COLLABORATIVE DRUG DISCOVERY

"10 Years of Collaborative Drug Discovery in the Cloud"

The CDD Vault®

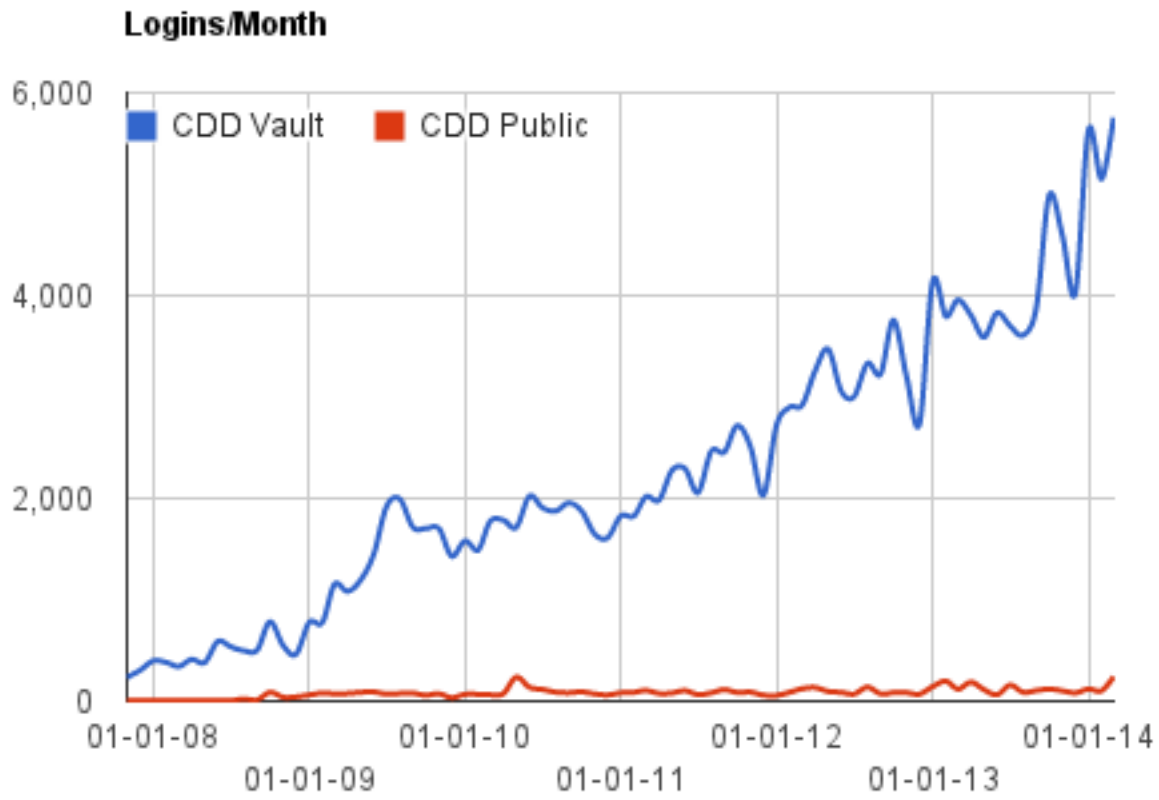
Finally…a Modern Approach to Drug Research Informatics

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!



Year 10: CDD Vault® Metrics

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

CDD First Spotlights

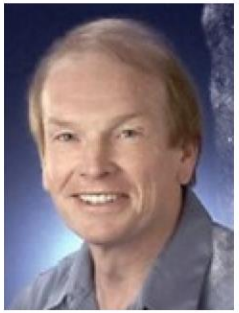
Dr. Ellen Berg, Asterand

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.

More CDD Recent Spotlights From:
https://www.collaborativedrug.com/spotlight-interviews/

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 Mockup: CDD Vault Predecessor

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	*Includes following Sub-Libraries:* • 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

Year 1: CDD Spun Out of Eli Lilly, UCSF Signs Up As First Customer

Protocol: cruzain edit

Description: Lorem ipsum dolor sit amet, consectetuer 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 ▲	Lab	#Compounds	#Hits	Delete Run
2004-04-19 00:00:00	mckerrow	11	9	

Year 3: Birth of CDD Vault V1.0

Molecule K11777.HCl:

Definition:

