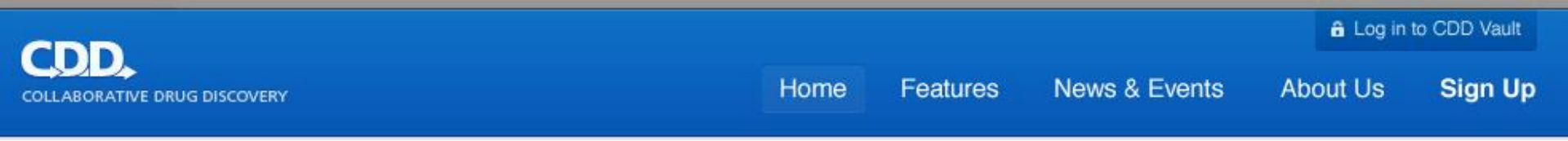


Collaboration: Theory and Practice

Sean Ekins, Ph.D., D.Sc.

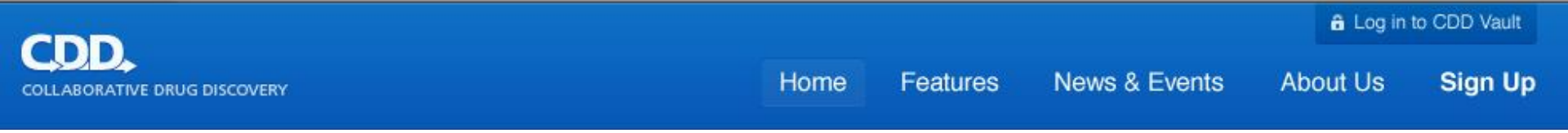
Collaborations Director,
Collaborative Drug Discovery, Inc.,
Burlingame CA.

sekins@collaborativedrug.com
www.collaborativedrug.com

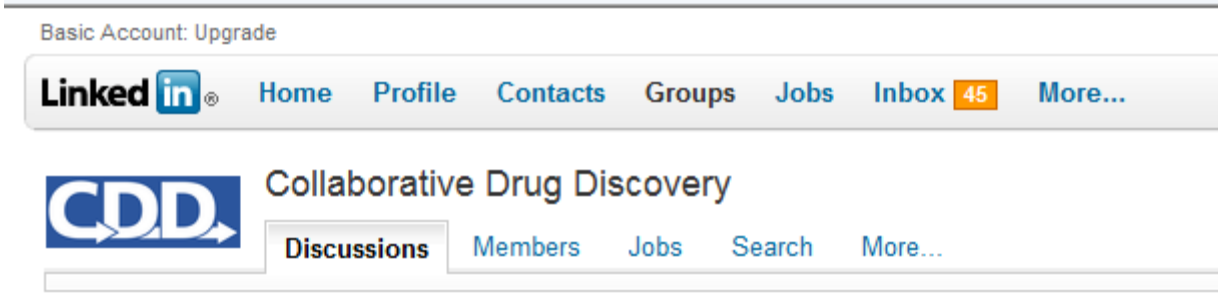
Collaborations in Chemistry, Fuquay-Varina, NC.
School of Pharmacy, Department of Pharmaceutical Sciences, University of Maryland.

In the long history of human kind (and animal kind, too) those who have learned to collaborate and improvise most effectively have prevailed.

Charles Darwin

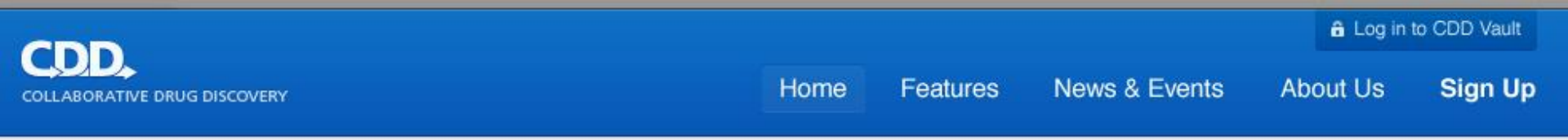


What does "Collaboration" mean to you?



Michael Pollastri • collaboration, to me, means that folks from disparate disciplines or skills work together towards the same end-goal. … A collaboration means free and open data sharing, transparent goals and intentions, and a relationship that allows open (frank) and constructive discussion.

Markus Sitzmann • The internet is the perfect place to share (certain) data and many of the new technologies and format available at the Web (REST, SOAP etc.) are perfect to use data collaboratively.



Open Innovation

Open innovation is a paradigm that assumes that firms can and should use external ideas as well as internal ideas, and internal and external paths to market, as the firms look to advance their technology

Chesbrough, H.W. (2003).
Open Innovation: The new imperative for creating and profiting from technology.
Boston: Harvard Business School Press, p. xxiv

Collaborative Innovation

A strategy in which groups partner to create a product - drive the efficient allocation of R&D resources. Collaborating with outsiders-including customers, vendors and even competitors-a company is able to import lower-cost, higher-quality ideas from the best sources in the world.

Open Source

While open source and open innovation might conflict on patent issues, they are not mutually exclusive, as participating companies can donate their patents to an independent organization, put them in a common pool or grant unlimited license use to anybody. Hence some open source initiatives can merge the two concepts

A starting point

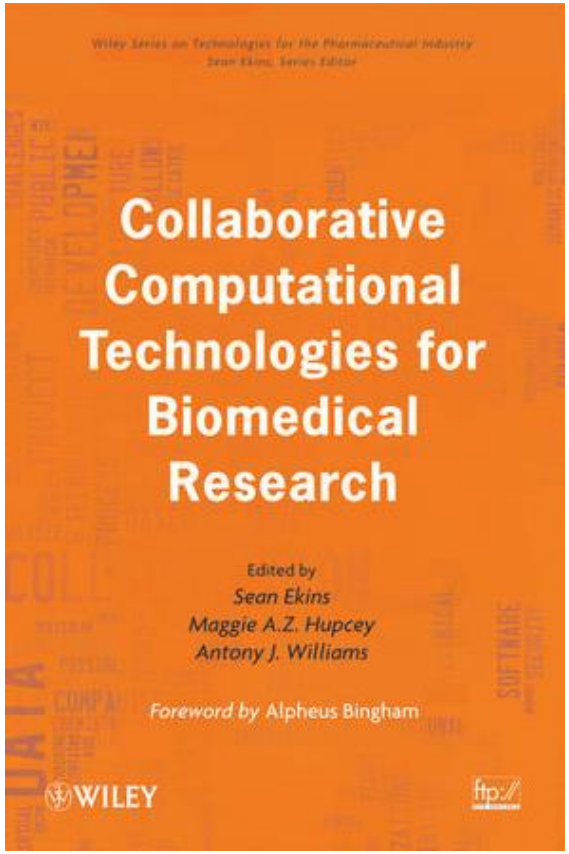
How to do it better?

What can we do with software to facilitate it ?

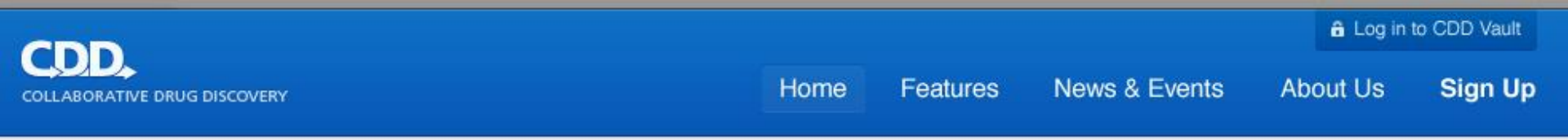
We have tools but need integration

The future is more collaborative

Part I. Getting People to Collaborate
Part II: Methods and Processes for Collaborations
Part III. Tools for Collaborations
Part IV. The Future of Collaborations



- **Groups involved traverse the spectrum from pharma, academia, not for profit and government**
- **More free, open technologies to enable biomedical research**
- **Precompetitive organizations, consortia..**



Collaboration is everywhere

Major collaborative grants in EU: Framework, IMI …NIH moving in same direction?

Cross continent collaboration CROs in China, India etc –
Pharma's in US / Europe

More industry – academia collaboration 'not invented here' a thing of the past

More effort to go after rare and neglected diseases -Globalization and connectivity of scientists will be key –

Current pace of change in pharma may not be enough.

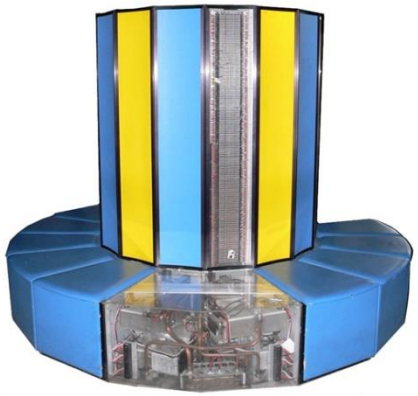
Need to rethink how we use all technologies & resources…

Hardware is getting smaller

Room size

1930's

2000s
Laptop



1980s

Netbook

Phone

Watch

An SGI Octane (1997-2000)

Desktop size

1990s

Not to scale and not equivalent computing power – illustrates mobility

Models and software becoming more accessible- free, precompetitive efforts - collaboration

PERSPECTIVE www.rsc.org/loc | Lab on a Chip

Precompetitive preclinical ADME/Tox data: set it free on the web to facilitate computational model building and assist drug development

Sean Ekins*abc and Antony J. Williams*d

Received 27th August 2009, Accepted 1st October 2009
First published as an Advance Article on the web 10th November 2009
DOI: 10.1039/b917760b

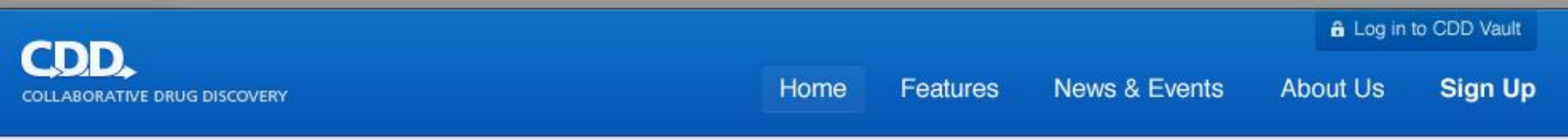
Lab Chip, 2010, **10**, 13–22

We propose that preclinical absorption, distribution, metabolism, excretion and toxicity data as well as pharmacokinetic properties from studies published in the literature (which use animal or human tissues *in vitro* or from *in vivo* studies) are precompetitive in nature and should be freely available on the web.

