R. Ken Coit College of Pharmacy

Department of Pharmacology & Toxicology
Southwest Environmental Health Sciences Center
Seminar Speaker

Tuesday, September 10, 2024
11:00 am
Room Skaggs 325: *In-Person Presentation*

Host: Nathan Cherrington and Steve Wright

Sean Ekins, PhD, DSc
CEO and Founder,
Collaborations Pharmaceuticals, Inc.

Applications of artificial intelligence for drug discovery

Collaborations Pharmaceuticals, Inc. is a privately owned company funded by NIH and DOD grants that performs research and development on innovative therapeutics for multiple rare and neglected infectious diseases. We develop and apply our artificial intelligence (AI) software to aid in drug discovery and toxicology assessment. We have used machine learning (ML) for generating ADME/Tox models as well as models for targets or phenotypic assays. These methods have allowed us to leverage public data to select additional compounds for testing, or build models after generating our own data. Such models have been applied for rare and neglected disease drug discovery. Recent advances in ML have led to newer model architectures including transformers (large language models, LLMs). These new architectures may offer promise, and we have undertaken evaluations relevant to our research. The applications of ML and AI to drug discovery projects will be described to highlight how these technologies can be utilized to address some of the challenges faced in developing treatments for the many diseases that are still without a treatment. In addition, some of the potential misuses of the technologies will be described.