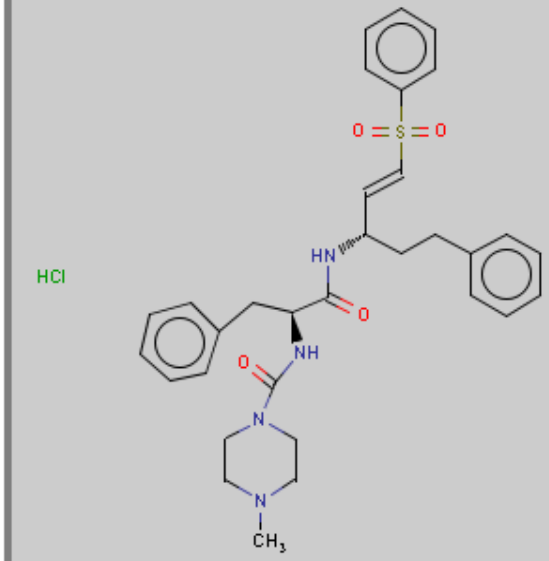
Name: K11777.HCl

Synonym: K11777.HCl

Description: Roush made hcl versionof K11777 8.2005

SMILES: Cl.CN1CCN(CC1)C(=O)N[C@@H](Cc2ccccc2)C(=O)N[C@@H](CCc3ccccc3)\C=C\S(=O)(=O)c4ccccc4

search



Double click image above to see alternate views

Batches: 2

Plates: 0

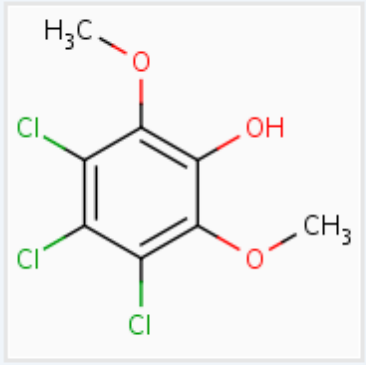
Protocols: 2

Protocol	Run Date	Readout	Value
Cruzain (rec) IC50 (uM)	Sep 12, 2005	IC50 (nM)	3.0
Cruzain (rec) IC50 (uM)	Aug 16, 2005	IC50 (nM)	1.0
T. brucei rhodesiense Rhodesain (rec) IC50 (uM)	Sep 12, 2005	IC50 (nM)	2.5
T. brucei rhodesiense Rhodesain (rec) IC50 (uM)	Aug 16, 2005	IC50 (nM)	1.0