. The value of the data being accessible will improve development of drug molecules with good ADME/Tox properties, facilitate computational model building for these properties and enable researchers to not repeat the failures of past drug discovery studies.

Could all pharmas share their data as models with each other?

- Improved Quality of data is essential
- Open PHACTS : partnership between European Community and EFPIA
- Freely accessible for knowledge discovery and verification.
  - Data on **small molecules**
  - Pharmacological profiles
  - ADMET data
  - Biological targets and pathways
  - Proprietary and public data sources.



CDD Company Time line

- 2003: Envisioned CDD
- 2004: Spun out of Lilly
- 2005: Eli Lilly co-invested in a syndicate with Omidyar Network and Founders Fund
- 2008: BMGF 2 year grant to support TB research ($1,896,923)
- 2010: STTR phase I with SRI TB – chem-bioinformatics integration ($150K)
- 2011: BMGF 3 year grant to support 3 academia: industry TB Collaborations (~$900,000)
  - MM4TB 5 year EU Framework 7 funded project (Euro 249,700)
  - Bio-IT World Best Practices Award, Editors Choice
  - SBIR phase I ($150K)
  - 5 year NIH NIDA contract

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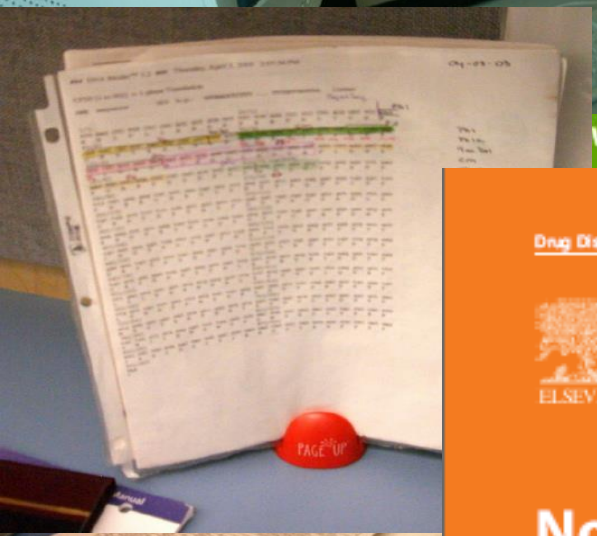
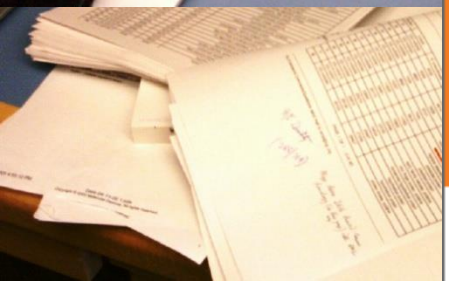
Typical Lab:
The Data Explosion Problem & Collaborations





Drug Discovery Today • Volume 00, Number 00 • February 2009 REVIEWS

ELSEVIER

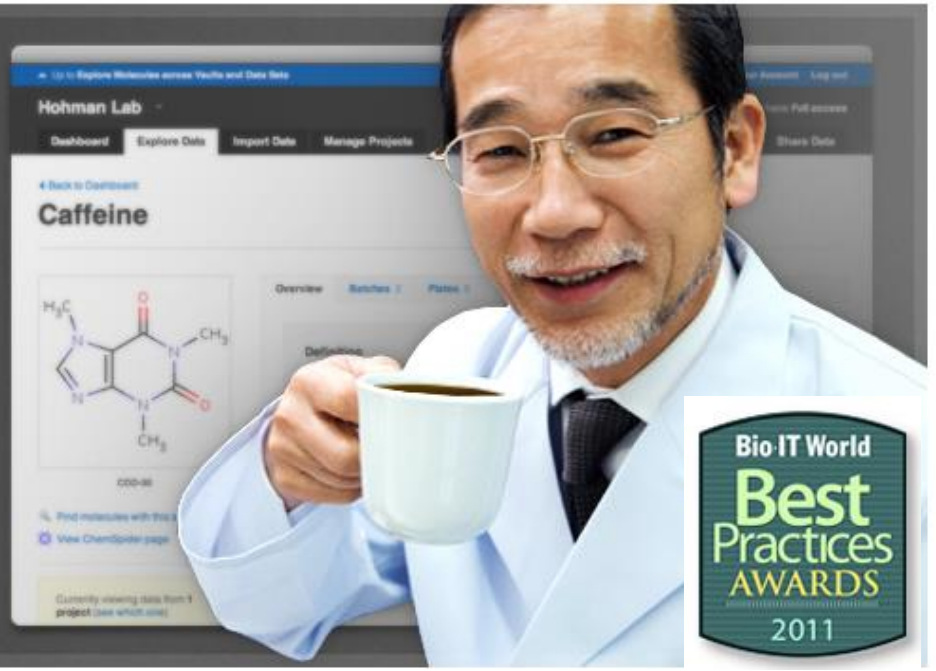
Novel web-based tools combining chemistry informatics, biology and social networks for drug discovery

Moses Hohman[1], Kellan Gregory[1], Kelly Chibale[2], Peter J. Smith[3], Sean Ekins[4,5,6] and Barry Bunin[1]

Streamline drug discovery with CDD's collaborative, web-based software.

CDD Vault is a web application for intelligent data management and secure collaboration. CDD makes drug discovery easier and more efficient for thousands of industry and academic scientists around the world.

Learn more | Sign up now



Simple and secure data management

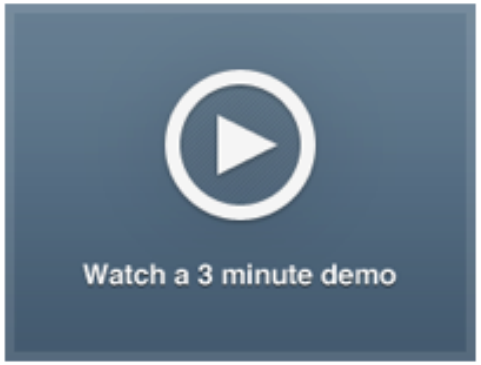
Securely store and easily mine experimental data, including bioassays and chemical structures, in a private data vault that CDD hosts for your group.

Learn more about managing your data with CDD Vault

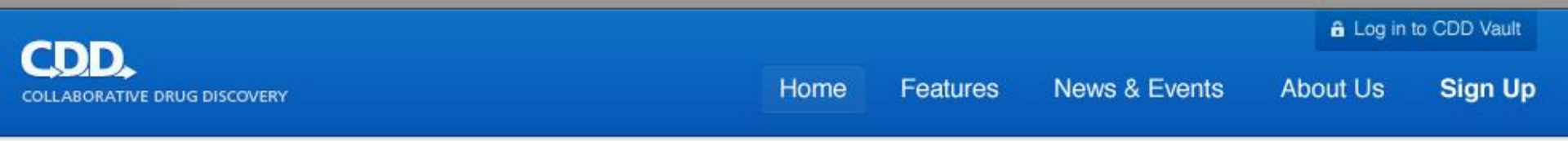
Collaborate securely with your partners

Not everyone wants to share data, but if you do, you retain full control over who can access which data

Learn more about collaborating with CDD Vault



"One of the biggest barriers for academic drug discovery is the poor access to



CDD is Secure & Simple

- Web based database (log in securely into your account from any computer using any common browser – Firefox, IE, Safari)
- Hosted on remote server (lower cost) dual-Xeon, 4GB RAM server with a RAID-5 SCSI hard drive array with one online spare
- Highly secure, all traffic encrypted, server in a secure professionally hosted environment
- Automatically backed up nightly
- **MySQL database**
- **Uses JChemBase software with Rails via a Ruby-Java bridge, (structure searching and inserting/ modifying structures)**
- **Marvin applet for structure editing**
- Export all data to Excel with SMILES, SDF, SAR, & png images

CDD Platform

CDD Vault – Secure web-based place for private data – private by default

CDD Collaborate – Selectively share subsets of data

CDD Public –public data sets - Over 3 Million compounds, with molecular properties, similarity and substructure searching, data plotting etc

will host datasets from companies, foundations etc

vendor libraries (Asinex, TimTec, ChemBridge)

<u>Unique to CDD</u> – simultaneously query your private data, collaborators' data, & public data, Easy GUI

