

Call for Pilot Projects on Early Drug Discovery & Artificial Intelligence

The High-throughput Institute for Discovery (HIT-ID) and the Institute for Biomedical Informatics (IBI) are pleased to announce a call for **pilot project proposals** that explore the transformative potential of **Artificial Intelligence (AI)** in **early-stage drug discovery**. This initiative aims to support innovative, high-impact projects that integrate AI-driven methodologies to accelerate, enhance, or redefine the early phases of drug development. This Pilot program is supported by the Stephen J. Heyman Fund for Artificial Intelligence Innovation.

Scope

We are seeking pilot projects that address key challenges or opportunities in early drug discovery through the use of AI technologies, including but not limited to:

- **Hit discovery and Virtual identification**
 - Predicting affinity between small molecules and targets
 - Using computational approaches to rank candidates
 - Virtual screening
 - Improve data analysis of existing screen data (eg image analysis)
- **Compound design and optimization**
 - De Novo design entirely new molecules
 - Optimize structures for potency, selectivity or synthetic feasibility
 - Predictive modeling for on target, off-target or drug-like properties

Proposals should demonstrate a clear scientific rationale, innovative AI application, and potential for translational impact. Projects that clearly bridge AI expertise and drug discovery knowledge are particularly encouraged. Collaborative proposals including two or more Schools across the University of Pennsylvania will be prioritized. Proposals that collaborate with and utilize the Perelman School of Medicine High-throughput screening core for wet validation of predictions will also be prioritized. Pilots will be for up to \$100,000 for one year. We anticipate funding up to two Pilots.

Submission Guidelines

Pilot submissions are due July 1, 2025. Please submit the following as a single PDF in the order listed below.

Cover page (1 page) including:

- Title
- Team members including all affiliations within the University of Pennsylvania
- Abstract stating problem and scientific rationale

Biosketches for each team member.

Project summary (1 page) including:

- Proposed work plan, timeline, and expected outcomes
- Description of AI methodology
- Long-term vision and how these results can lead to new funding

Budget for the one-year timeline.

Deadline for submissions: July 1, 2025

Send proposals to: tori.gordillo@pennmedicine.upenn.edu