CDD Vault Today: Advanced SAR and Data Mining Tools

CDD · Dose-response plot

View plot | Flag outliers



CDT-0000003

Assay: P. Falciparum IC50 v2

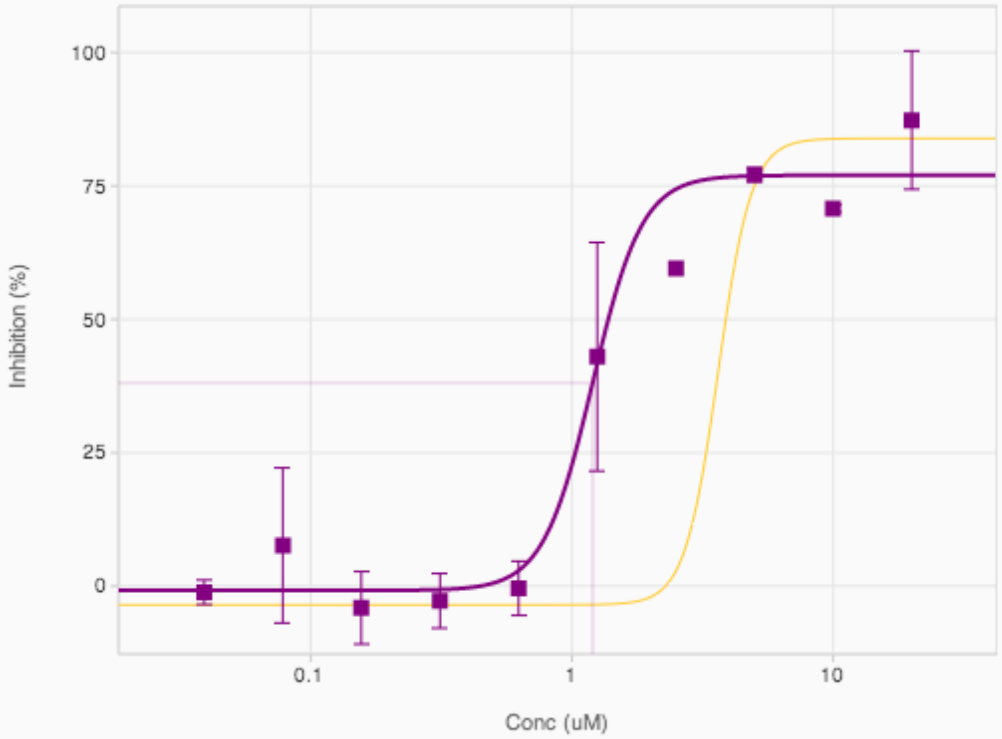
Screen: 2013-05-29
Lot: AA-001

IC_{50} (uM)	1.20
Hill slope	4.58
R^2	0.836
Baseline (%)	-0.813
Maximum (%)	77.0
Curve class	1.20
N = 27	

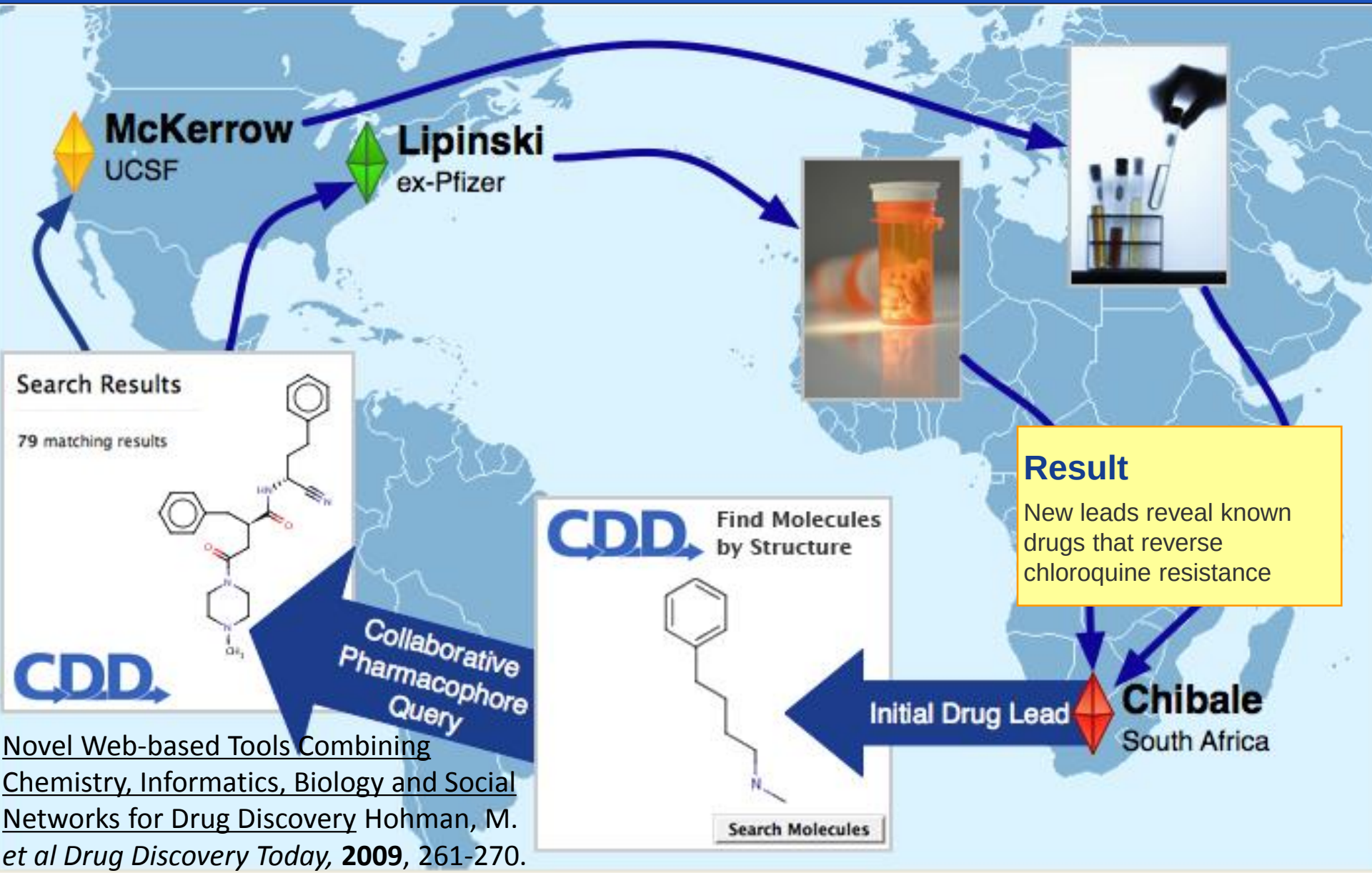
Reference substance:

IC_{50} (uM)	3.63
Hill slope	6.83
R^2	0.943
Baseline (%)	-3.51
Maximum (%)	83.9

Reset Zoom · Save as PDF · Tips

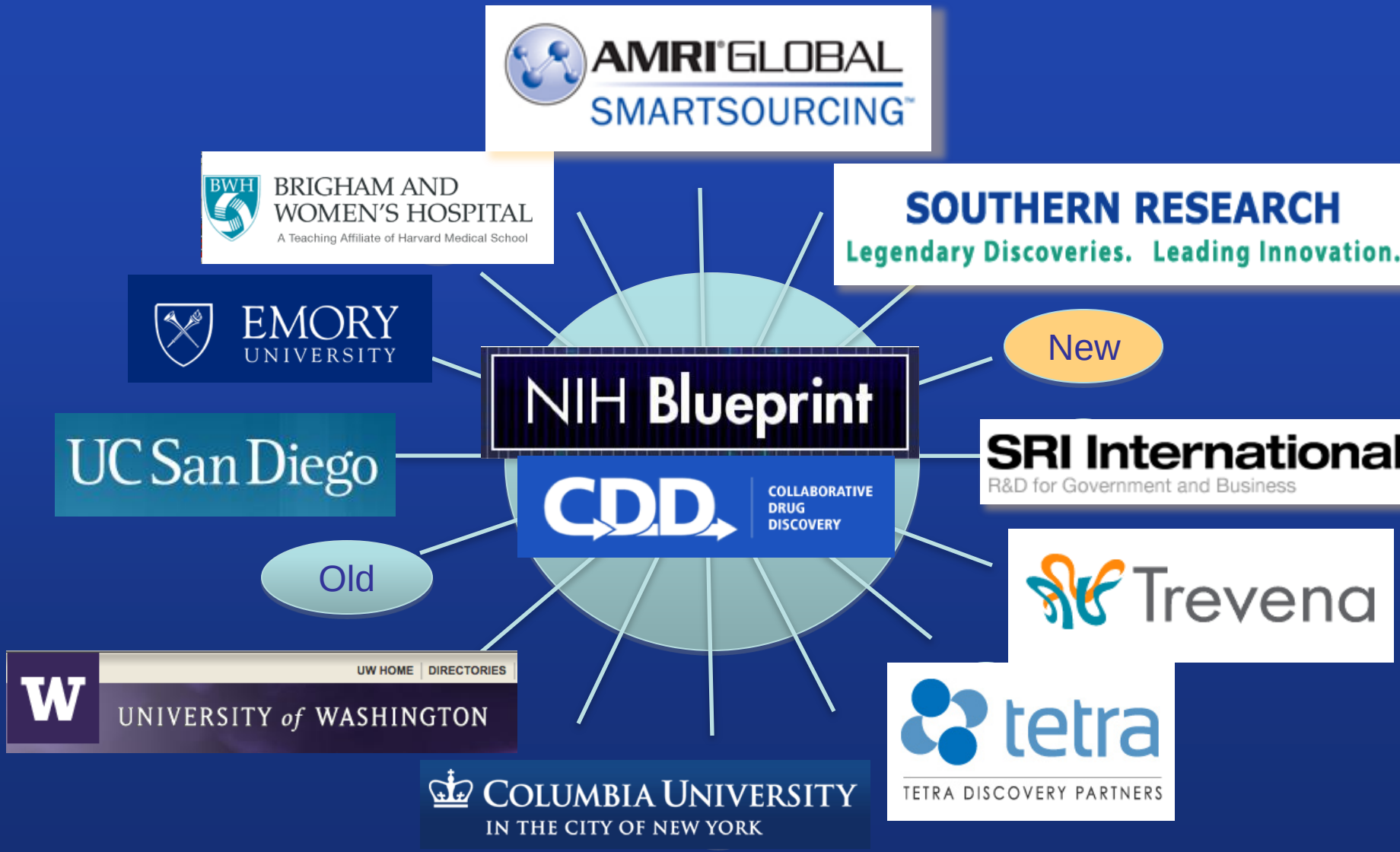


Year 5: Collaborations "Cross the Chasm"

