



COLLABORATIVE
DRUG
DISCOVERY

“10 Years of Collaborative Drug Discovery in the Cloud”

The CDD Vault[®]



Finally...a Modern Approach to Drug Research Informatics

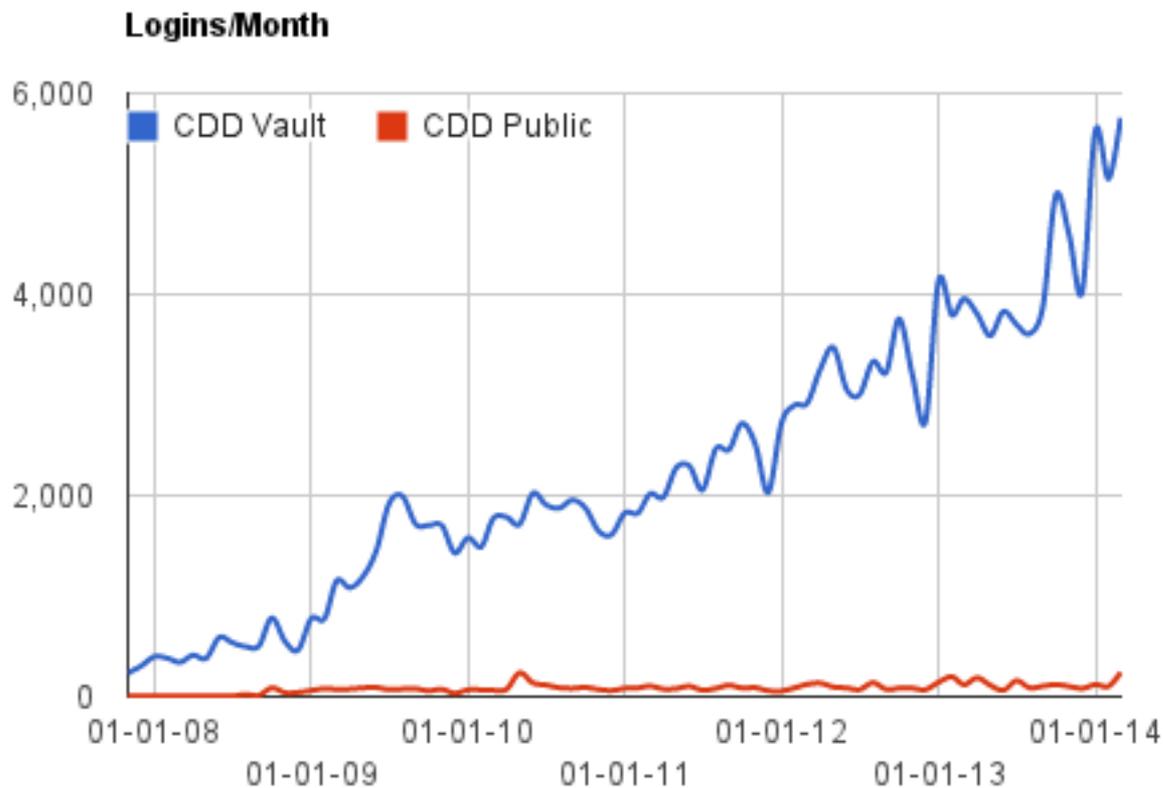
Collaborative Drug Discovery (CDD), Inc
Barry A. Bunin, PhD



COLLABORATIVE
DRUG
DISCOVERY

10 Years Evolving CDD Vault

Login/month: One Month in 2014 = All Year in 2008!





- 212,785 Logins
- 22,488,307 Molecules
- 249,764,130 Bioassay Datapoints

Dr. Ellen Berg, Asterand

JULY 19, 2011

Ellen Berg was a cofounder of BioSeek, Inc. and served as its Chief Scientific Officer. She was appointed as General Manager, Bio Seek LLC after the merger of BioSeek and Asterand in 2010. Dr. Berg has more than 20 years of research experience in pathophysiologic mechanisms of inflammation and immunity. Her expertise in complex cell-based biological assays led to the development of the company's proprietary BioMAP® technology for target validation and drug characterization using primary human cell systems.



Jim Wikel, Ex-Eli Lilly, Apex Therapeutics

MAY 19, 2011

Jim Wikel is the Chief Chemist at Apex Therapeutics, and has served in a variety of positions at Eli Lilly from 1971 to 2004. Read about Jim's inspirational path from a tiny coal mining town of West Virginia to Head of Structural and Computational Sciences at Lilly, in this CDD Spotlight.



Dr. James McKerrow, UCSF

MARCH 29, 2011

As CDD's first major customer, Dr. McKerrow guided us in our early days and introduced us to the Gates Foundation, making him perfect for our first CDD Spotlight.



Spotlight Interviews

Prof. Jonathan Baell of "PAINS" Filters Fame from Monash University

OCTOBER 7, 2013

People are just finding compounds with a bit of activity and really publishing screening hits as though they are genuine optimizable candidates. And these things can be subversive and they can look real, so these publications are kind of getting accepted and unfortunately there's a lot of noise out there, a lot of pollution, and [...]



Dr. Robert Volkmann, Vice President of Chemistry – Mnemosyne & SystaMedic

AUGUST 15, 2013

What you've done is you've designed a product that works for people like me. It not only works great for me but also works great for our biologists and our CRO chemists in India. ... I just take it for granted that CDD will work and it will work as planned. So I guess for [...]

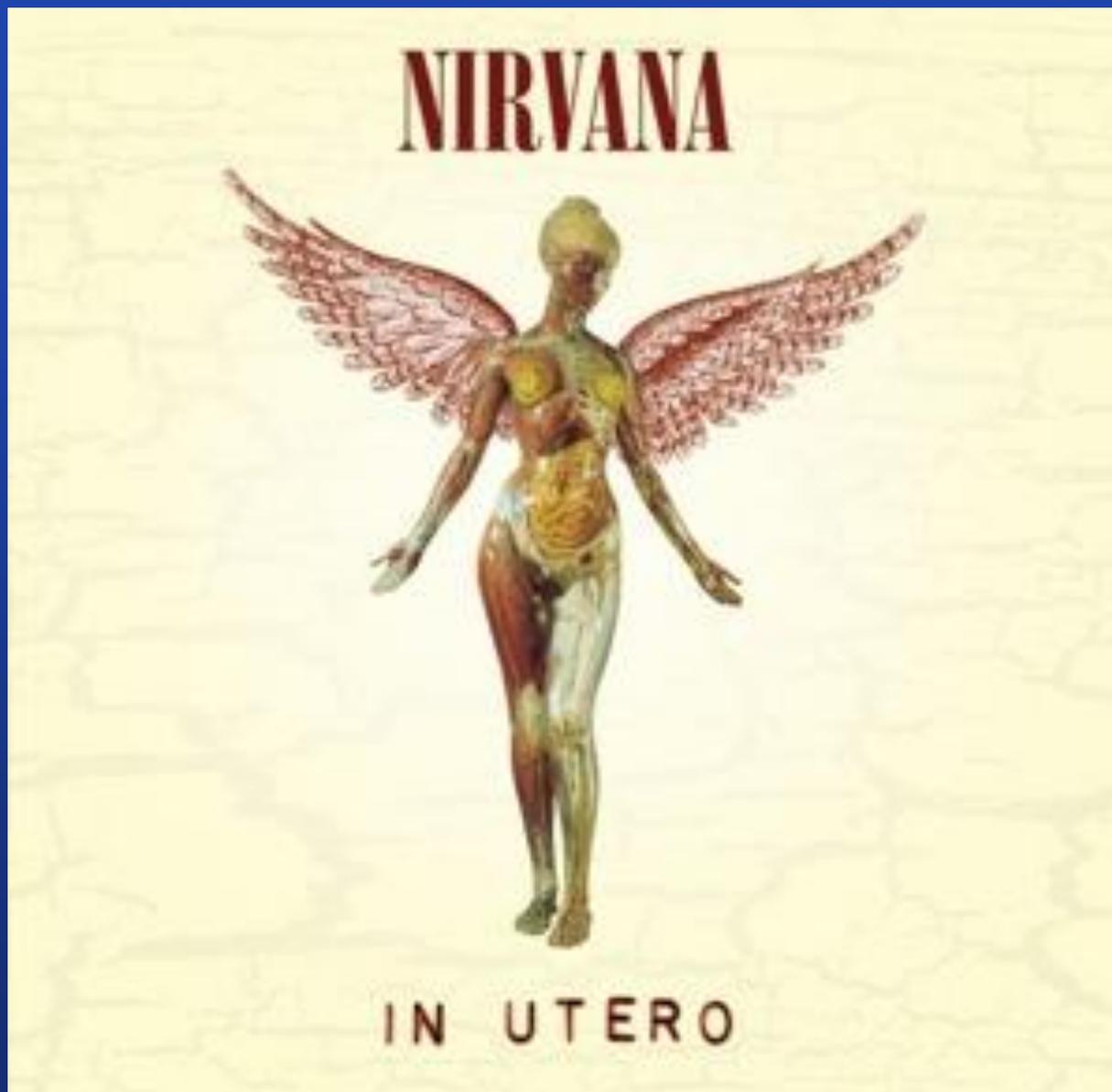


Orphagen CEO Scott Thacher, Ph.D. + Director of Chemistry Ruo Steensma, Ph.D.

JULY 12, 2013

"We had Excel sheets all over the place and data from different projects that were just separated in different folders and after a while," says Dr. Ruo Steensma, "It got to the point that it was just hard to manage. We chose CDD, and we're really happy with the service and the cost and the way the database is evolving."







CHEMbot Bazaar

Home

My Library

My Models

My Projects

Message Center



What is the "CHEMbot Bazaar"?

[Edit My Public Items]

CHEMbot Bazaar

My Public Items

Public Libraries

Public Models

Public Projects

The following Structure Libraries are available to all CHEMbot Premium Subscribers:

Library Name	Description	Owner	Last Updated
CHEMbot Public Library	<p>Includes following Sub-Libraries:</p> <ul style="list-style-type: none"> commercial drug compound sets therapeutic diversity sets target class diversity sets 	CHEMbot System	7/18/03, 4:03p
Public Library 1	Includes 12 commercially available anti-depressant compound sets	user3986	7/22/03, 3:45p
Public Library 3	6COX Target, 10 compound sets	user8b9y	7/24/03, 5:14p
Public Library 4	VEGF Target, 36 compound sets	user2899	7/28/03, 3:12p

Protocol: cruzain  [edit](#)

Description: Lorem ipsum dolor sit amet, consectetur adipiscing elit. Nam lacinia diam sit amet libero. Phasellus tincidunt quam id nibh. Fusce porttitor suscipit ipsum. Sed diam erat, facilisis at, egestas at, condimentum sed, nulla. In odio metus, luctus ac, iaculis quis, sollicitudin in, ipsum. Nam diam. Proin eget lectus. Integer vitae nunc nec nunc vehicula congue. Donec lacus elit, euismod in, tempus eget, porttitor at, lorem.