CDD · CDD - Sean Ekins

Sean Ekins: Your Account · Log out

Dashboard | Explore Data | Import Data | Manage Projects

You are a Vault Administrator

CDD has some new updates. · See what's changed

Recent Activity | Messages | Vault Settings | People

Your Recent Protocols

Create a new protocol

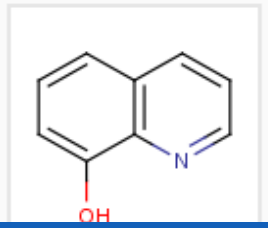
See all protocols

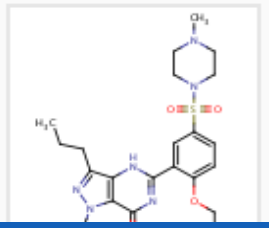
Protocol	Type	Molecules
Joel malaria Diarylureas	in vitro data	33
Scripps Pubchem cpds Pubchem Scripps	Library	0
joel BBB data	predictions	
purple box TB Alliance cpd library	real compounds	
Asinex pharmacophore hits search with first pharmacophore	virtual pharmacophore	

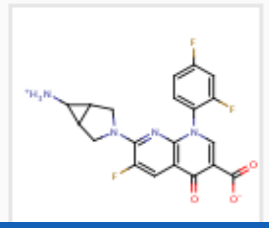
Your Recent Molecules

Create a new molecule

See all molecules







CDD · Barry Bunin's Vault

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Dashboard | Explore Data | Import Data | Manage Projects

You are a Vault Administrator

Create a new ...

Currently viewing data from 1 project and 2 public data sets (see which ones)

Projects all · none

Barry Bunin's Vault

CCK hit and lead optim

Show/hide projects

Shared Data all · none

A new one

In vivo exhaustion mitig

In vivo productivity assa

Public Data all · none

Approved Drugs

Search | Saved Searches | Molecules | Protocols | Plates | References

Search by protocols

(any protocol type) | (any protocol)

Add a term

by structures

by molecule keywords

(any protocol)
Barry Bunin's Vault
(any Barry Bunin's Vault protocol)
Bio Protocol
CCK A receptor binding affinities
CCK Rat Model
CCK-A Dose Response Curve
Copy of CCK A receptor binding affinities
Approved Drugs
(any Approved Drugs protocol)
Drug Bank
FDA
Lipinski FDA List
Orange Book
Physician's Desk Reference
PDSP Ki Database
(any PDSP Ki Database protocol)
1200015E14Rik
17Beta-HSD Type 3
5-HT Transporter

Heavy atom count : to

Polar surface area : to

Rotatable bonds : to

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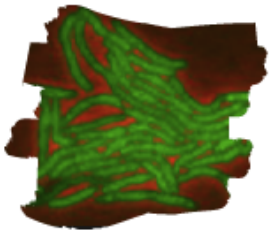
More Medicines for Tuberculosis



The More Medicines for Tuberculosis (MM4TB) consortium evolved from the highly successful FP6 project, New Medicines for TB (NM4TB), that delivered a candidate drug for clinical development two years ahead of schedule. Building on these firm foundations and exploiting its proprietary pharmacophores, MM4TB will continue to develop new drugs for TB treatment. An integrated approach will be implemented by a multidisciplinary team that combines some of Europe's leading academic TB researchers with two major pharmaceutical companies and four SMEs, all strongly committed to the discovery of anti-infective agents...

>More

Welcome to the mm4tb website

This is a preliminary version of the website, where you will find basic information about our project.
The full version of the website will be ready soon, please visit us again in the near future to learn more!

>Project Par

École Polytechnique Fédérale de Lausanne, Switzerland
Uppsala University, Sweden
University of Cambridge, United Kingdom
Institut Pasteur, France
Università degli Studi di Padova, Italy
Vichem Chemie Research Ltd., Hungary
Indian Institute of Science, India
Università degli Studi Piemonte Orientale "A. Avogadro", Italy
Tydock Pharma, Italy
Eidgenössische Technische Hochschule Zürich, Switzerland
Sanofi-Aventis, France
SCIPROM Sàrl, Switzerland

A. N. Bakh Institute of Biochemistry of the Russian Academy of Science, Russian Federation
Comenius University, Slovakia
John Innes Centre, Norwick, United Kingdom
Cellworks, Bangalore, India
Collaborative Drug Discovery, USA
Universidad del Pais Vasco/ Euskal Herriko Unibertsitatea, Spain
University of Zaragoza, Spain
Alere Technologies GmbH, Germany
University of Cape Town, South Africa

- 20 groups academia + AZ, Sanofi-Aventis, Tydock Pharma
- Goal to discover drugs for TB
- Use CDD to share data / collaboration
- Bi annual face to face meetings

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BILL & MELINDA GATES foundation

ALL LIVES HAVE EQUAL VALUE

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Topics

What Is TB?

Test your knowledge of the disease with this interactive photo gallery.

1 2 3

Tuberculosis

New funding and interest in tuberculosis is producing encouraging results, but there is still more work to be done. We support the goals of the Global Plan to Stop TB, which aims to treat 50 million people with TB and prevent 14 million deaths from the disease by 2015. Read more.

SELECTED GRANTS

Click the map to view Tuberculosis grants or explore the world map.

RELATED INFO

Progress Against Tuberculosis
(PDF, 1.2MB, 4 pages)
Strategy Overview: Tuberculosis
(PDF, 664KB, 6 pages)
Our Commitment to Sharing Information

- 3 Academia/ Govt lab – Industry screening partnerships
- CDD used for data sharing / collaboration

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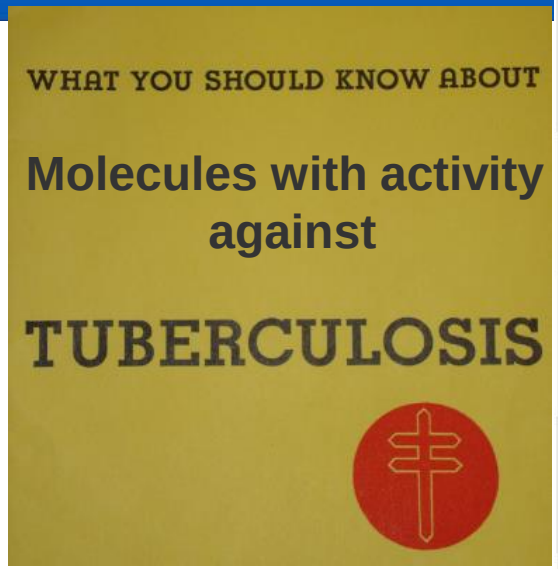


~20 public datasets for TB
Including Novartis data on TB hits

>300,000 cpds

Patents, Papers Annotated by CDD

Open to browse by anyone

☑	**TB: TAACF Assay Results** PI: Bernard Munos Published: 2/12/2008 Antibacterial activity of a publicly available library of 812 compounds against Mycobacterium tuberculosis (H37Rv) in Alamar Blue whole cell assay	TB Early Phase Drug Discovery Program	812
☑	**TB: Literature Review** PI: Ballel, et al. Published: 4/17/2009 Tuberculosis SAR data compiled in a survey of agents active against M. tuberculosis, including those with both known and unknown modes of action (Ballel, et al. "New Small-Molecule Synthetic Antimycobacterials" in Antimicrobial agents and chemotherapy, June 2005). Updated 4/17 with TubercuList/TBDB/other target links and impro references.	TB Literature Data	49
☑	**TB MIC Prathipati GVKbio** PI: Sean Ekins Published: 12/10/2008 SAR MIC data from a recent publication by Prathipati et al at Novartis (PMID: 19053518). Consists of a dataset culled from the GVKbio database. The dataset was published as supplemental information at the journal website.	CDD - Sean Ekins	2880
☑	**TB MIC Prathipati NIAID** PI: Sean Ekins Published: 12/10/2008 Literature TB MIC SAR data from a recent publication by Prathipati et al at Novartis (PMID: 19053518). Consists of a dataset culled from the NIAID website. The datase was published as supplemental information on the journal website.	CDD - Sean Ekins	3748
☑	**Sacchettini et al., review** PI: Sean Ekins Published: 2/18/2009 First and second line antituberculosis agents from Tables 1 and 2 in Sacchettini J.C., Rubin E.J. and Freundlich J.S. Drugs versus bugs: in pursuit of the persistent preda Mycobacterium tuberculosis, Nature Reviews Microbiology, 6, 41-52, (2008).	CDD - Sean Ekins	14
☑	**MLSMR** PI: Robert Goldman Published: 5/8/2009 A diverse collection of over 200,000 compounds collected by the Molecular Libraries Small Molecule Repository (MLSMR) were made available to the Southern Research Molecular Libraries Screening Center in Spring 2008 for primary testing against Mtb H37Rv. The most active compounds from this primary screen were selected and tes at 10 concentrations in both a dose response assay against H37Rv as well as a cytotoxicity counterscreen using vero cells.	Southern Research Institute	214507
☑	**TB: Makarov et al., NM4TB consortia** PI: Sean Ekins Published: 5/8/2009 Structure activity relationship data for 1,3-benzothiazin-4-ones (BTZ). Data obtained from the paper "Benzothiazinones Kill Mycobacterium tuberculosis by Blocking Arabinan Synthesis" published in Science by Makarov et al., 2009 and colleagues at the NM4TB consortia (PMID: 19299584).	CDD - Sean Ekins	32
☑	**TB Efficacy Data from Published Literature** Published: 5/28/2009 TB Efficacy Data from Published Literature sources. SAR data for 6771 unique, as well as common compounds from over 300 PubMed references. Data includes PubMed citations, targets, cells and organisms testes, MIC, % Inhibition, EC50-EC100, IC50, etc.	CDD: TB Curated Literature	6771
☑	**TB Toxicity Data from Published Literature** Published: 5/28/2009 TB Toxicity Data from Published Literature sources. SAR data for 638 unique, as well as common compounds from PubMed references. Data includes PubMed citations, targets, cells and organisms testes, cell viability, LD50, CC50, MNTD, etc.	CDD: TB Curated Literature	638
☑	**TB Pharmacokinetic Data from Published Literature** Published: 5/28/2009 TB Pharmacokinetic Data from Published Literature sources. SAR data for 28 unique, as well as common compounds. Data includes PubMed citations, targets, cells and organisms tested, bioavailability, Vm, Vd, Cmax, etc.	CDD: TB Curated Literature	28
☑	**TB Absorption Data from Published Literature** Published: 5/28/2009 TB Absorption Data from reference article Inhibition of siderophore biosynthesis by 2-triazole substituted analogues of 5'-O-[N-(salicyl)sulfamoyl]adenosine: antibacter	CDD: TB Curated Literature	24