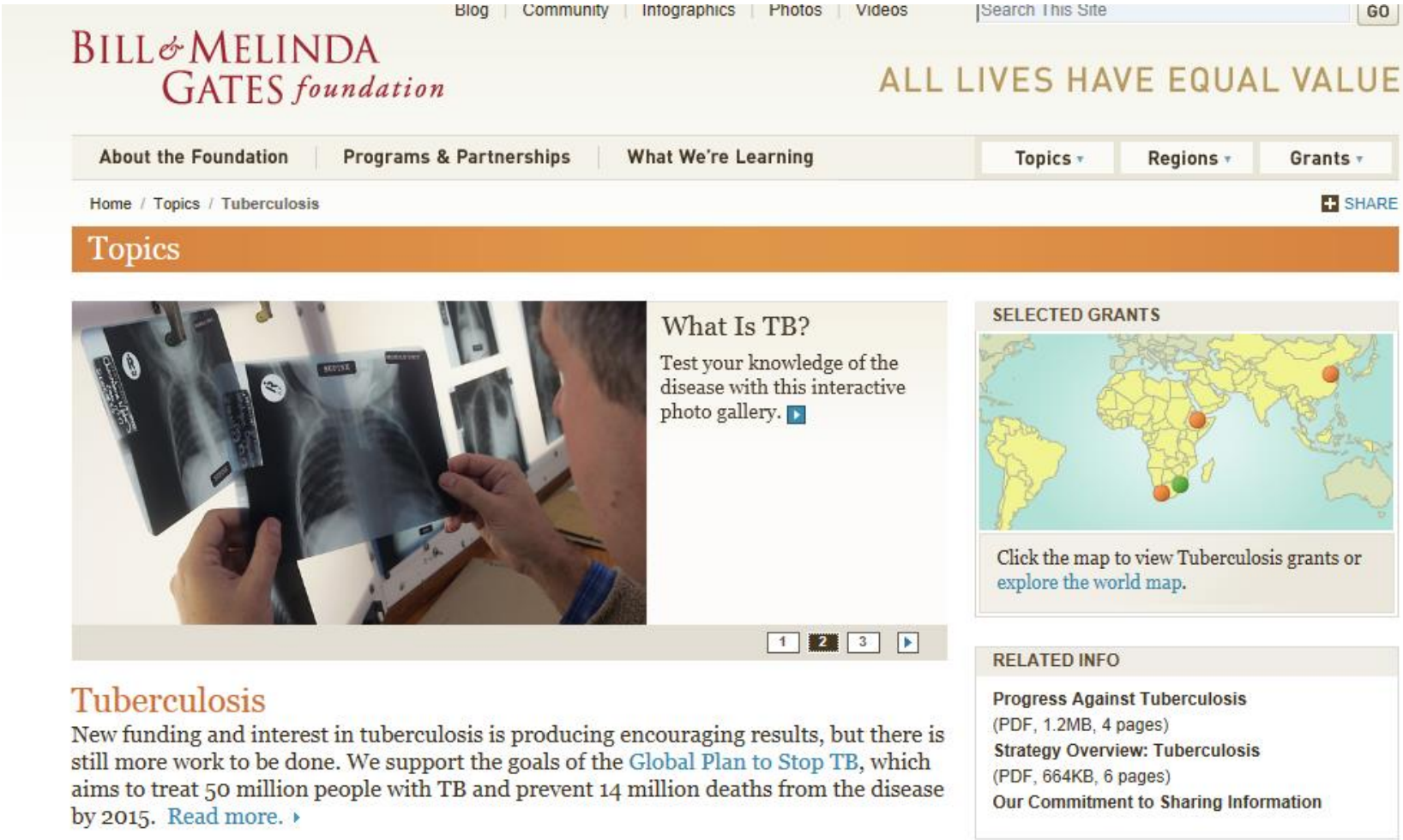


Novel Web-based Tools Combining Chemistry, Informatics, Biology and Social Networks for Drug Discovery Hohman, M. *et al Drug Discovery Today,* **2009**, 261-270.