Expected Fields:

Result	Units	Description	Hit Threshold
IC50	nM	50% inhibition concentration	500.0
du4-71	ratio	activity relative to du4-71	

Compounds assayed: 11 **Hits:** 9  [summarize all data](#)**Runs of this protocol**  [add run](#)

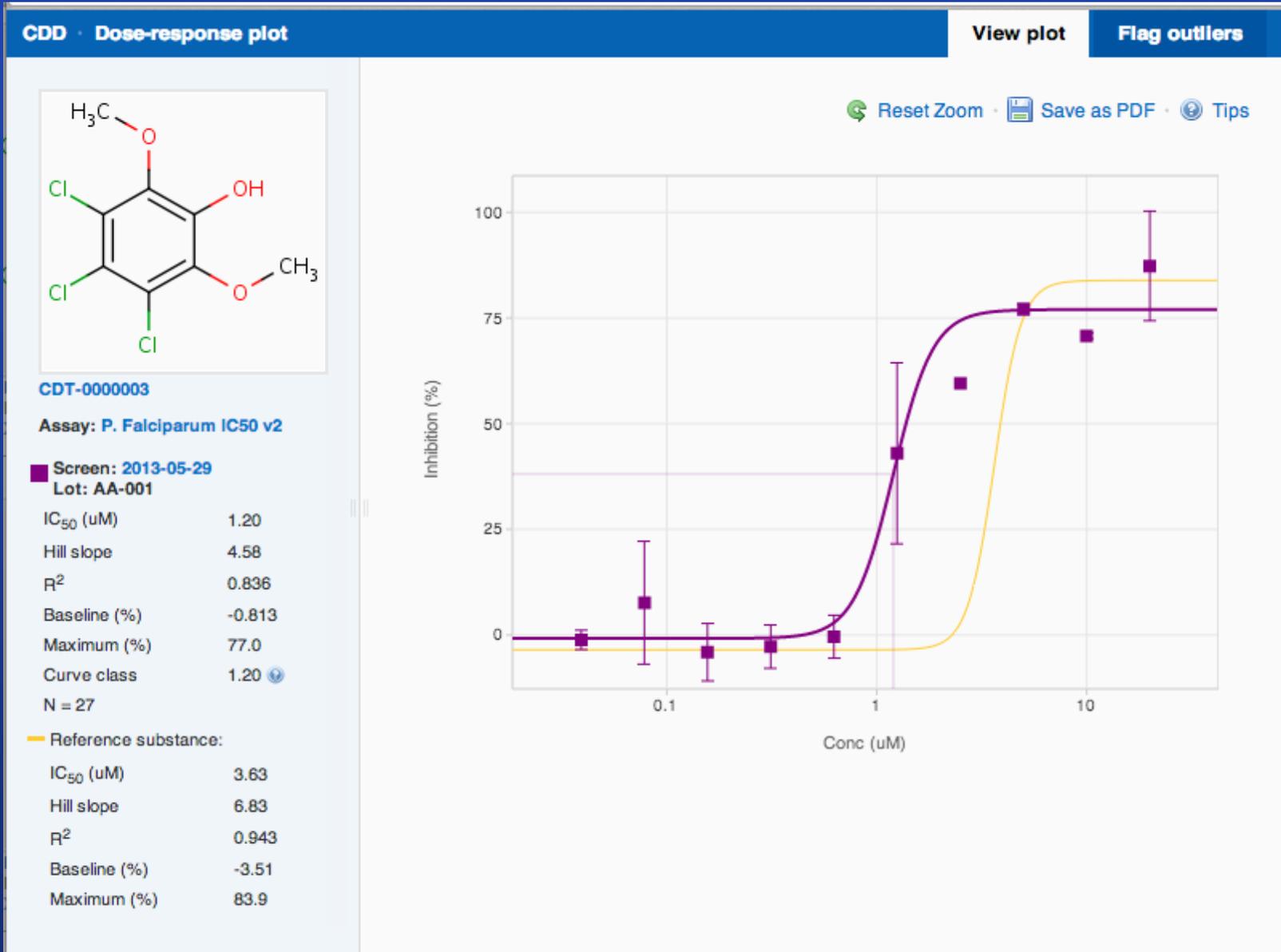
 Date 	<u>Lab</u>	<u>#Compounds</u>	<u>#Hits</u>	<u>Delete Run</u>
2004-04-19 00:00:00	mckerrow	11	9	

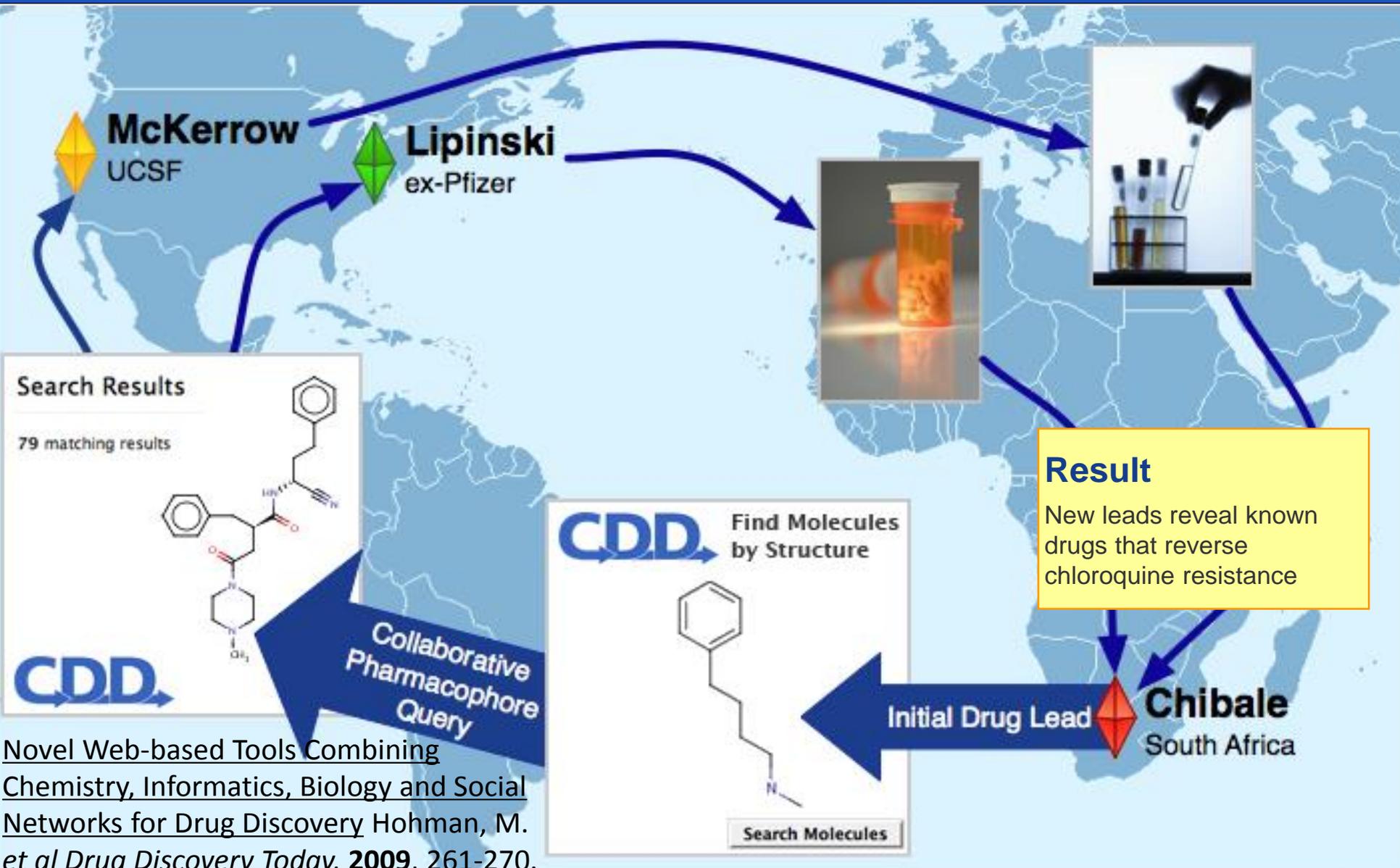


COLLABORATIVE
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DISCOVERY

Year 3: Birth of CDD Vault V1.0







Novel Web-based Tools Combining Chemistry, Informatics, Biology and Social Networks for Drug Discovery Hohman, M. *et al Drug Discovery Today*, 2009, 261-270.



COLLABORATIVE
DRUG
DISCOVERY

NIH Blueprint – CDD Partnership

Securely sharing data



AMRI GLOBAL
SMARTSOURCING™



**BRIGHAM AND
WOMEN'S HOSPITAL**
A Teaching Affiliate of Harvard Medical School

SOUTHERN RESEARCH
Legendary Discoveries. Leading Innovation.



**EMORY
UNIVERSITY**

New

NIH Blueprint

SRI International
R&D for Government and Business

UC San Diego

CDD COLLABORATIVE
DRUG
DISCOVERY

Old

Trevena

W UW HOME DIRECTORIES
UNIVERSITY of WASHINGTON

tetra
TETRA DISCOVERY PARTNERS

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

Blog | Community | Infographics | Photos | Videos | Search This Site GO

BILL & MELINDA GATES foundation ALL LIVES HAVE EQUAL VALUE

About the Foundation | Programs & Partnerships | What We're Learning | Topics ▾ | Regions ▾ | Grants ▾

Home / Topics / Tuberculosis + SHARE

Topics



What Is TB?
Test your knowledge of the disease with this interactive photo gallery. [▶](#)

1 2 3 ▶

SELECTED GRANTS



Click the map to view Tuberculosis grants or [explore the world map.](#)

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.](#) ▶

RELATED INFO

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

- 6 Academic/Non-Profit/Govt labs +
- 7 Big Pharmas (each w/ own Legal and IT Process)
- CDD for secure data sharing / collaboration – disclosure legally blessed leads



Welcome, Jim
McKerrow-CDD Database

Save Query as:

 >>

Export to Excel

Export to SDFFile

Collaborate

E-mail

X MY DATABASE

People I'm Sharing with (Data Recipient):

E-mail Identity
aisaksen@appabove.com
bbunin@collaborativedrug.com
mbazargan@collabrx.com

People Sharing with Me (Data Sender):

E-mail Identity
lsafty@gmail.com
brett.wong@tufts.edu
kgregory@collaborativedrug.com

Manage your collaboration accounts.