1702 hits in >100K cpds

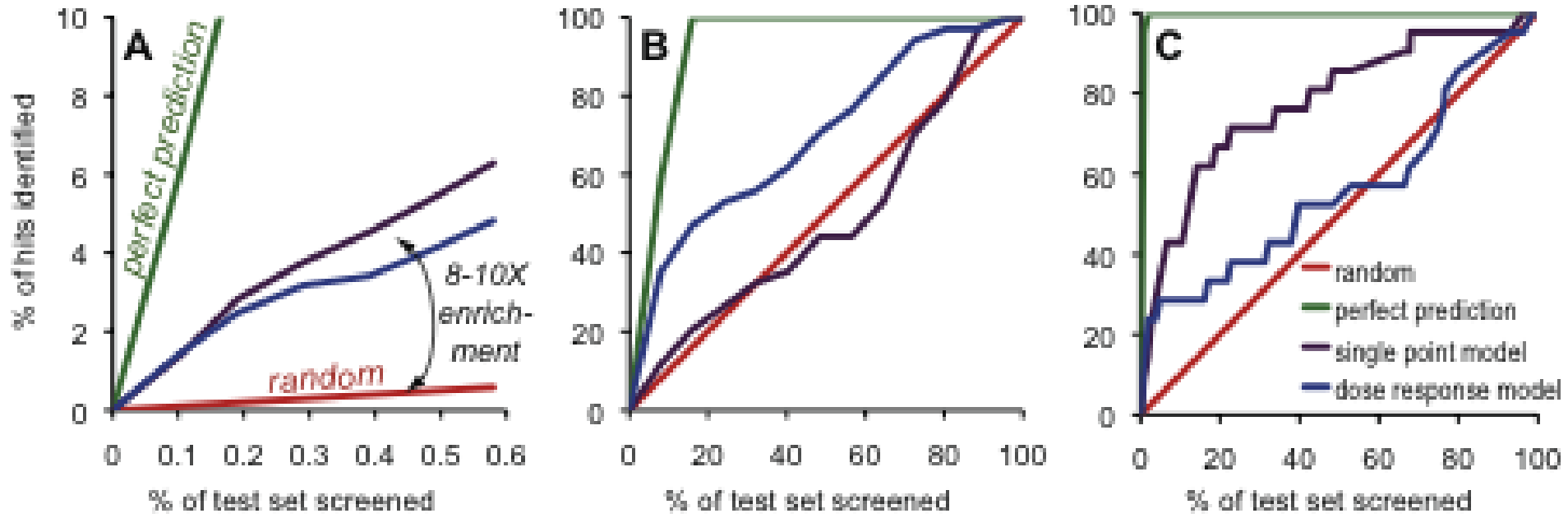
100K library

34 hits in 248 cpds

Novartis Data

21 hits in 2108 cpds

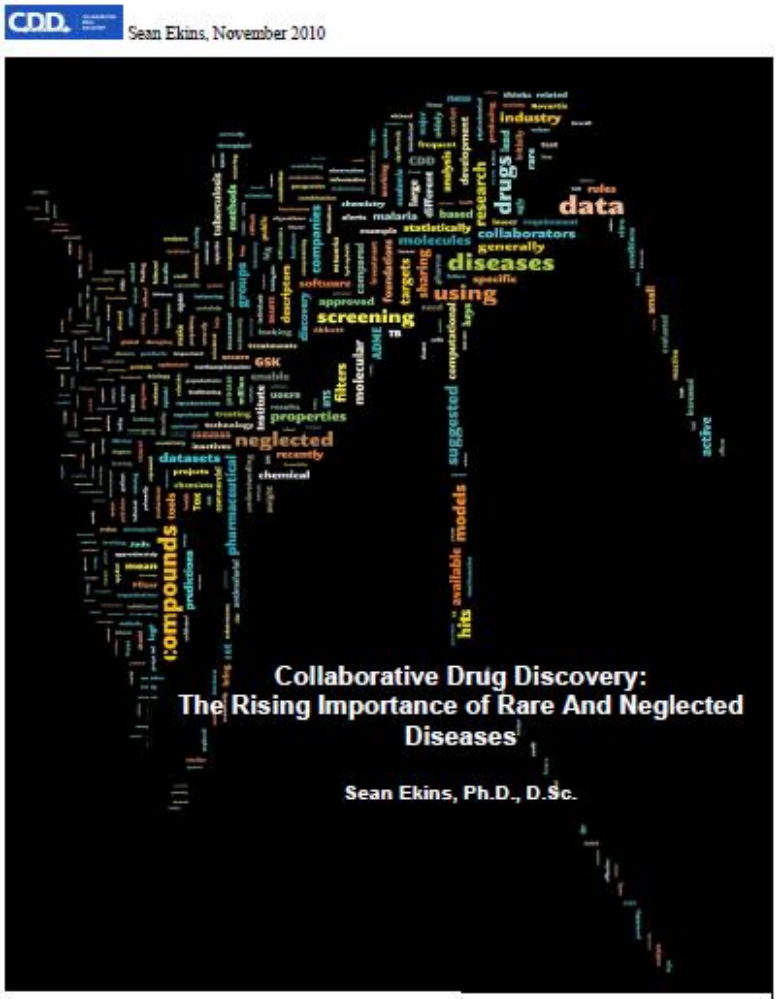
FDA drugs



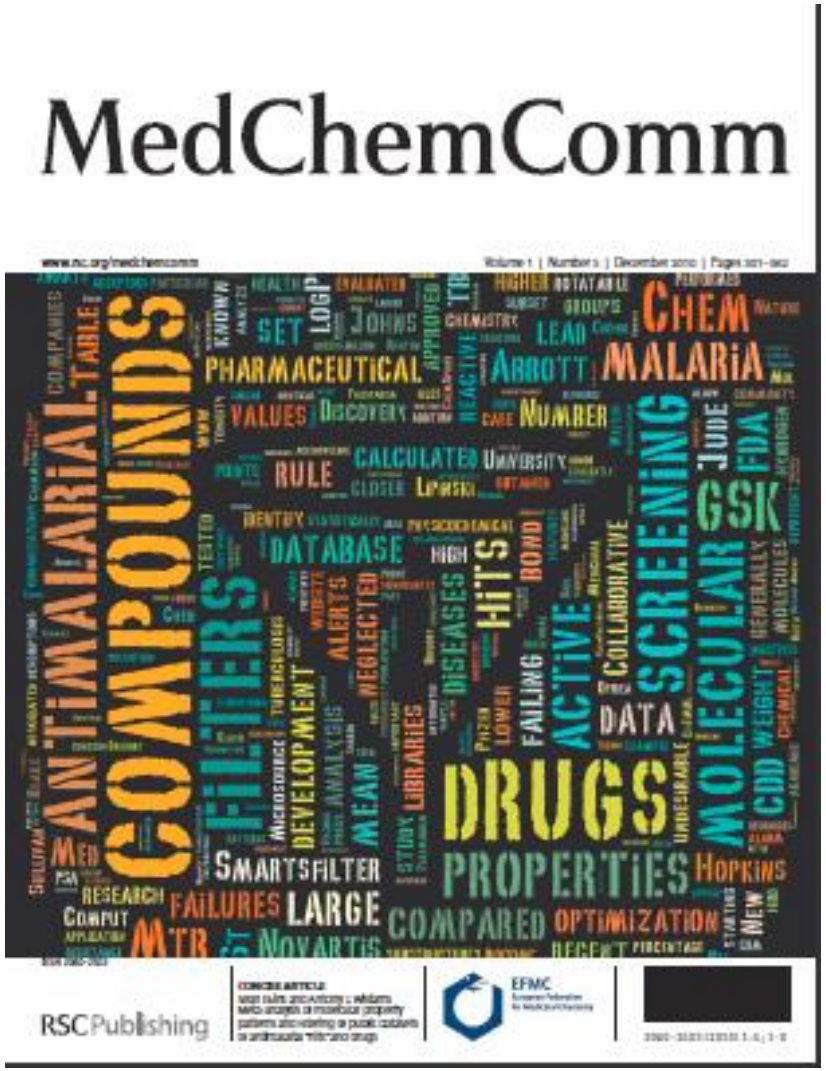
Suggests models can predict data from the same and independent labs
Initial enrichment – enables screening few compounds to find actives

Ekins et al., Mol BioSyst, 6: 840-851, 2010
Ekins and Freundlich, Pharm Res. 2011

Analysis of malaria data



http://www.slideshare.net/ekinssean



Ekins S and Williams AJ, MedChemComm, 1: 325-330, 2010.

