



# Sean Ekins, Ph.D, D.Sc. (Serial collaborator)

## Research Interests:

Work on neglected disease drug discovery, rare diseases, drug transporter models, ADME/Tox modeling

Developing mobile apps for chemistry

Advocate for open science

**Used pharmacophores and computational chemistry software since 1996**

## Recent work:

Identifying a target for FDA approved drugs in Ebola

Using machine learning to identify new *in vitro* actives against Ebola

Developed a model for NTCP (transporter involved in Hepatitis B Virus uptake) and finding drugs that inhibit it

Identified FDA approved drugs that target Topo I in Mtb

Identified new EMA approved *in vivo* active compound for Chagas disease.

Multiple NIH STTR, SBIR grants currently funded

Consultant on NIH grants with others.

# Current Positions & Roles

Senior Consultant  
Since 2007



Consulting ADME/Tox,  
drug discovery  
cheminformatics

Chief Scientific Officer  
Since 2008



Grant PI, bringing in funding,  
neglected disease drug  
discovery research – use  
cheminformatics

Chief Science Officer  
Since 2013



Facilitate science & SAB, write  
grants, collaborate

CEO, President, Co-Founder  
Since 2012



Grant PI, rare disease-  
Sanfilippo Syndrome

CEO, Founder  
Since 2015



Collaborations Pharmaceuticals, Inc.

Write grants and collaborate  
on rare and neglected  
diseases, cheminformatics

Blogger  
Since 2011



Blog about drug discovery

# How I got here..

## Education

HND Applied Biology, Nottingham Polytechnic (UK)  
MSc Clinical Pharmacology, Aberdeen University (UK)  
PhD Clinical Pharmacology, Aberdeen University (UK)  
DSc Science, Aberdeen University (UK) (2005)



Timeline  
1988



1996

## Past companies:

Postdoc



1996

Senior Scientist



1998

Senior Computational Chemist



1999

Assoc. Dir. Concurrent Pharma (now Vitae)



2001

2001

VP GeneGo (bought by Thomson Reuters),



2004

2006

and more smaller companies...



2008

# Education needed

- Broad science background
- Pharmacology focus
- Computational focus (application of software, develop ideas for new tools)– picked up as a postdoc and over time
- Zero programming, zero formal training in cheminformatics
- Learn how to collaborate
- Read and write as much as you can on topic
- Publish (open), give talks...
- Use social media to market your science, gain visibility
- Review for journals
- Share

The screenshot shows the PLOS Computational Biology website. At the top, there's a navigation bar with 'Browse', 'Publish', and 'About' links, along with a search bar and a 'sign in' button. Below this, a statistics bar shows 40,624 views, 2 citations, 24 saves, and 1,134 shares. The main article is titled 'Ten Simple Rules of Live Tweeting at Scientific Conferences' by Sean Ekins and Ethan O. Perlstein, published on August 21, 2014. Below the article, there's a section for 'F1000Research' with a 'SUBMIT YOUR RESEARCH' button and 'My Research' and 'SIGN IN' links. The article content includes a 'RESEARCH NOTE' section with a 'REVISED' status, a common feature pharmacophore for FDA-approved drugs inhibiting the Ebola virus, and author information for Sean Ekins, Joel S. Freundlich, and Megan Coffee. There's also a 'Grant information' section stating that no grants were involved. A 'CrossMark' logo is visible. To the right, there's an 'Open Peer Review' section showing a 'Referee Status' of 'checked' and 'Invited Referees' with a count of 1 and 2. Below this, there's a 'KUDOS' logo with the tagline 'Greater Research Impact' and a 'Who We Help' dropdown menu. The user profile for 'Dr Sean Ekins' is visible in the top right corner.