Collaborate: Differentiation Vault Admin is Privy to All Projects

Currently viewing data from **9 projects**, **1 shared data set**, and **1 public data set** (see which ones)

Projects all · none

- alpha
- AT Vault
- Barry Bunin's Vault
- Biochemistry assays
- Biotech Collaborative F
- Cancer Kinase Target F
- CCK hit and lead optim
- Dihydropyridine deriva
- Just India CRO**

[Show/hide projects](#)

Shared Data all · none

- A new one
- In vivo exhaustion mitiga
- In vivo productivity as**

Public Data all · none

- ADMEdata.com - A Cor**

(any protocol type) (any protocol)

Add a term

Remove this term

by structures substructure similarity \geq 70%

[Launch the Structure Editor](#)
to build a structure for this search

by molecule keywords

any field

Example: mol1 OR synonym2 AND NOT userfield3

Save this search...

by chemical properties

Molecular weight : to

log P : to

H-bond donors : to

H-bond acceptors : to

Lipinski violations : to

pKa : to

Exact mass : to

Heavy atom count : to

Polar surface area : to

Rotatable bonds : to

Search Molecules



Collaborate: India CRO User Doesn't Even Know Other Projects Exist

+ Create a new ...

Showing data from **1 project** and **1 public data set** (see which ones)

Projects all · none

Just India CRO

[Show/hide projects](#)

Shared Data all · none

A new one

In vivo exhaustion mitiga

In vivo productivity assa

Public Data all · none

ADME: ADMEdata.com

FDA APPROVED, TOX:

FDA APPROVED: Appro

FDA APPROVED: NCG

FDA APPROVED: Orph

GPCR: PDSP Ki Databa

Search | [Saved Searches](#) | [Collections](#) | [Molecules](#) | [Protocols](#) | [Plates](#) | [References](#)

Protocols ⓘ

(select protocol) or (select category)

+ Add a term ⊖ Remove term

Structures ⓘ substructure similarity ≥ 70%

Launch the Structure Editor
to build a structure for this search

Collections ⓘ

In (select a collection)

+ Add a term ⊖ Remove term

Chemical Properties ⓘ

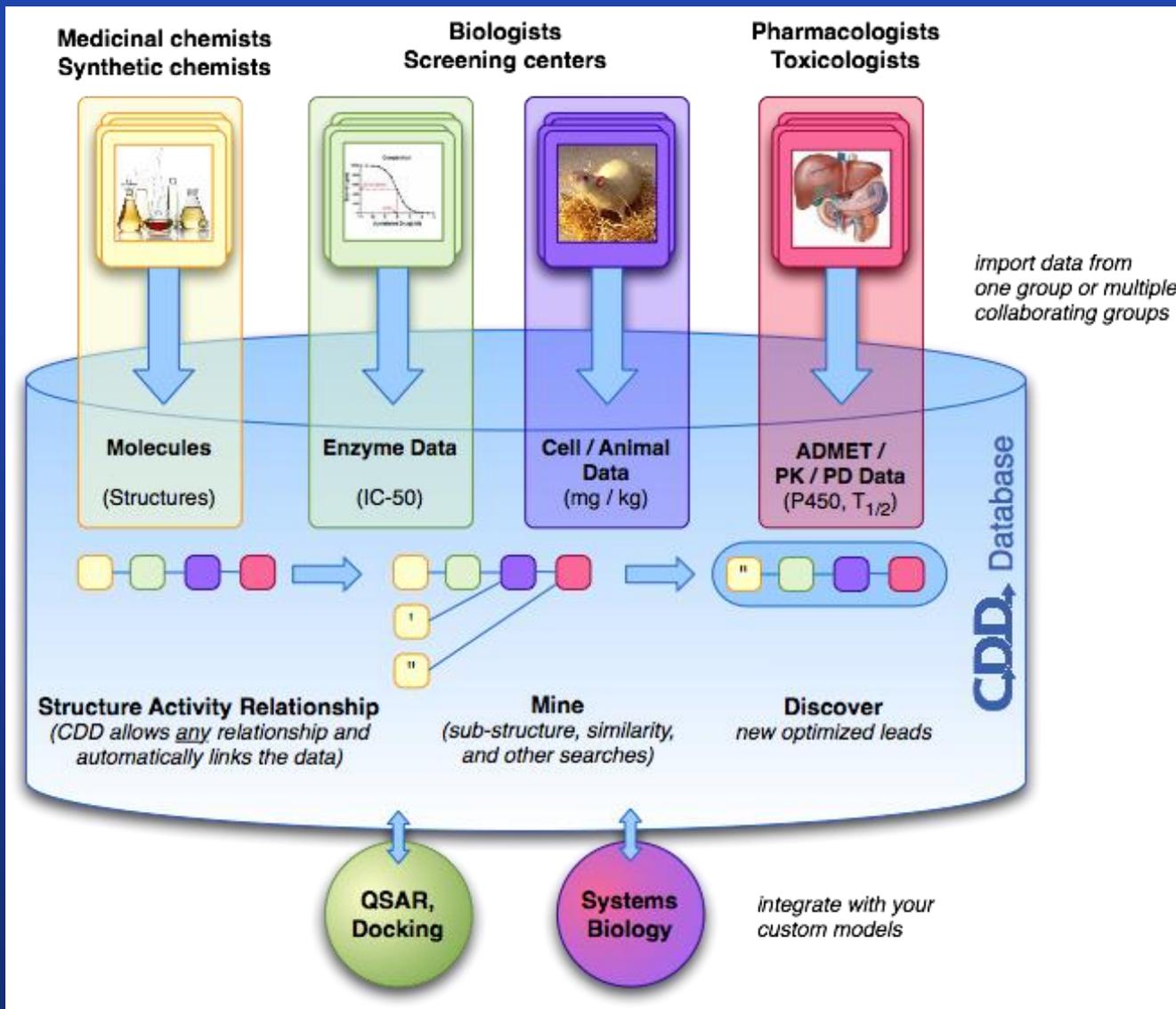
(select property) Min: Max:

Keywords ⓘ Any field

Example: mol1 OR synonym2 AND NOT userfield3

Save this search...

Search Molecules



search -

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Reload Print Mail New Tab Close

Address <http://www.collaborativedrug.com/cdd/page/search.jsp#resultAnchor> Go Links >>

Google wsgsr Search 14 blocked Check AutoLink AutoFill Options wsgsr

CN(C)CC(=O)Cc1ccccc1

Search Molecules

Display Option:
Number of search results per page

Clear Result Export to Excel Export to SDFFile Save Query as: >>

Results: 1 molecules containing C[C@H](CCc1ccccc1)NC(=O)CCc2ccccc2
having T. cruzi: In vitro assay run with readout Days Survival > 5 (days)
and having Cruzain (rec) IC50 (uM) run with any readouts

table rosetta show structures

Molecule	Structure	Cruzain (rec) IC50 (uM) DU4-71 (%)	Cruzain (rec) IC50 (uM) IC50 (nM)	Cruzain (rec) IC50 (uM) IC50 (uM)	Cruzain (rec) IC50 (uM) Ki (uM)	Cruzain (rec) IC50 (uM) kobs/I (see excel) (M)	T. cruzi: In vitro assay Days Survival (days)
K11002				0.01			8.0--25.0

Internet

17 structures · Show 100 ▾

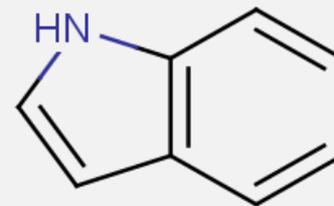
Change display options Plot results Export results Add results to project

File format: XLS - Excel
 CSV - Comma-Separated Values
 SDF - Structure-Data File

Export or cancel

Structures ⓘ

substructure similarity ≥ 70% ▾



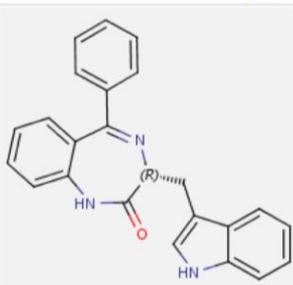
Select... all · none

Molecule ↑

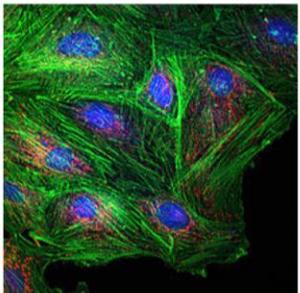
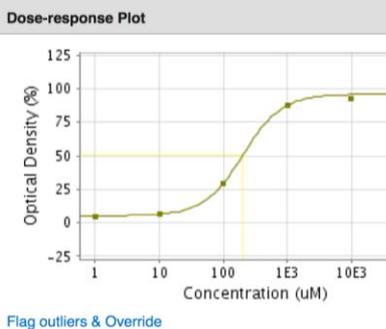
flag outliers

CCK-A Dose Response Curve

IC50 (uM) 201.42 Image



9 from table 1 (Merck Compound)
Barry Bunin's Vault
SMILES

	1	2	3	4	5	6	7	8	9	10	11	12
A	30.0 z: -0.078	8.9 z: -0.744	23.0 z: -0.299	4.0 z: -0.899	0.2 z: -1.019	78.0 z: 1.438	50.0 z: 0.554	37.0 z: 0.143	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
B	81.0 z: 1.533	65.0 z: 1.027	58.0 z: 0.806	89.0 z: 1.785	79.0 z: 1.469	81.0 z: 1.533	83.0 z: 1.596	67.0 z: 1.091	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
C	53.0 z: 0.649	4.0 z: -0.899	5.4 z: -0.854	8.0 z: -0.772	1.0 z: -0.993	6.0 z: -0.835	7.0 z: -0.804	1.2 z: -0.987	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
D	10.0 z: -0.709	4.0 z: -0.899	2.7 z: -0.940	0.61 z: -1.006	4.3 z: -0.889	6.7 z: -0.813	2.1 z: -0.959	1.9 z: -0.965	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
E	34.0 z: 0.049	20.0 z: -0.393	6.0 z: -0.835	11.0 z: -0.678	0.12 z: -1.021	8.2 z: -0.766	60.0 z: 0.870	2.2 z: -0.955	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
F	94.0 z: 1.943	84.0 z: 1.627	77.0 z: 1.406	61.0 z: 0.901	59.0 z: 0.838	71.0 z: 1.217	91.0 z: 1.848	68.0 z: 1.122	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
G	24.0 z: -0.267	58.0 z: 0.806	11.0 z: -0.678	67.0 z: 1.091	29.0 z: -0.109	44.0 z: 0.364	66.0 z: 1.059	37.0 z: 0.143	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025
H	2.2 z: -0.955	5.8 z: -0.842	1.4 z: -0.981	8.9 z: -0.744	3.6 z: -0.911	4.2 z: -0.892	9.3 z: -0.731	7.5 z: -0.788	100.0 z: 2.133	98.0 z: 2.069	0.01 z: -1.025	0.01 z: -1.025

Z'-factor: 0.969 (controls)
Z'-factor: -1.928
Legend
 Positive control
 Negative control