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Open algorithms, descriptors, closed data – can we unlock it?

Using Open Source Descriptors and Algorithms for Modeling ADME Properties

Rishi R. Gupta†, Eric M. Gifford†, Ted Liston†, Chris L. Waller†, Moses Hohman*, Barry A. Bunin* and Sean Ekins*

†Pfizer Global Research and Development, Eastern Point Road, Groton, CT 06340

*Collaborative Drug Discovery, 1633 Bayshore Highway, Suite 342, Burlingame, CA 94010

ABSTRACT

Aim: Computational models could be more readily shared with collaborators if they were generated with open source descriptors (e.g. Chemistry development kit, CDK) and modeling algorithms.

Method and Results: We evaluated open source descriptors and model building algorithms using a training set of ~50K molecules and a test set of ~25K molecules with human liver microsomal metabolic stability (HLM) data. A C5.0 decision tree model demonstrated that open CDK+SMARTS keys (Kappa = 0.43, sensitivity = 0.57, specificity 0.91, positive predicted value (PPV) = 0.64) are equivalent to models built with commercial MOE2D+SMARTS keys (Kappa = 0.43, sensitivity = 0.58, specificity 0.91, PPV = 0.63). Extending the dataset to ~ 200K molecules confirmed this observation. The same combination of descriptor set and modeling method was applied to a variety of other ADME endpoints such as solubility etc. and the results were encouraging.

Conclusion: Open source descriptors and algorithms

METHOD

Datasets:

Human Liver Microsomal Stability (HLM) data on ~200K compounds. Compounds were synthesized and tested in the HLM assay at Pfizer. Datasets were binned as per the guidance provided by experts in the Pharmacokinetics, Dynamics and Metabolism (PDM) business unit (Table1).

Datasets:

- Data was binned in 3 bins as shown in Table 1.
- A 3 bin classification model as well as a continuous model on the full dataset was built.
- The distribution of the data in each class in this and the other datasets is shown in Table 2.

Table 1. Classification bins for HLM assay

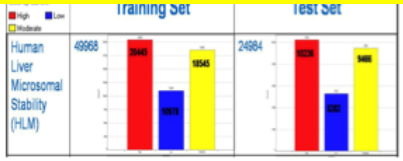
Table 3. Details on the HLM data modeling grid showing performance of various modeling methods versus descriptors.

	SVM	RP Forest Uni Class	RP Forest	Rulequest Cubist C5.0
CDK	Kappa = 0.14 Sensitivity = 0.11 Specificity = 0.96 PPV = 0.43	Kappa = 0.16 Sensitivity = 0.54 Specificity = 0.70 PPV = 0.33	Kappa = 0.11 Sensitivity = 0.85 Specificity = 0.33 PPV = 0.25	Kappa = 0.39 Sensitivity = 0.54 Specificity = 0.91 PPV = 0.61
MOE2D and SMARTS Keys	Not evaluated	Not evaluated	Not evaluated	Kappa = 0.43 Sensitivity = 0.58 Specificity = 0.91 PPV = 0.63 (Baseline)

	CDK +fragment descriptors	MOE 2D +fragment descriptors
Kappa	0.65	0.67
sensitivity	0.86	0.86
specificity	0.78	0.8
PPV	0.84	0.84

MDR training 25,000
testing 18,400

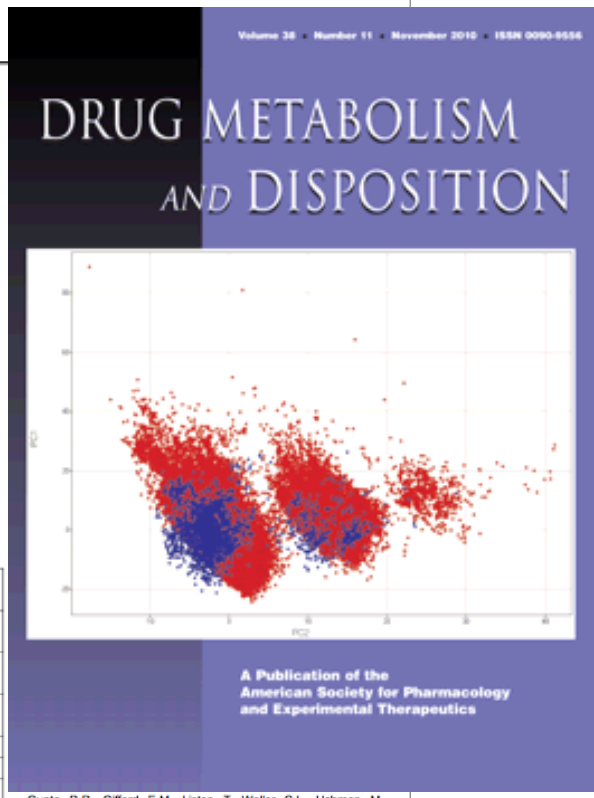
Figure 1. This schematic describes the "*in silico* screening" methodology where a predictive *in silico* model can be used to pre-screen the compounds before they can go through the actual *in vitro* screening.



Descriptors:

- Pfizer modified Molecular Operating Environment 2D set (MOE2D, 2008) (463 descriptors).
- CDK (http://cdk.sourceforge.net/) (Steinbeck et al., 2006) fingerprints (195 descriptors).
- SMARTS keys (355 Keys)

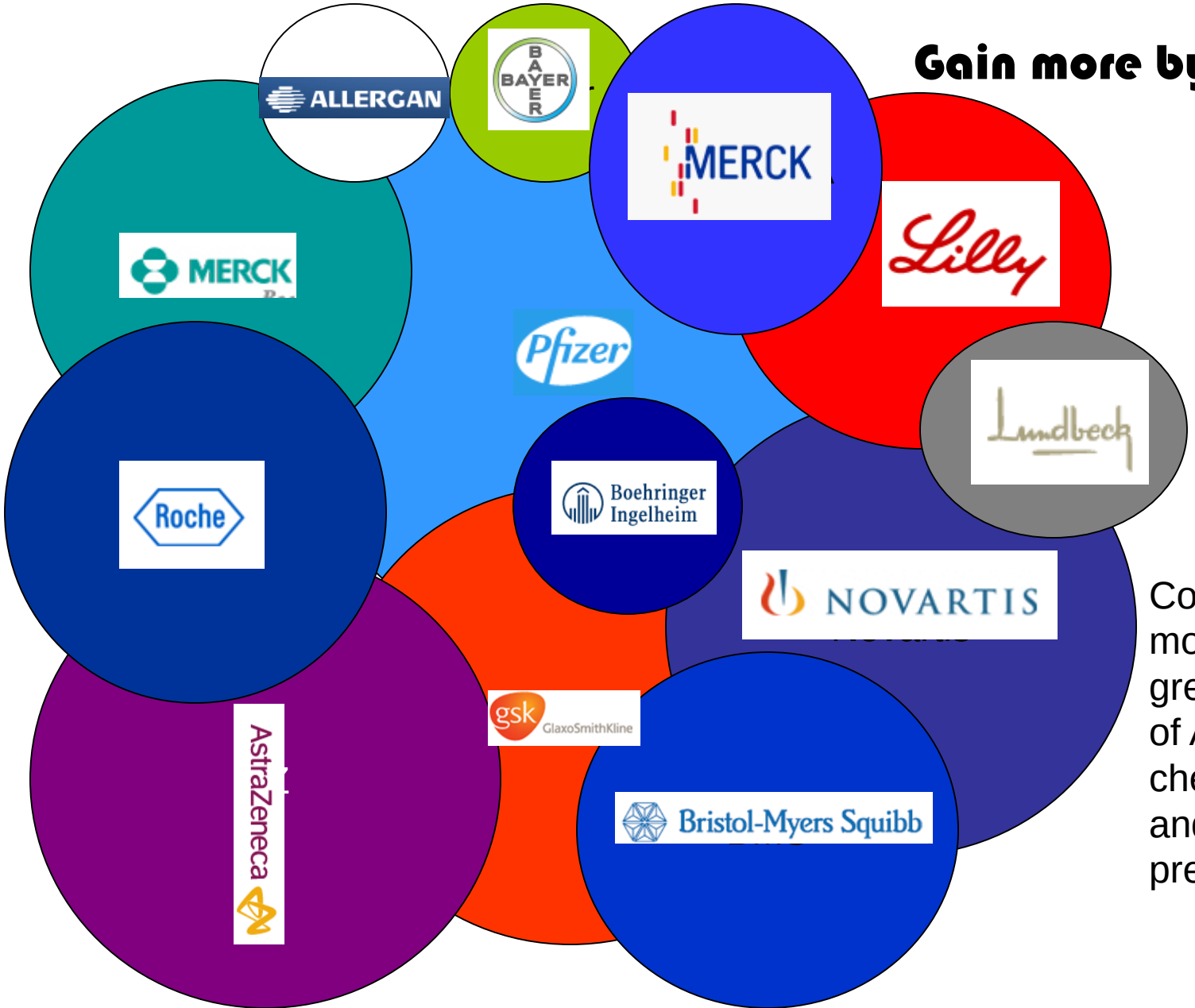
	Keys
# of Descriptors: 578	# of Descriptors: 818
# of Training Set compounds: 193,650	# of Training Set compounds: 193,930
XValidation Results: 38,730 compounds	XValidation Results: 38,786 compounds
Training R^2: **0.79**	Training R^2: **0.77**
20% Test Set R^2: **0.69**	20% Test Set R^2: **0.69**
Blind Data Set (2310 compounds):	**Blind Data Set (2310 compounds):**
R^2 = **0.53**	R^2 = **0.53**



Gupta, R.R., Gifford, E.M., Liston, T., Waller, C.L., Hohman, M., Bunin, B.A. and Ekins, S.; Using Open Source Computational Tools for Predicting Human Metabolic Stability and Additional ADME/Tox Properties, Drug Metabolism and Disposition, 2010 (in press).

