engagements. Managed teams of chemists, biologists, physacists, and engineers persuing drug discovery projects. Co-author of 2 publications and inventor on 2 patents.

2021 - 2024 — **Principal Scientist** — CADD, Bristol Myers Squibb

- **Drug Discovery & Development**: Contributed to small molecule and protein degradation drug discovery projects in collaboration with medicinal chemists and biologists. Contributed to successful hit ID and lead optimization campaigns by quickly identifying hits and progressing leads to IND enablement.
- **Software Projects**: Lead development of ML and cheminformatics infrastructure for small molecule activity prediction, ADMET modeling, uncertainty estimation, Bayesian optimization, virtual screening, automated retrosynthesis, large-scale enumeration, generative design, and immunogenicity prediction.
- **Leadership**: Key driver of computation-driven lead optimization strategy for company. Acted as AI lead on projects by designing, implementing, and continuously improving computational strategies to drive compound selection. Leadership recognized with BMS "Leadership Award in Synthetic and Medicinal Chemistry" in 2023. Co-author of 1 publication and inventor on 3 patents.

Research Highlights

Large-Scale Simulation & Deep Learning: Data for training drug discovery AI models is scarce and biased. This work uses simulation to expand model applicability domains. **Representative Publication**: Lemos, et al. "SAIR: Enabling Deep Learning for Protein-Ligand Interactions with a Synthetic Structural Dataset", *BioRxiv*, **2025**

Bayesian Optimization: Problems in drug discovery and development often require iterative experimentation. This work leverages BO to translate data to actionable insights and guide optimization of assays, reactions, molecular structures, and formulations. **Representative Publication**: Shields, et al. "Bayesian Reaction Optimization as A Tool for Chemical Synthesis", *Nature*, **2021**, *590*, 89–96.

Organometallic Chemistry: This work utilizes organometallic chemistry, quantum mechanical modeling, and ultrafast spectroscopy to understand and improve photocatalytic systems for synthesis. **Representative Publication**: Shields, et al. "Long-Lived Charge Transfer States of Nickel(II) Aryl Halide Complexes Facilitate Bimolecular Photoinduced Electron Transfer" *J. Am. Chem. Soc.*, **2018**, *140*, 3035–3039.

Synthetic Methods Development: Development, study, and application of broadly useful methods for small molecule chemical synthesis. **Representative Publication**: Shields, et al. "Direct C(sp^3)–H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals" *J. Am. Chem. Soc.*, **2016**, *138*, 12719–12722.

Complete Publication Record: Link