## Author Dashboard

Click column headings to sort

My research			Information you added to explain and enrich your publication				Actions you took to share your publication			Your results					Citations
Publication title	More details...	Published	Short title	Lay summary	Impact statement	Add resources	Tweets posted	Facebook posts	Email shares	Share referrals	Kudos views	Click throughs	Full text downloads	Altmetric score	Web of Science® Times Cited*
Thiophenecarboxamide Derivatives Activated by EthA Kill Mycobacterium tu...	Bar chart	2015	✗	✗	✗	✗	✗	✗	✗	0	1	0	?	10	-
Finding small molecules for the 'next Ebola'	Bar chart	2015	✗	✗	✗	✗	✗	✗	✗	0	0	0	?	-	-
Open Source Bayesian Models. 1. Application to ADME/Tox and Drug Discove...	Bar chart	2015	✓	✓	✓	✓	2	✗	✗	14	13	1	?	23	1
Open Source Bayesian Models. 2. Mining a "Big Dataset" To Create and Val...	Bar chart	2015	✓	✓	✓	✓	2	✗	✗	24	88	1	?	23	-

# Key Collaborators in Cheminformatics

Who will be next?



## Jim Wikel

1st

Scientific Advisor at Collaborative Drug Discovery, Inc.  
Indianapolis, Indiana Area | Pharmaceuticals

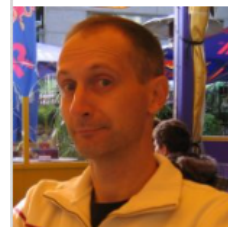
Current Apex Therapeutics Inc, Indiana University School of Medicine,  
Collaborative Drug Discovery, Inc.

Previous Coalesix, Eli Lilly

Education Marshall University

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330  
connections



## Peter Swaan

1st

Professor of Pharmaceutical Sciences at University of  
Maryland, Baltimore

Baltimore, Maryland Area | Higher Education

Current University of Maryland, Baltimore

Previous University of Maryland, Baltimore (UMB), The Ohio State  
University, SmithKline Beecham

Education University of California, San Francisco

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408  
connections



## Matthew Krasowski MD, PhD

## Joel Freundlich

1st

Associate Professor

Greater New York City Area | Higher Education

Current UMDNJ-New Jersey Medical School

Previous Jacobus Pharmaceuticals, Locus Pharmaceuticals, Praecis Pharmaceuticals

Education Massachusetts Institute of Technology

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304  
connections



## Antony Williams

1st

Scientist at National Center of Computational Toxicology  
at EPA

Raleigh-Durham, North Carolina Area | Publishing

Current US Environmental Protection Agency (EPA), ChemConnector

Previous Royal Society of Chemistry, ACS Division of Chemical  
Information, ChemZoo

Education University of London

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500+  
connections



## Alex Clark

1st

President at Molecular Materials Informatics

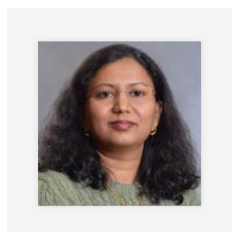
Montreal, Canada Area | Research

Previous Chemical Computing Group, IntelliChem, University of  
California, Riverside

Education University of Auckland

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482  
connections



## Sandhya Kortagere

1st

Associate Professor at Drexel University College of  
Medicine

Greater Philadelphia Area | Research

Previous Drexel University College of Medicine, UMDNJ, Weill Cornell  
Medical School

Education National Institute of Mental Health and Neuro Sciences

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362  
connections

## Ni Ai

1st

Assistant professor at Zhejiang University, China

Greater New York City Area | Research

Previous Snowdon Inc, University of Medicine & Dentistry of New Jersey, Taxis Pharmaceuticals

Education Department of Pharmacology at Robert Wood Johnson Medical School, University of Medicine &  
Dentistry of New Jersey (UMDNJ)

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34  
connections

# Future ?



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**BIG MODELS**

**THOUSANDS OF BIG MODELS**

Need new algorithms, data visualization, mining approaches

Need for broad Biology & Chemistry knowledge – open minds, BIG thinkers

# Contact me

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collabchem



sean.ekins

LinkedIn



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