Protocols ⓘ

CCK-A ▾

→ with run (any run) ▾

→ with readout definition IC50 (uM) < ▾ 10 uM

→ and show all ▾

- CDD Vault – Successful Software as a Service
 - Chemical Registration & SAR for budget sensitive labs
 - Unique Collaborative Features (*Differentiation*)
 - Secure, Scalable, Proven (>212,785 logins)
- While being true to the initial vision
 - External data (public + client) securely integrated with private data
 - Economics of integrated specialization in Internet for drug discovery
- *...and Maintaining a Simple Design Aesthetic: “CDD Vault gives us the ability to see the data as it’s put into the database with very little training. So it’s easy and intuitive to do.”*
- *- Jim Wikel*



COLLABORATIVE
DRUG
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CDD Vault: Exciting Future Directions

CDD Vision

A powerful calculation and graphing extension to the CDD Vault

CDD Vision provides the ability to automatically process data according to custom calculations you define, like:

- Compound selectivity
- Ligand efficiency
- Binding Efficiency Index
- Inventory (automatically debit amount remaining)
- Averaging of values, like IC50, across runs

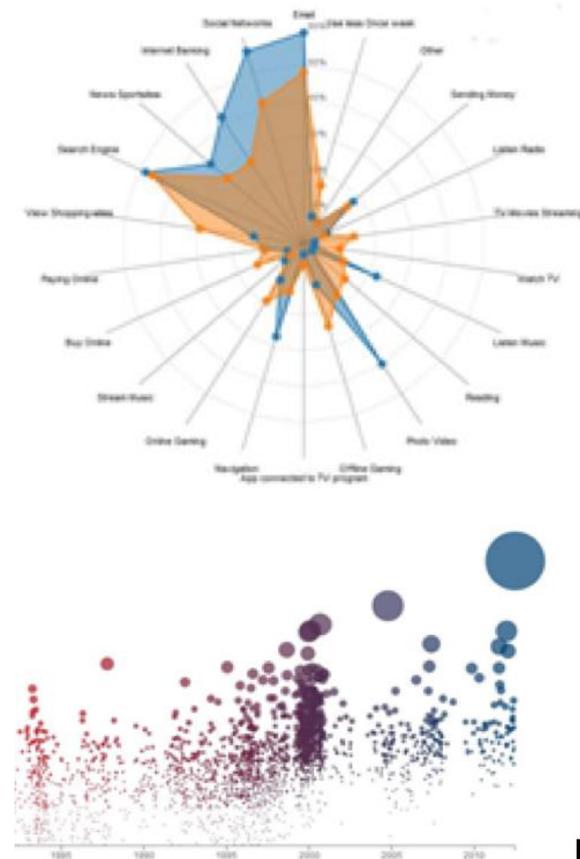
Name:

Data Type: Display Format:

Unit:
Example: nM, kg, rfu

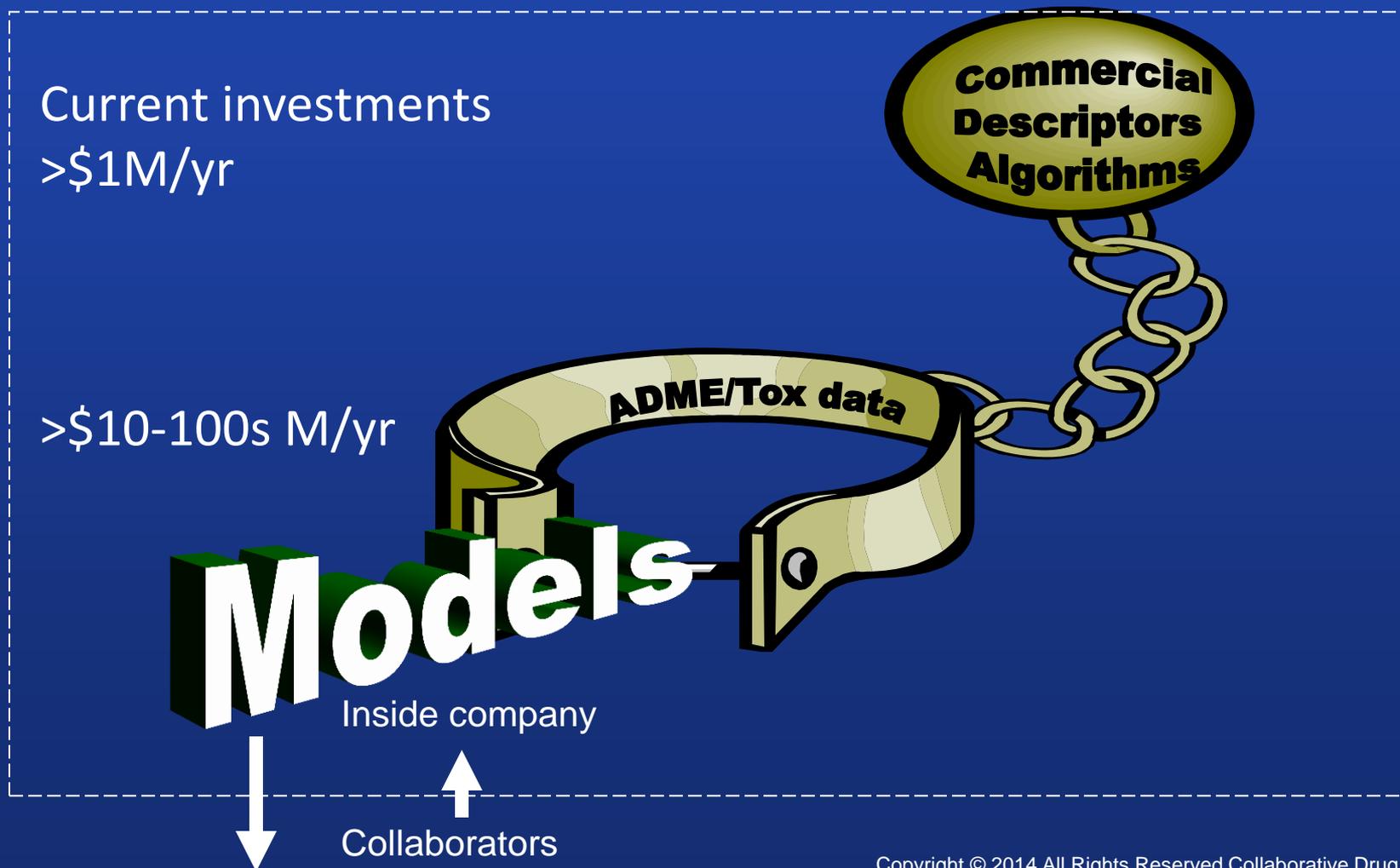
Formula =

or



CDD Open Source Descriptors & Models: Extensions on Secure CDD Vault Collaborations

1. Spend < 20% on descriptors and algorithms (Free with CDD Vault)
2. Selectively share your models with collaborators and control access
3. Have someone else host the models / predictions



80 Selected: Plot Export

Build a QSAR Model

Use all molecules from:

Active molecules: **Your 80 selected results**

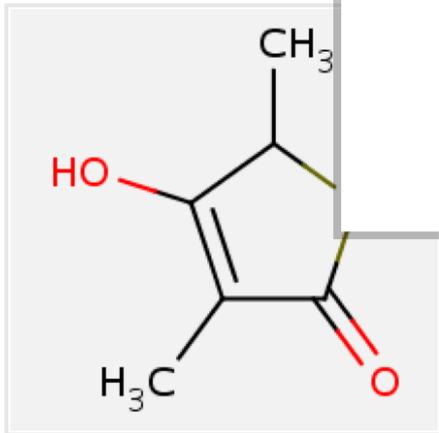
Name:

Project:

or



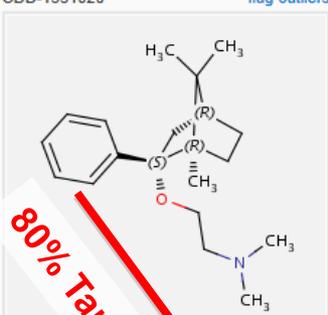
CDD-341021



CDD-341021
Collaborative Drug Discovery, Inc.
CXSMILES (CDD Compatible)

Plate Fields		Dose Response
Name	Well	MIC99 (nM)
Screen-05	B07	< 1.00
Screen-05	B08	
Screen-05	B09	
Screen-05	B10	
Screen-05	B11	
Screen-05	B12	
Screen-05	B07	< 1.00
Screen-05	B08	
Screen-05	B09	
Screen-05	B10	
Screen-05	B11	

6 Selected Results: [Plot results](#) [Export results](#) [Add results to collection](#) [Add results to project](#)

Select...	Molecule	Collections	NCATS Known Targets + ChEMBL Predicted Targets	Known Mechanism of action	Original de... indication	commercially available
all - none	CDD-1351020 flag outliers	Malaria predictions Active, seans picks for further followup	<p>GABA transporter 3 (CHEMBL5208) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5208</p> <p>GABA transporter 2 (CHEMBL4889) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4889</p> <p>Betaine transporter (CHEMBL3715) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3715</p> <p>GABA transporter 1 (CHEMBL1903) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1903</p>			
					5-Hydroxytryptamine 2A/2C receptor (5-HT2A/2C) antagonist	yes

80% Tanimoto Search

Original Target

EMBL-EBI [Terms](#) [Use](#) [Privacy](#) [Cookie](#)

Databases Tools Research Training Industry About Us Help Site Index

- ChEMBLdb
- Malaria Data
- ChEMBL-NTD
- Kinase SARfari
- GPCR SARfari
- DrugEBlity
- ChEMBL Group
- Downloads
- Web Services
- FAQ
- ChEMBLdb Statistics
 - DB: ChEMBL_14
 - Targets: 9,003
 - Compound records: 1,384,479
 - Distinct compounds: 1,213,239
 - Activities: 10,129,256
 - Publications: 46,133

EBI > Databases > Small Molecules > ChEMBL Database

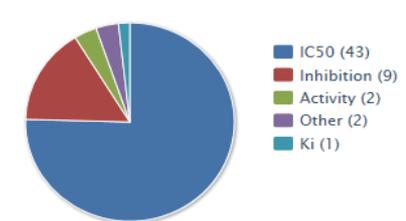
Target Report Card

Target Name and Classification

Target ID	CHEMBL3715
Target Type	PROTEIN
Preferred Name	Betaine transporter
Synonyms	Sodium- and chloride-dependent betaine transporter; BGT-1; Na(+)/Cl(-)-betaine/GABA transporter; Solute carrier family 6 member 12
Organism	Homo sapiens
Protein Target Classification	transporter electrochemical na-sympoter neurotransmitter betaine_gaba

Target Associated Bioactivities

ChEMBL Activity Types for Target CHEMBL3715



ator (CHEMBL250) target/inspect/CHEMBL250			
ator (CHEMBL4127) target/inspect/CHEMBL4127			
	Transient receptor potential cation channel vanilloid 1 (TRPV1) antagonist	Acute and chronic pain	

From:
Southan, C. et al, *Drug Discovery Today*. 2013 Jan; 18(1-2): 58-70.