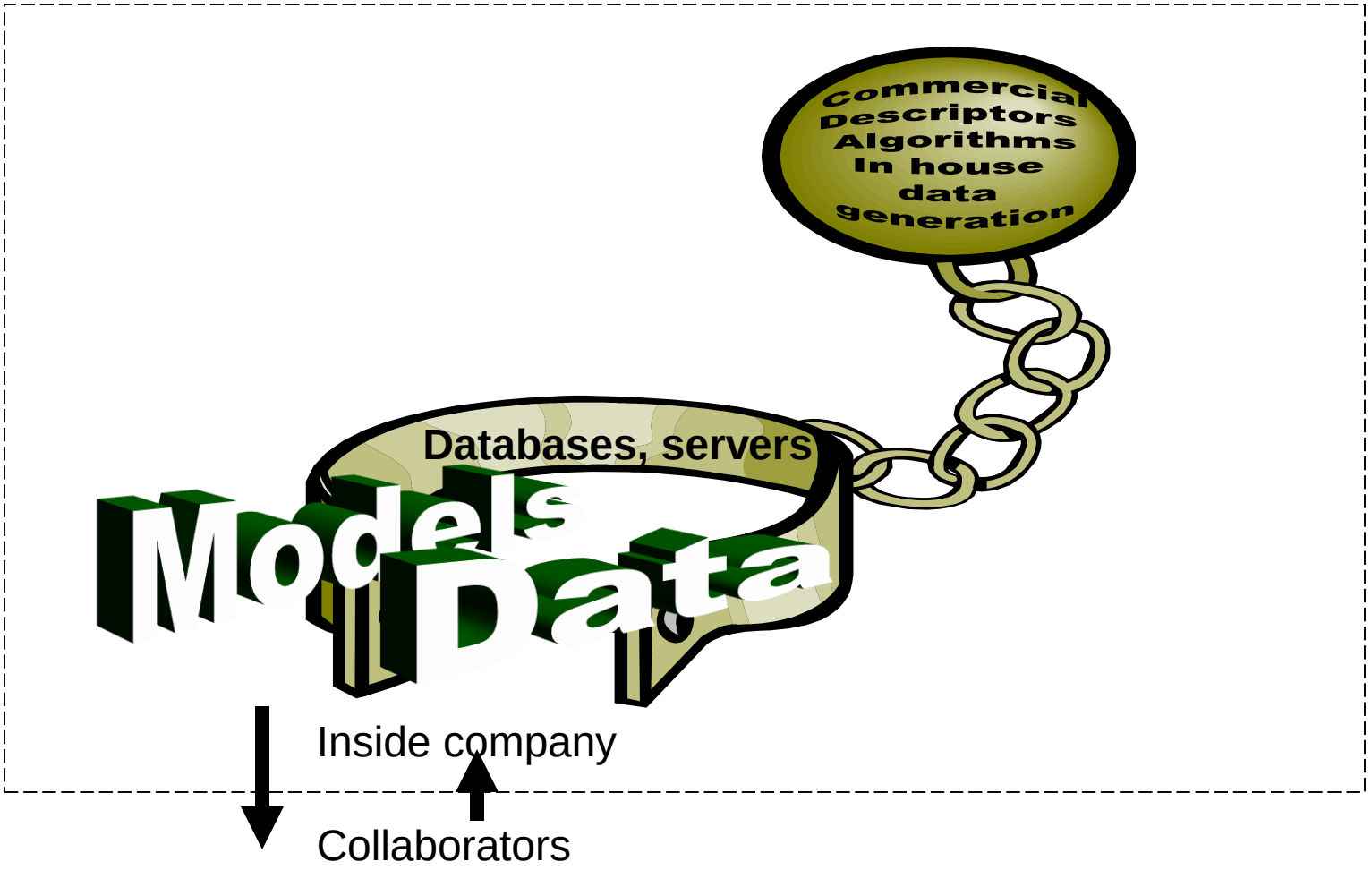
Gupta RR, et al., Drug Metab Dispos, 38: 2083-2090, 2010

