



Sean Ekins



Title: Drug Discovery For Rare And Neglected Diseases

Research emphasis:

Sean is Founder and CEO of [Collaborations Pharmaceuticals, Inc.](#) which is focused on using machine learning approaches for rare and neglected disease drug discovery. He is also on the SAB of the [Pitt Hopkins Research Foundation](#) and Adjunct Professor at 3 US universities. Since 2005 he has been awarded >20 NIH/DOD grants as well as performs as a consultant on many others. He has authored or co-authored >300 peer reviewed papers, book chapters, and edited 5 books. For over 23 years he has been at the forefront of using software in drug discovery and toxicology research. He has a passion for finding new collaborators and helping rare disease research.

Application:

- Rare diseases
- Neglected Diseases
- Machine learning
- Toxicology

Collaboration potential:

- Learning from small molecules in any area
- Identify drug hits for new or old targets
- Analyze HTS screening data
- Identify chemical probes or drugs for your bacteria, virus, fungi, parasite etc.

Selected publications:

Ekins S, Industrializing rare disease therapy discovery and development, *Nature Biotechnol*, 35: 117-118, 2017.

Ekins S, Lingerfelt MA, Comer JE, Freiberg AN, Mirsalis JC, O'Loughlin K, Harutyunyan A, McFarlane C, Green CE and Madrid PB, Efficacy of Tilorone Dihydrochloride against Ebola Virus Infection, *Antimicrobial Agents Chemotherapy* 25 : 62, 2018.

Russo DP[#], Zorn KM[#], Clark AM, Zhu H and Ekins S, Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction, *Mol Pharm*, 15(10):4361-4370, 2018

Martinez-Brokaw CD, Radke JB, Pierce JG, Ehlers A, Ekins S, Wood KE, Maakestad J, Rymer JA, Tamama K and Krasowski MD, Accidental intoxications in toddlers: lack of cross-reactivity of vilazodone and its urinary metabolite M17 with drug of abuse screening immunoassays. *BMC Clin Pathol*. 2019 Feb 18;19:2.

CEO, Collaborations
Pharmaceuticals, Inc.

M.Sc. University of Aberdeen
Ph.D. University of Aberdeen
D.Sc. University of Aberdeen

Address: 840 Main Campus Drive,
Lab 3510
Raleigh, NC 27606

Phone: 215-687-1320

Email:
sean@collaborationspharma.com

[www.faculty_url.com](#)