How to Make the World's Scientific Data as Actionable as Running Excel Spreadsheets?

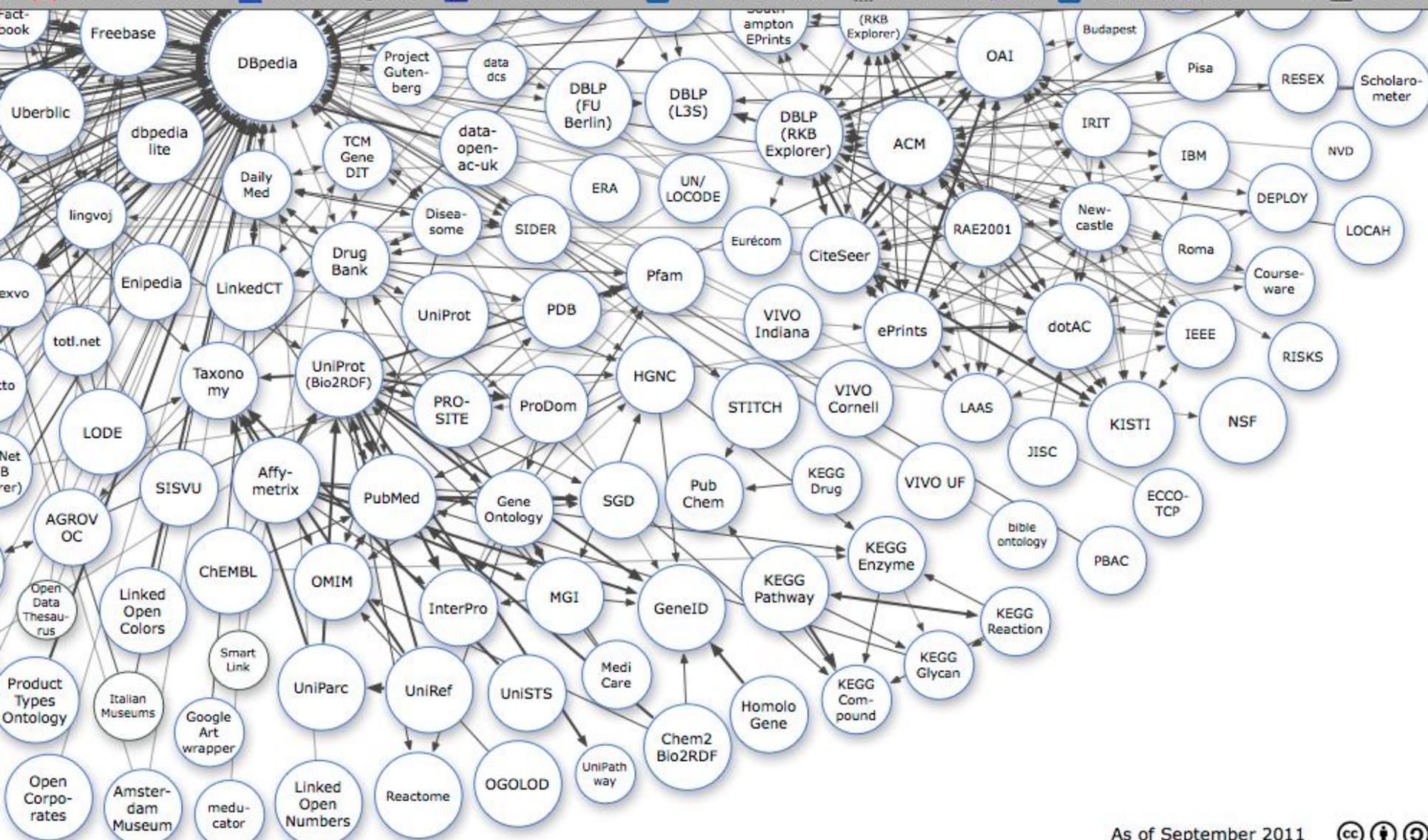
l-09-19/lod-cloud.html



Google



Re: LOI for PAR... Customizing Re... Latest Headlines CDD Public | Col... Innectus Corpor... Collaborative Dr... Bookmarks



File Set Operation Define Share

Operators for Protein

- GO Terms
- Organism
- ChemBL Assays (→ Assay)
- ChemBL Activities (→ Molecule)
- MetaCyc Pathways (→ Pathway)
- Uniprot accession
- Metacyc accession
- KEGG accession

		Molecular weight	
17alpha-Estradiol	CDD-9	272.382	ChemBL Targets
a771726	CDD-10	270.2073	Cyclooxygenase-2 (CHEMBL230)
abacavir	CDD-11	288.3051	Perilipin-5 (CHEMBL1741196)
acarbose	CDD-12	645.6048	
acebutolol	CDD-13	336.4259	
acetaminophen	CDD-14	151.1626	Vascular endothelial growth factor receptor 3 (CHEMBL1955)
acetazolamide	CDD-15	222.245	Maternal embryonic leucine zipper kinase (CHEMBL4578)
acetoexamide	CDD-16	324.395	
			Pyruvate kinase (CHEMBL5149)
			Phosphoglycerate kinase glycosomal (CHEMBL1741167)

datahub
The easy way to get, use and share data

Datasets Groups About Search

/ Datasets / ChEMBL-RDF (@ Uppsala ...

Groups
Linking Open Data Cloud

Social
Google+
Twitter
Facebook

License
Creative Commons Attribution
OPEN DATA

ChEMBL-RDF (@ Uppsala University)
RDF version of the CC-SA-BY ChEMBL database by the team of John Overington at the EBI, Hinxton/UK (<http://www.ebi.ac.uk/chembl/>).

Data and Resources

- SPARQL endpoint**
Uppsala SPARQL end point. [Explore](#)
- Bzip2-ed N3 dump**
No description for this resource. [Explore](#)
- Example target**
No description for this resource. [Explore](#)

DBpedia

Description

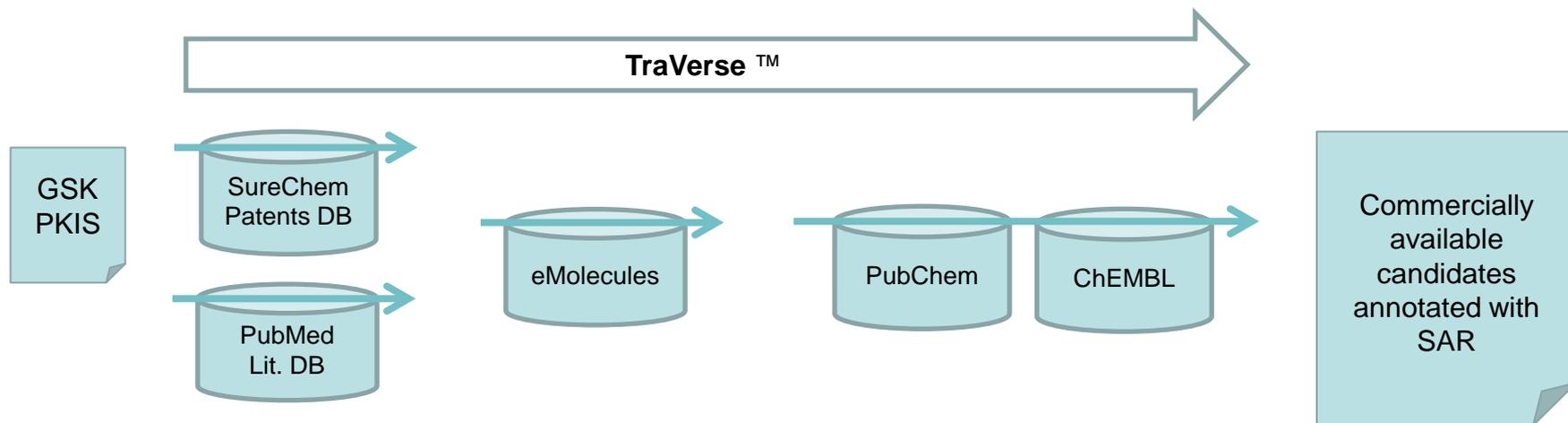
From the front page:

DBpedia.org is a community effort to extract structured information from Wikipedia and to make this information available on the Web. DBpedia allows you to ask sophisticated queries against Wikipedia and to link other datasets on the Web to Wikipedia data.

The DBpedia knowledge base currently describes more than 3.64 million things, out of which 1.83 million are classified in a consistent Ontology, including 416,000 persons, 526,000 places, 106,000 music albums, 60,000 films, 17,500 video games, 169,000 organisations, 183,000 species and 5,400 diseases. The DBpedia data set features labels and abstracts for these 3.64 million things in up to 97 different languages; 2,724,000 links to images and 6,300,000 links to external web pages; 6,200,000 external links into other RDF datasets, 740,000 Wikipedia categories, and 2,900,000 YAGO categories. The DBpedia knowledge base altogether consists of over 1.2 billion pieces of information (RDF triples) out of which 335 million were extracted from the English edition of Wikipedia and 865 million were extracted from other language editions.