NIH Blueprint – CDD Partnership
Securely sharing data



Bill & Melinda Gates Foundation (BMGF)
CDD Industry-Academic TB Collaborations



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

Welcome, Jim
McKerrow-CDD Database

Save Query as: >>

Export to Excel | Export to SDFile | Collaborate | E-mail

X **MY DATABASE**

People I'm Sharing with (Data Recipient):

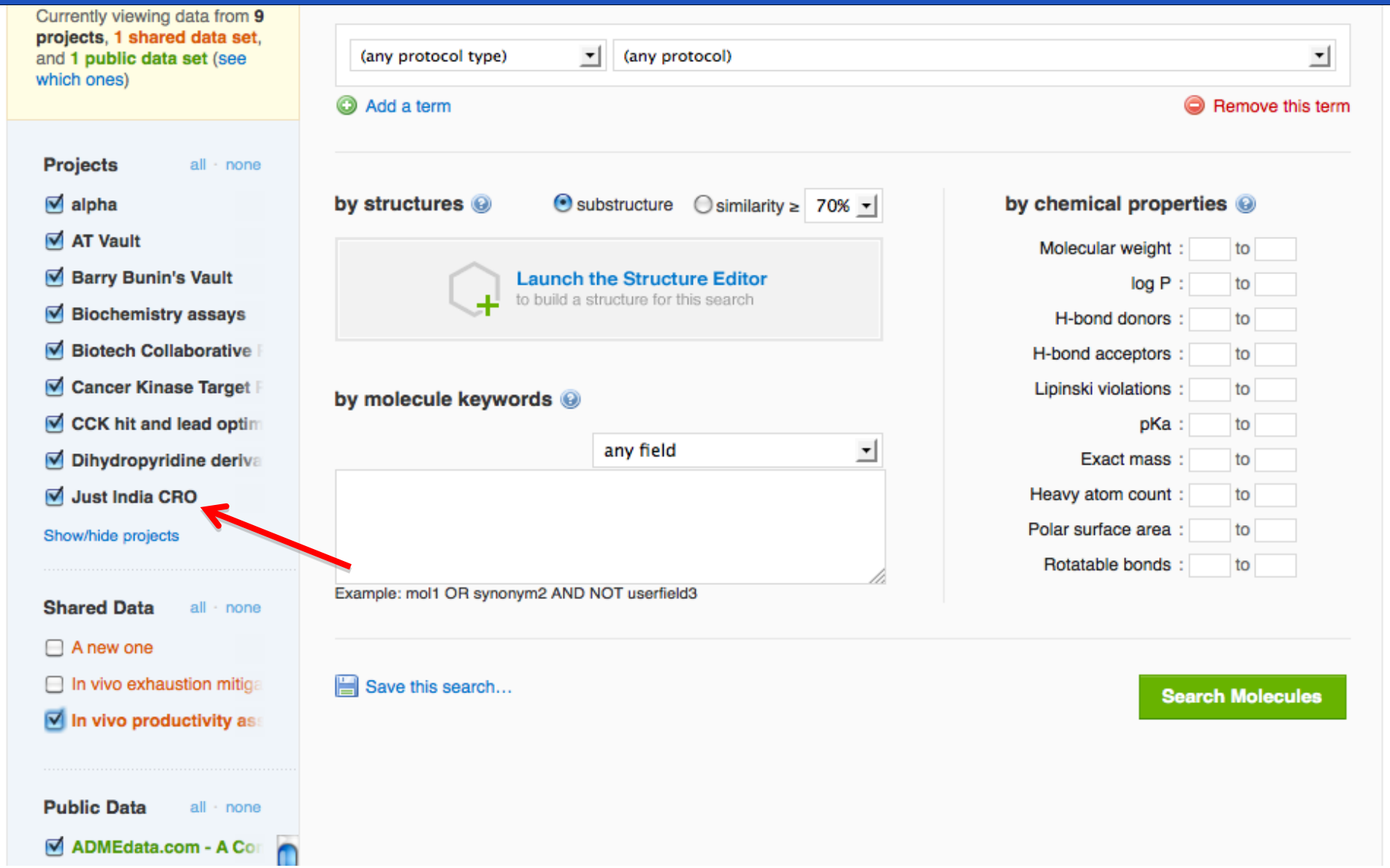
E-mail Identity
aisaksen@appabove.com
bbunin@collaborativedrug.com
mbazargan@collabrx.com