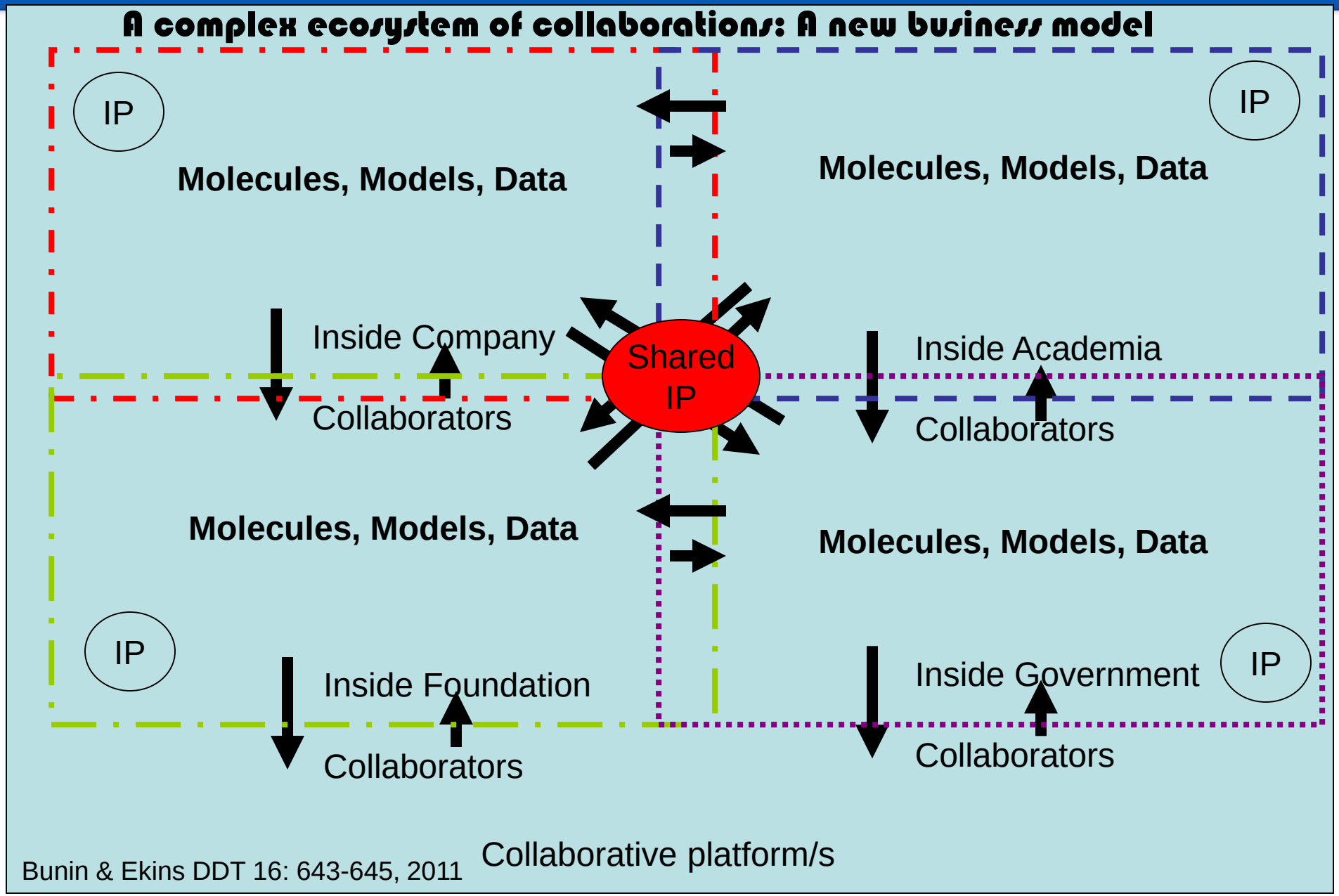
Gain more by sharing mor



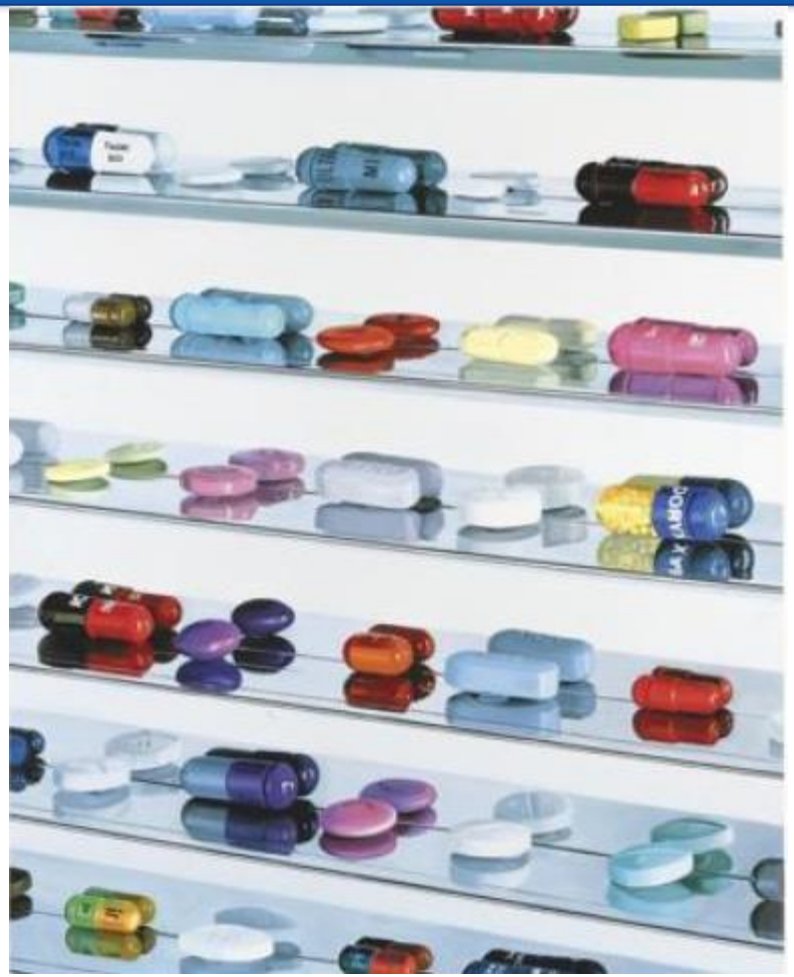
Could combining models give greater coverage of ADME/ Tox chemistry space and improve predictions?

1. Spend less on data generation, descriptors and algorithms – use more open source – use models to help refine testing, external collaborators test your drugs
2. Selectively share data & models with collaborators and control access
3. Have someone else host the models / predictions
4. Predicting properties without the need to know the structures used in models





Bunin & Ekins DDT 16: 643-645, 2011



DAMIEN HIRST
B.1965
PHARMACEUTICALS

All pharmas have assets on shelf that reached clinic

“Off the Shelf R&D”

Get the crowd to help in repurposing / repositioning these assets

How can software help?

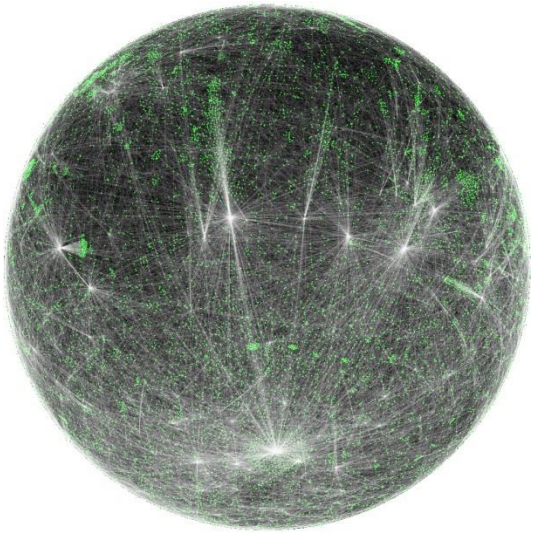
- Create communities to test

- Provide informatics tools that are accessible to the crowd - enlarge user base

- Data storage on cloud – integration with public data

- Crowd becomes virtual pharma-CROs and the “customer” for enabling services

Could our Pharma R&D look like this



Massive collaboration networks – perhaps enabled by Apps

Crowdsourcing will it have a role in R&D, drug discovery possible by anyone with a phone

Pharmaceutical Research, Vol. 27, No. 3, March 2010 (© 2010)
DOI: 10.1007/s11095-010-0059-0

Editorial

Reaching Out to Collaborators: Crowdsourcing for Pharmaceutical Research

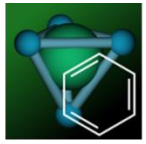
Sean Ekins[1,2,3,4,6] and Antony J. Williams[5]

Ekins & Williams, Pharm Res, 27: 393-395, 2010.

Received October 23, 2009; accepted January 5, 2010; published online January 27, 2010

Mobile Apps for Drug Discovery

- Make science more accessible = >communication
- Mobile – take a phone into field and do science more readily than a laptop
- GREEN – energy efficient computing
- MolSync + DropBox + MMDS = Share molecules as SDF files on the cloud = collaborate


Mobile Molecular DataSheet


MolSync

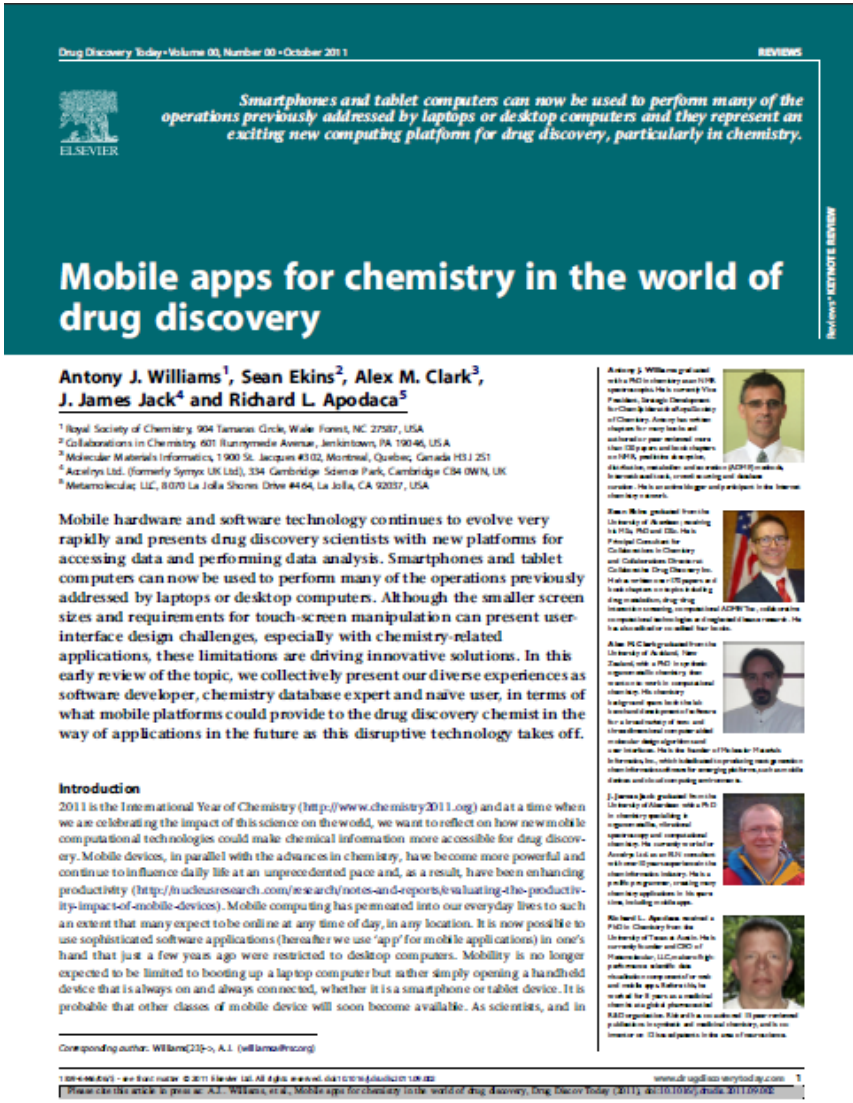

MolPrime


ChemSpider Mobile


Green Solvents

Reaction101


Yield101


Drug Discovery Today • Volume 00, Number 00 • October 2011 REVIEWS
ELSEVIER

Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers and they represent an exciting new computing platform for drug discovery, particularly in chemistry.

Mobile apps for chemistry in the world of drug discovery

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Mobile hardware and software technology continues to evolve very rapidly and presents drug discovery scientists with new platforms for accessing data and performing data analysis. Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers. Although the smaller screen sizes and requirements for touch-screen manipulation can present user-interface design challenges, especially with chemistry-related applications, these limitations are driving innovative solutions. In this early review of the topic, we collectively present our diverse experiences as software developer, chemistry database expert and naive user, in terms of what mobile platforms could provide to the drug discovery chemist in the way of applications in the future as this disruptive technology takes off.