Data and Resources

- Download page (N-Triples, bz2-compressed)** 🔥
Download page (N-Triples, bz2-compressed) [Explore](#)
- SPARQL endpoint** 🔥
SPARQL endpoint [Explore](#)



“Look for interesting scaffolds and motifs”



“Reposition for neglected disease indications”

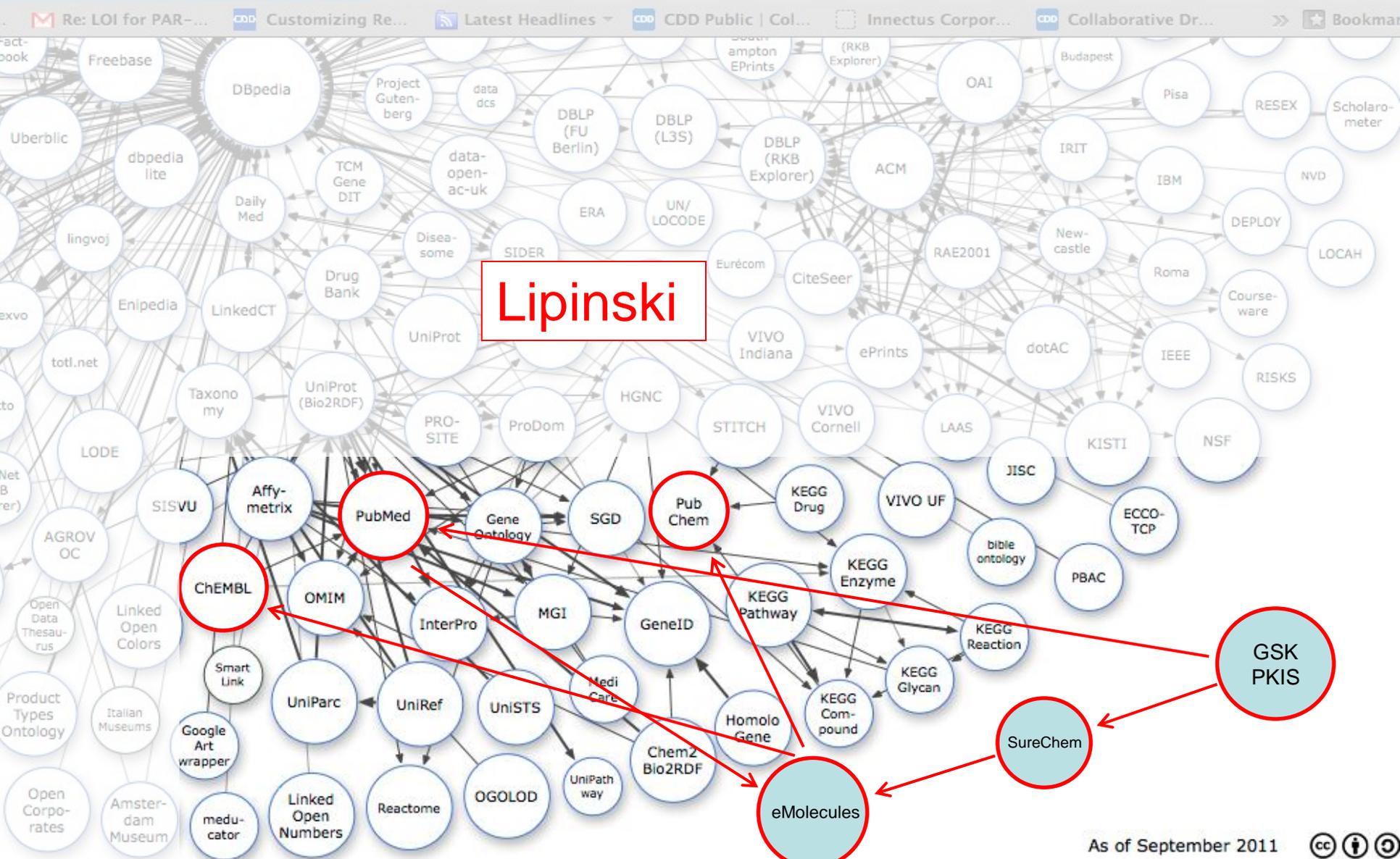


“Inexpensively test better informed hypothesis”

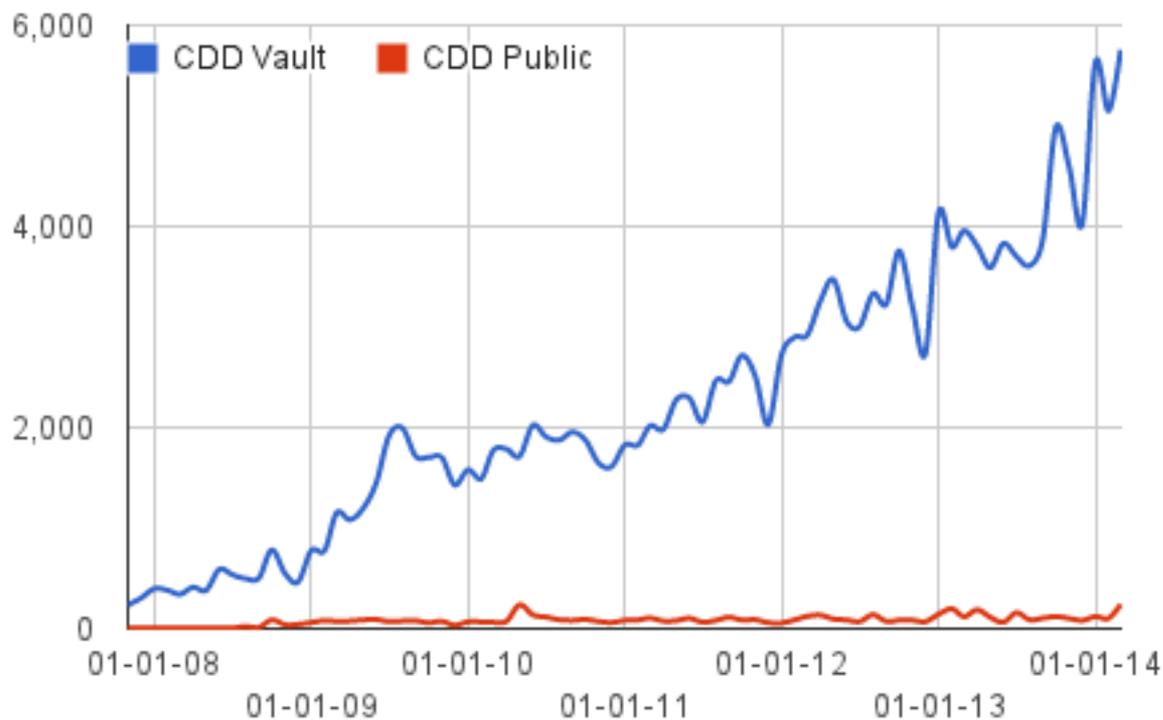


Better Drug Candidates

Dr. Christopher Lipinski
Retired Senior Research Fellow
Pfizer

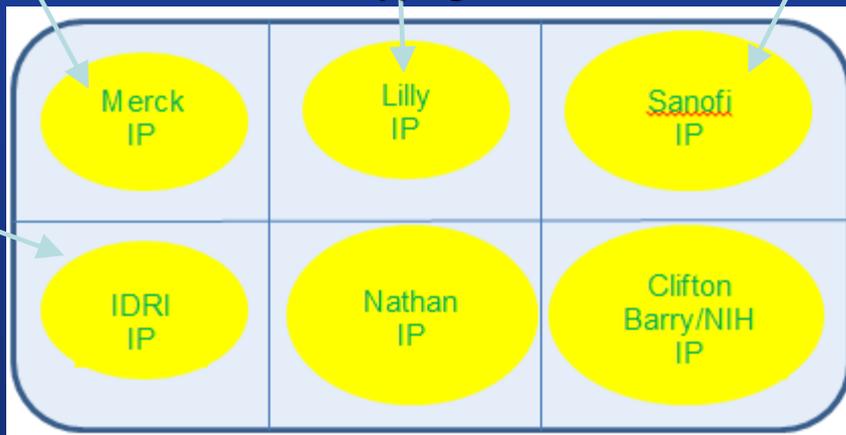


Logins/Month





CDD
ShareSpace



Trusted, Neutral
Facilitator



Collaborative CDD Vault ELN – Future Directions “Content Around Data”

Collaborative Drug Discovery

http://www.collaborativedrug.com

CDD · Collaborative Drug Discovery, Inc. Kellan Gregory: Account · Help · Log out

Dashboard Explore Data Import Data Reports Manage

Back to Protocols

T. cruzi % Inhibition - Assay Optimization Vault: Collaborative Drug Discovery, Inc.

View readouts for this protocol
Export readouts for this protocol
Copy protocol details
Manage access to this protocol
Delete this protocol

Showing data from 1 of 1 project

Owner: Kellan Gregory
Created: October 31,
Updated: April 21, 2009

Run Data Protocol Details Projects 1 Files 1

Create a New Experiment

Experiment ID: KG-1
Author: Kellan Gregory
Date Created: October 30, 2013
Status: Started
Project: Project One
Date: [] Remove Drag
Goal: [] Remove Drag
Design: [] Remove Drag
Results: [] Remove Drag
Conclusions: [] Remove Drag

Add new field Add Date

Create this run or cancel

2 Runs

ELN

Experiment ID	Author	Date Created	Status	Molecules	Plates
KG-1-2	Kellan Gregory	2013-10-30	Witnessed	80	1
KG-1-1	Anna Spektor	2013-10-29	Archived	80	1 Save to PDF

Files can be dragged and dropped into the text box areas, making them more free-form. Database remembers your last set of fields.

Collaborative Drug Discovery

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Dashboard Explore Data Import Data Reports Manage

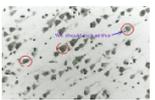
Back to Protocols

October 30, 2013 experiment of T. cruzi % Inhibition Assay Optimization Vault: Collaborative Drug Discovery, Inc.

All Data Experiment Details Files 1

View readouts
View scatter plot
Export readouts
Move experiment to another project
Delete this protocol

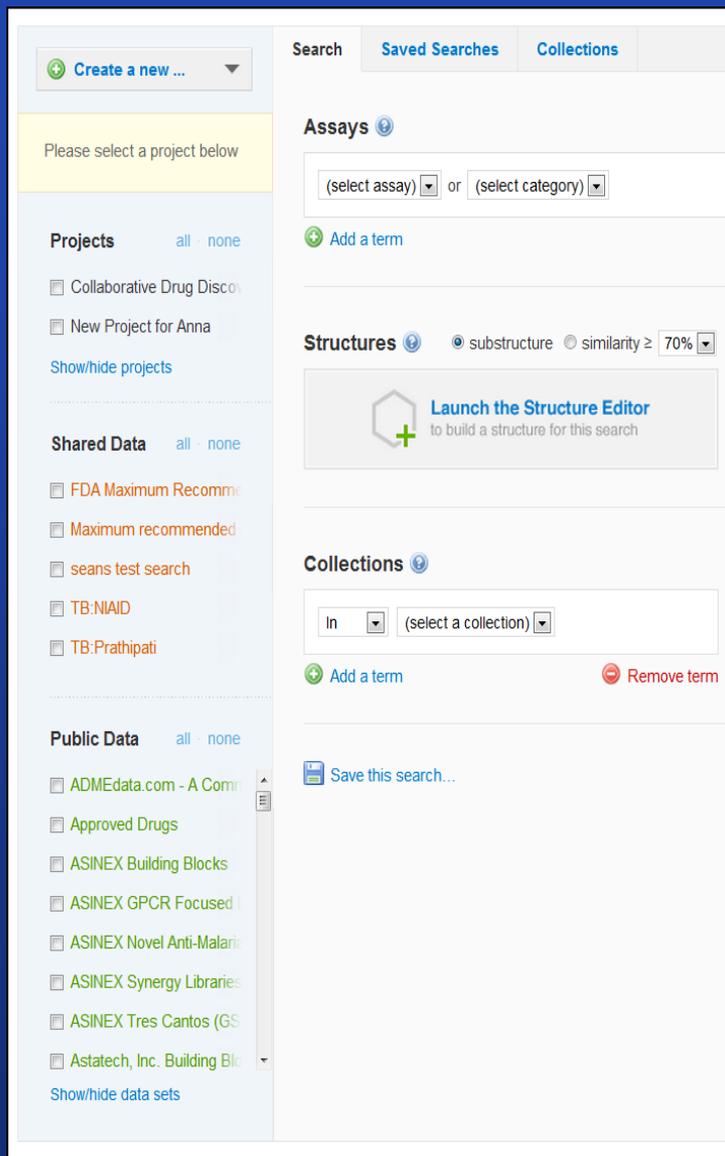
Project: New One
Owner: Kellan Gregory
Created: October 31,
Updated: April 21, 2009

Experiment ID: KG-1
Author: Kellan Gregory
Date Created: October 30, 2013
Status: Started
Date: October 29, 2013
Goal: Learn basic cell culture technique for skeletal muscle... and find a cure for something! Abnormalities in MLC patterns may play a role in the development of muscular dystrophy. I need a cell culture model to study such patterns. I must be able to culture skeletal muscle from chick embryos so that I can manipulate culture conditions and look for changes in the normal pattern of expression. Ajouter quelquechose d'autre...
Design: 1. Obtained 1 doz. fertile 7 day chicken eggs. After wetting the egg shells with ethanol I transferred them to the laminar flow hood, carefully cracked the shells, and aseptically removed embryos to a petri dish with ice-cold Hank's Balanced Salt Solution (HBSS) NOTE: two eggs were sterile. I lost one trying to fish it out of the shell, therefore I started with nine embryos. hoy
2. Aseptically removed heads and discarded. Removed skin from breast by peeling with forceps, and used straight vanna scissors to remove breast "fllets." Pieces were placed in a sterile watch glass with 0.5 ml HBSS
3. Minced tissue with sterile curved scissors into 0.5mm3 bits...
Results:  
Some brief description or maybe something more in depth...
Conclusions: Isolated conclusion from a report on mapping magnetic fields
Background information:
Initial hypothesis: Magnetic field strength will be proportional to the strength of the current running through a straight wire and inversely proportional to the distance from the wire.
The data collected correlated strongly to the hypotheses, albeit with percent errors reaching as high as 20% uncalibrated. (Other sections of this report detailing this information have been removed from this example.)

Control Layouts Positive control (hit) Negative control Reference molecule

Experiment Default 96-well Control Layout
Experiment Default 384-well Control Layout
Experiment Default 1536-well Control Layout

Add a plate-specific control layout



The screenshot shows the CDD web interface with the following sections:

- Search:** Includes tabs for "Search", "Saved Searches", and "Collections".
- Assays:** Features a search box with "(select assay)" and "(select category)" dropdowns, an "Add a term" button, and a "Launch the Structure Editor" button with the text "to build a structure for this search".
- Structures:** Includes radio buttons for "substructure" and "similarity ≥ 70%", and a "Launch the Structure Editor" button.
- Collections:** Features a search box with "In" and "(select a collection)" dropdowns, "Add a term" and "Remove term" buttons, and a "Save this search..." button.
- Left Sidebar:** Contains sections for "Projects" (with "all" and "none" filters), "Shared Data" (with "all" and "none" filters), and "Public Data" (with "all" and "none" filters). Each section lists various data sources with checkboxes.

- **Projects 4: See data from other Vaults**
 - Visible in the sidebar, organized by Vault.
 - Read-only.
 - No new data can be directly deposited.
 - Users must switch Vaults and have proper access rights to deposit data for molecules (idea that data must be associated to the library owner's Vault).
 - <= See CDD Vault Sidebar for clarification



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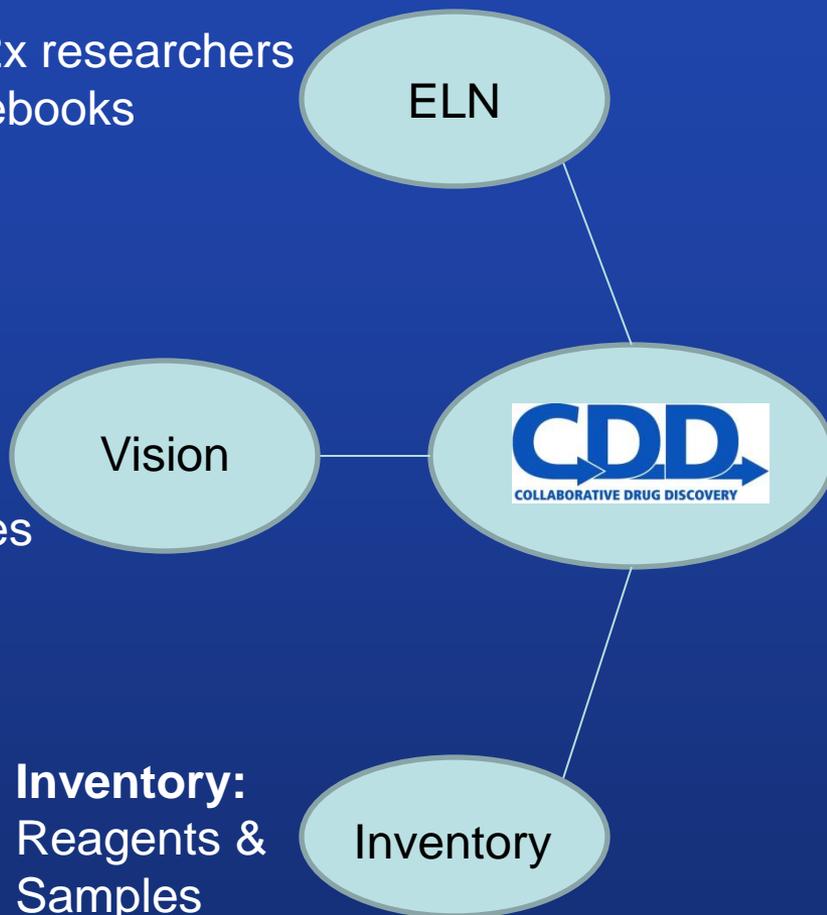
CDD Vault – Full Solution Roadmap for the Collaborative Drug Discovery Workspace

CDD Public + Collaborative Vault:
Maintain Public Good +
Efforts to Advance our
Field

Note: Beyond What
the Market Naturally
Supports

CDD Vision: Powerful
Calculations &
Visualization Capabilities

ELN: ~2x researchers
use notebooks



Inventory:
Reagents &
Samples

Engaging the user community to guide CDD Vault development:

- Amgen – Henry Johnson
- Carmot Therapeutics – Dan Erlanson
- Genentech – Jeff Blaney
- Reset Therapeutics – Paul Humphries
- Tetra Discovery – Mark Gurney

Complements existing SAB w/ expert industry CDD Vault evangelists

➤ Who else would be great?

COMMUNITY

Users

Testimonials >

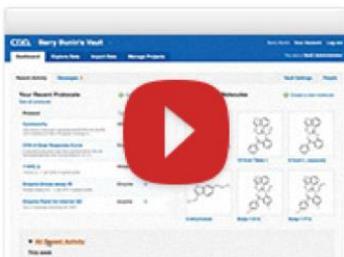
Case Studies

Spotlight Interviews

Partners

Public Access

START YOUR FREE TRIAL



Click here to watch a 3 minute

CDD Vault User Testimonials



"CDD Vault gives us the ability to see the data as it's put into the database with very little training. So it's easy and intuitive to do."

JIM WIKEL

Apex Therapeutics
CDD Scientific Advisory Board



"CDD easily allows us to securely collaborate, while keeping some data private, all in one system."

ELLEN BERG, PHD

Asterand



"CDD Vault is a lifesaver. We really needed a way to capture the data we were creating and be able share and analyze it — before we were capturing data on spreadsheets."

MALCOLM KENDALL

President & CEO, Indel Therapeutics, Inc.

KELLAN GREGORY

Director of Product Management

Kellan Gregory is CDD's Director of Operations. He has a degree in Chemical Engineering with an emphasis in biotechnology from Tufts University. Kellan was co-author in an HIV study with Dr. Paul A. Volberding, and interned with BioRad and Libraria. He has not written two books and founded two companies like Barry Bunin, PhD. Unlike Sylvia Ernst, PhD, he did not help with commercial introductions of both Beilstein and Pipeline Pilot. And he's at least 99 articles and 3 books behind Sean Ekins, Ph.D. who has experience working with two big Pharmas. But you know what? If you want a product expert with the most experience using data and databases, the strongest people skills and the ability to tell you straight up what will and will not work, Kellan Gregory – with his growing team of specialists in the community interests group – is your best collaborator. Kellan also creates practical specifications for our product enhancements by prioritizing thousands of requests from hundreds of CDD customers.

**KRISHNA DOLE**

Head of Scientific Informatics

Krishna Dole has a decade of experience creating collaborative scientific software. He has developed software for drug discovery, population biology, geomorphology and phylogenetics. Prior to joining CDD in 2007, he coauthored mx, an open source biodiversity informatics application that remains under active use and development. On the software side, he has been working with the Ruby on Rails framework for over 6 years, and has published a plugin and submitted bugfixes to Rails itself. Like all of CDD's software developers he is an enthusiastic user of automated testing, the agile process, and behavior driven development. At CDD he draws on his broad experience to guide the design and implementation of scientific features. Krishna has a double BA in Biology and Earth Sciences/Environmental Studies from UC Santa Cruz.



DAVID BLONDEAU

Head of Software Development and Security Officer

David Blondeau is the Head of Software Development and Security Officer at Collaborative Drug Discovery, Inc. A strong proponent of software engineering best practices, David leads the development of CDD with a passion for pragmatic innovation, usability, security, and performance. David has more than 10 years experience building and delivering mission-critical software applications. He started his career at Intalio Inc., where he led the development of an enterprise-class business process management (BPM) application server that, among many other things, has been deployed to track the health of every farm animal in Netherlands since 2005. He then went on to architect another BPM solution for Siebel Systems before branching into web application development. When not enhancing CDD's platform, David runs long distances and has completed several marathons. This actually gives him plenty of time to think about CDD. David received his M.S. in Computer Science and Mathematics from ENSEEIHT in Toulouse, France.

**ANNA COULON SPEKTOR**

Customer Success Manager

Anna Coulon Spektor is CDD's Customer Success Manager. Anna has extensive experience managing client relationships for top 10 pharma companies, helping to organize and analyze their data efficiently and effectively. Anna also coordinates CDD training, and creates customized data strategies and solutions. Anna began her career as a chem- and bio-informatics consultant and has experience of other software such as IDBS' ActivityBase. Not only is she proficient in database software and solutions in the pharma sector, she understands the world of academia, having obtained a Master of Science in Biomedical Engineering, and a degree in Molecular Biology from the University of Chicago, and having spent 10 years as an academic researcher.



CDD Vault®

Finally, a modern approach to drug research informatics

CDD Vault is a hosted biological and chemical database that securely manages your private and external data. Accomplish more with an intuitive solution designed by scientists.