Introduction

2011 is the International Year of Chemistry (http://www.chemistry2011.org) and at a time when we are celebrating the impact of this science on the world, we want to reflect on how new mobile computational technologies could make chemical information more accessible for drug discovery. Mobile devices, in parallel with the advances in chemistry, have become more powerful and continue to influence daily life at an unprecedented pace and, as a result, have been enhancing productivity (http://nucleusresearch.com/research/notes-and-reports/evaluating-the-productivity-impact-of-mobile-devices). Mobile computing has permeated into our everyday lives to such an extent that many expect to be online at any time of day, in any location. It is now possible to use sophisticated software applications (hereafter we use 'app' for mobile applications) in one's hand that just a few years ago were restricted to desktop computers. Mobility is no longer expected to be limited to booting up a laptop computer but rather simply opening a handheld device that is always on and always connected, whether it is a smartphone or tablet device. It is probable that other classes of mobile device will soon become available. As scientists, and in

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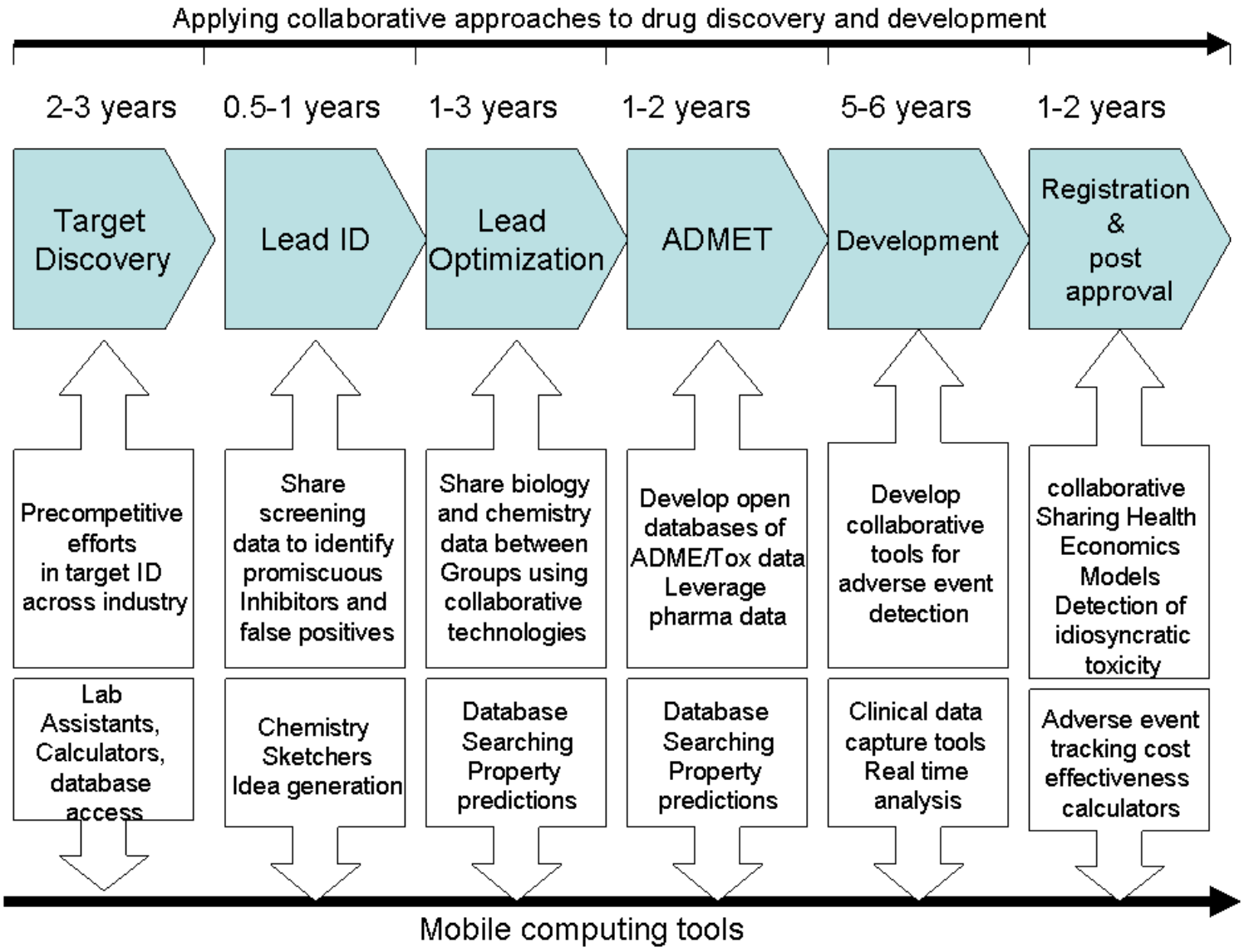
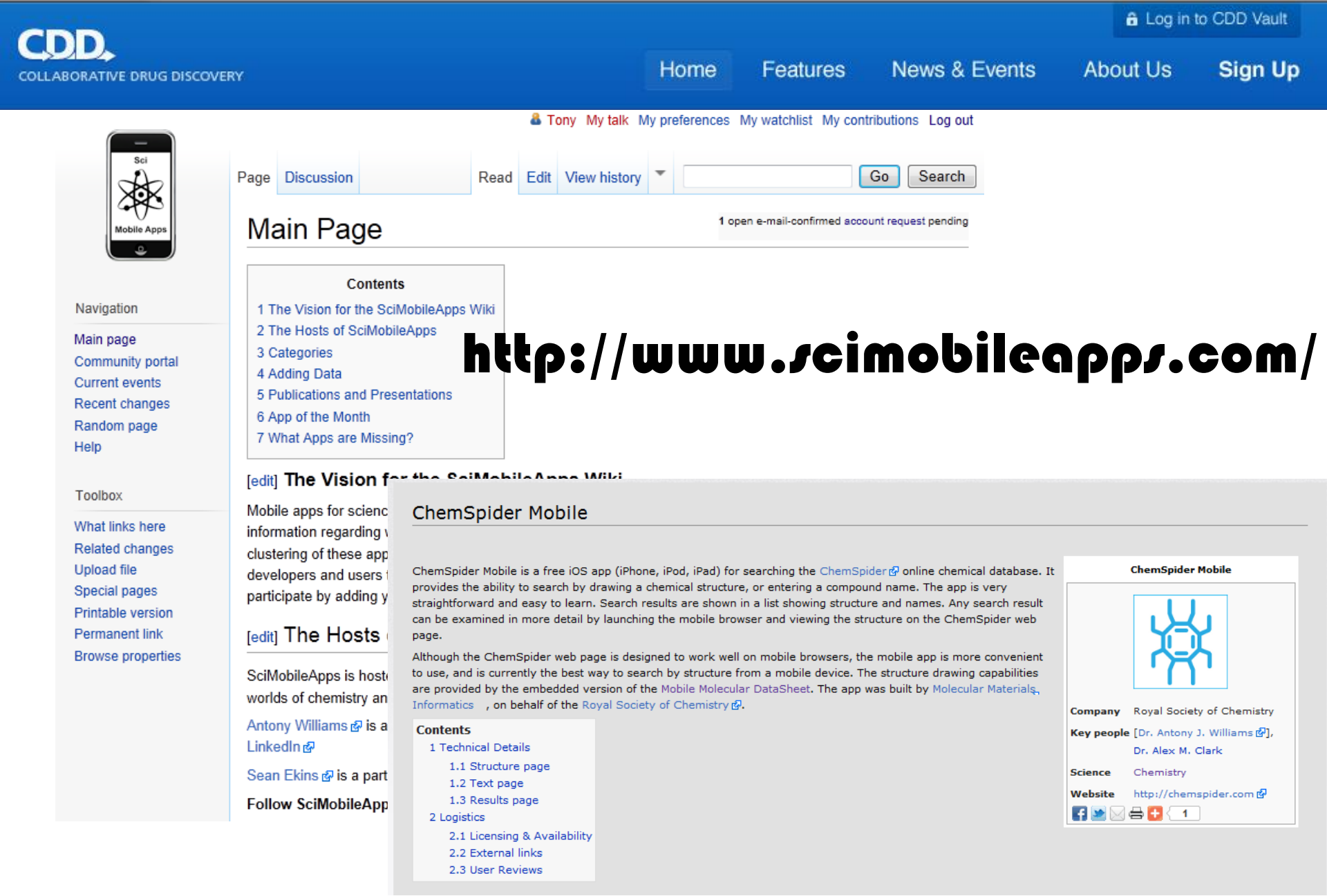
1359-6446/$37 - see front matter © 2011 Elsevier Ltd. All rights reserved. doi:10.1016/j.drudis.2011.09.002
Please cite this article in press as: A.J. Williams, et al., Mobile apps for chemistry in the world of drug discovery, Drug Discov Today (2011), doi:10.1016/j.drudis.2011.09.002

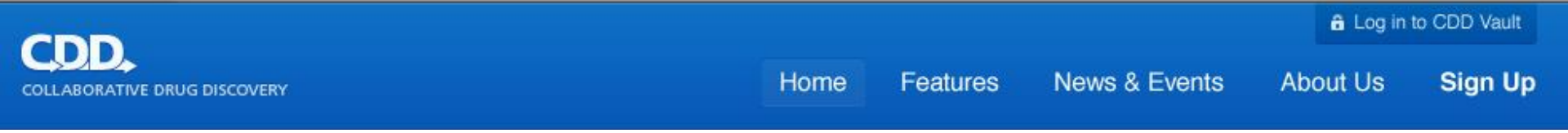
Williams et al DDT in press 2011



Williams et al., DDT in Press, Arnold and Ekins, PharmacoEconomics 28: 1-5, 2010



Also a sister Wiki for scientific databases www.scidbs.com



What is needed

- **More sharing**
- **Support those making data open**
- **Support companies /groups promoting software for datasharing**

Collaborators

Colleagues at CDD
Antony Williams (RSC)
Joel Freundlich, (UMDNJ)
Gyanu Lamichhane, Bill Bishai (Johns Hopkins)
Jeremy Yang (UNM)
Nicko Goncharoff (SureChem)
Chris Lipinski
Takushi Kaneko (TB Alliance)
Carolyn Talcott and Malabika Sarker (SRI International)
Chris Waller, Eric Gifford, Ted Liston, Rishi Gupta (Pfizer)
Alex Clark (MMDS)

GSK
ChemAxon, Accelrys

Bill and Melinda Gates Foundation
Collaborators at MM4TB