A SYSTEM YOUR ENTIRE TEAM CAN ACTUALLY USE

- ✓ Intuitive web interface
- ✓ Economical cloud deployment
- ✓ Biologists and chemists interacting

[Benefits over legacy platforms >](#)



BEATS JUGGLING SPREADSHEETS OF SCREENING DATA

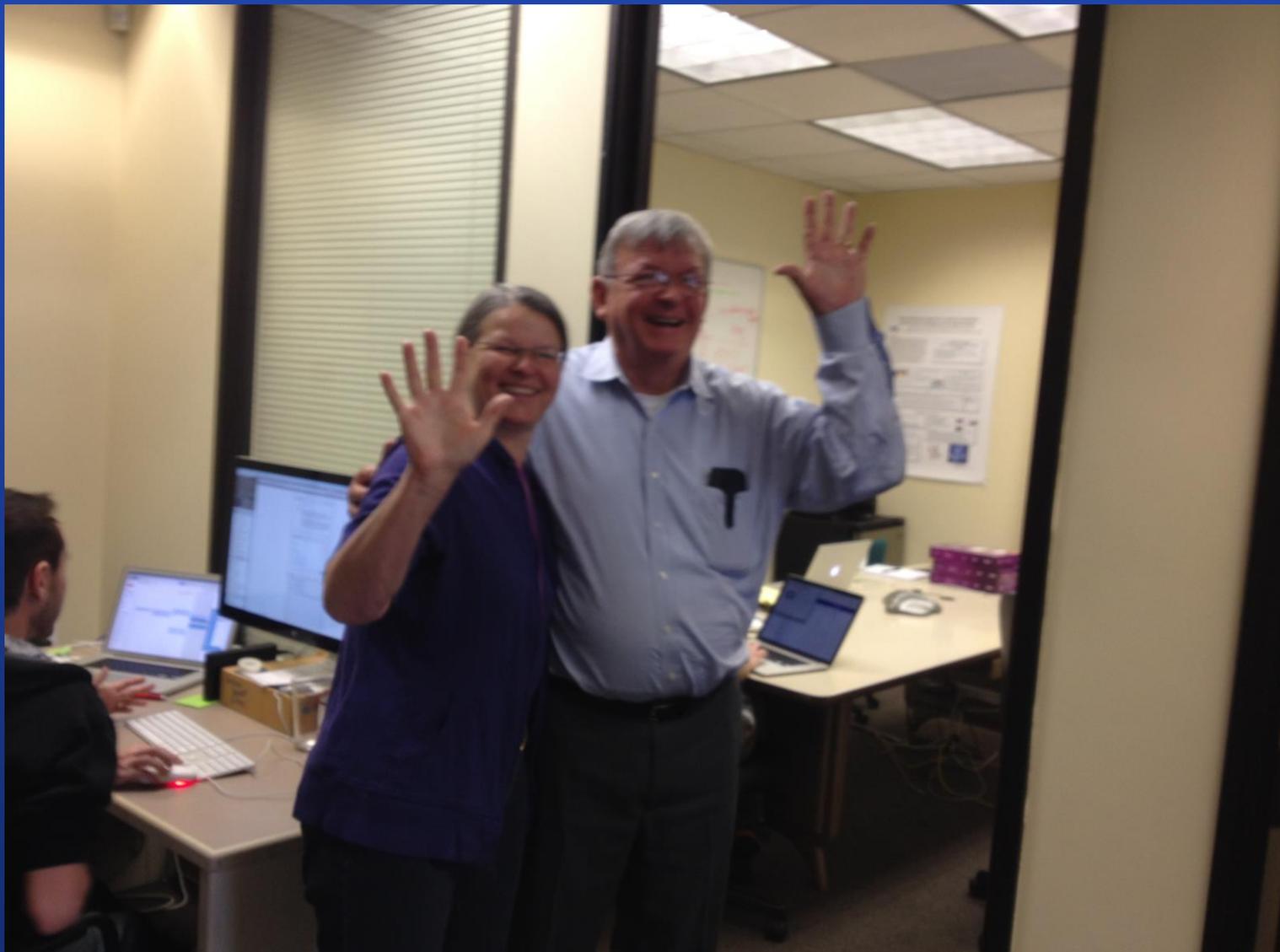
- ✓ Eliminates the risk of data loss
- ✓ Unified data yields better results
- ✓ Easier to find, analyze, and share data

[Benefits for new projects >](#)



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CDD "Rule of 10"



GSK and Online Communities Create Unique Alliance to Stimulate Open Source Drug Discovery for Malaria

- GSK becomes first company to freely share chemical structures on 13,500 molecules from its compound library
- Alliances formed with leading scientific research communities from private industry and public-domain data provider

May 19, 2010/Burlingame, CA/ GlaxoSmithKline (GSK) had teamed up with leading public-domain data providers European Bioinformatics Institute (EMBL-EBI), the U.S. [National Library of Medicine \(NLM\)](#) and the US-based informatics service provider Collaborative Drug Discovery (CDD) to make freely available key scientific information on more than 13,500 compounds that could ultimately lead to new treatments for malaria.

The release of this data marks the first time that a pharmaceutical company has made available the structures of so many compounds and is made possible through the collaboration of the web hosts and their





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2 Big Pharmas with 25 Organizations in Single, Secure MM4TB-CDD Vault®



EPFL	AstraZeneca India Private Limited	Uppsala University	University of Pavia	University of Cambridge
Queen Mary University of London	Institut Pasteur	Bach Institute of Biochemistry (RAS)	University of Padova	Comenius University
Vichem Chemie	John Innes Centre	Indian Institute of Science	Cellworks Research India Private Limited	University of Piemonte Orientale
Collaborative Drug Discovery (CCD)	University of the Basque Country	Tydock Pharma Srl	Universidad de Zaragoza	ETHZ
Alere Tech. GmbH	Sanofi Aventis R&D	University of Cape Town	SCIPROM	Institut Pasteur de Lille (INSERM)



COLLABORATIVE
DRUG
DISCOVERY

Commercial Collaboration Case Study: Cash Conscientious Harvard Spinout

CDD Vault Case Studies

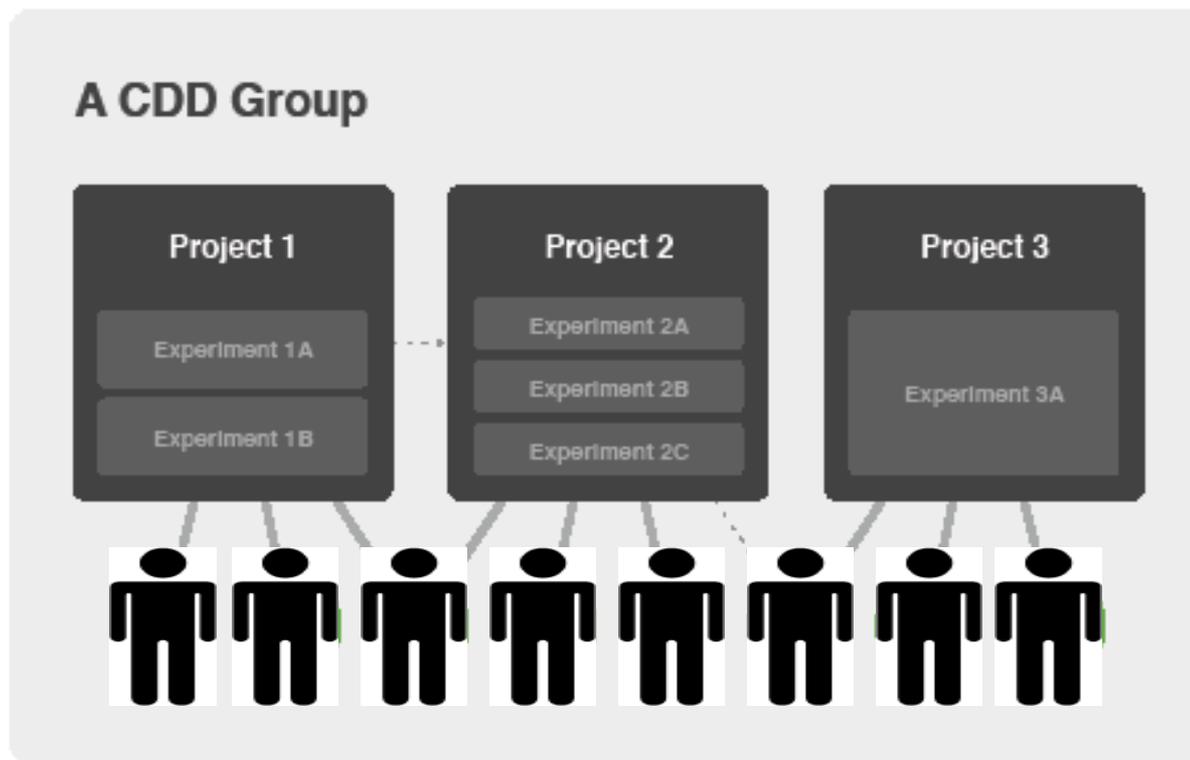
Acetylon Pharmaceuticals

This Harvard spinout company uses CDD Vault to manage both academic-industry and China CRO collaborations. After becoming a customer in 2009, they have grown to a dozen CDD Vault users presently, all while filing for an IND for their HDAC inhibitor and raising \$27M in a Series-B financing in the meantime.



Acetylon Pharmaceuticals and Celgene Corporation Announce an Exclusive Strategic Collaboration to Advance the Science of Epigenetics

Strategic Collaboration Includes Option for Celgene to Acquire Acetylon



Projects provide subdivisions of data and data privacy

- 2013: CDD Vault securely hosted >9 years – with 99.98% up-time
- 2013: CDD surpassed >100,000 logins
- 2012: CDD FISMA compliant and accredited
- 2012: NIH picked CDD Vault for Neuroscience Blueprint Network
- 2012: CDD securely hosted >160,000,000 datapoints
- 2011: CDD won Bio-IT World Editors' Choice Best Practices Award
- 2011: MM4TB 5 year EU funded project with AstraZeneca, Sanofi-Aventis
- 2010: GSK, Novartis, Pfizer, and NIH Collaborations announced
- 2009: CDD Vault surpasses >1 Million Compounds
- 2008: Gates Foundation 2 year grant (extended to 5 years)
- 2005: Eli Lilly co-invested in a syndicate with Omidyar Network and Founders Fund
- 2004: CDD spun out of Lilly, UCSF signs up as first customer

➤ *Quo Vadis: “Whither goest thou”*



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Behind Firewall

Both hosted and behind firewall options

Experiment Data

Assay Details

Projects 1

Files 0

Assay Definition

 [Edit assay definition](#)

Name: ABL Kinase Private Data QSAR Model

Category: QSAR Model

Description:

Parameters

Name	Data Type	Unit	Description
Score	Number		The relative score (higher is better)
Applicability	Number		The applicability of the model based on feature similarity.