People Sharing with Me (Data Sender):

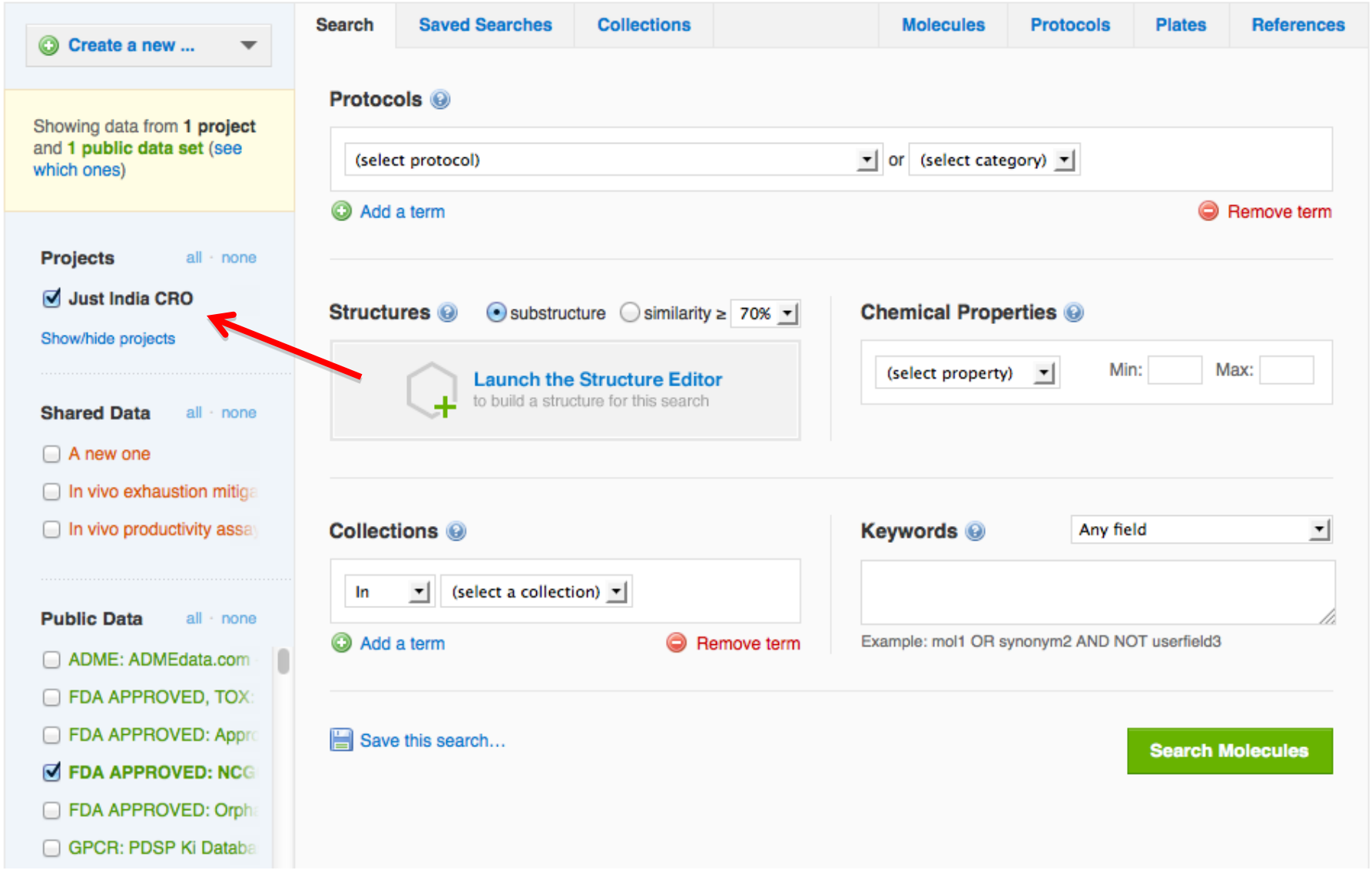
E-mail Identity
lsafty@gmail.com
brett.wong@tufts.edu
kgregory@collaborativedrug.com

Manage your collaboration accounts.

Collaborate: Differentiation
Vault Admin is Privy to All Projects

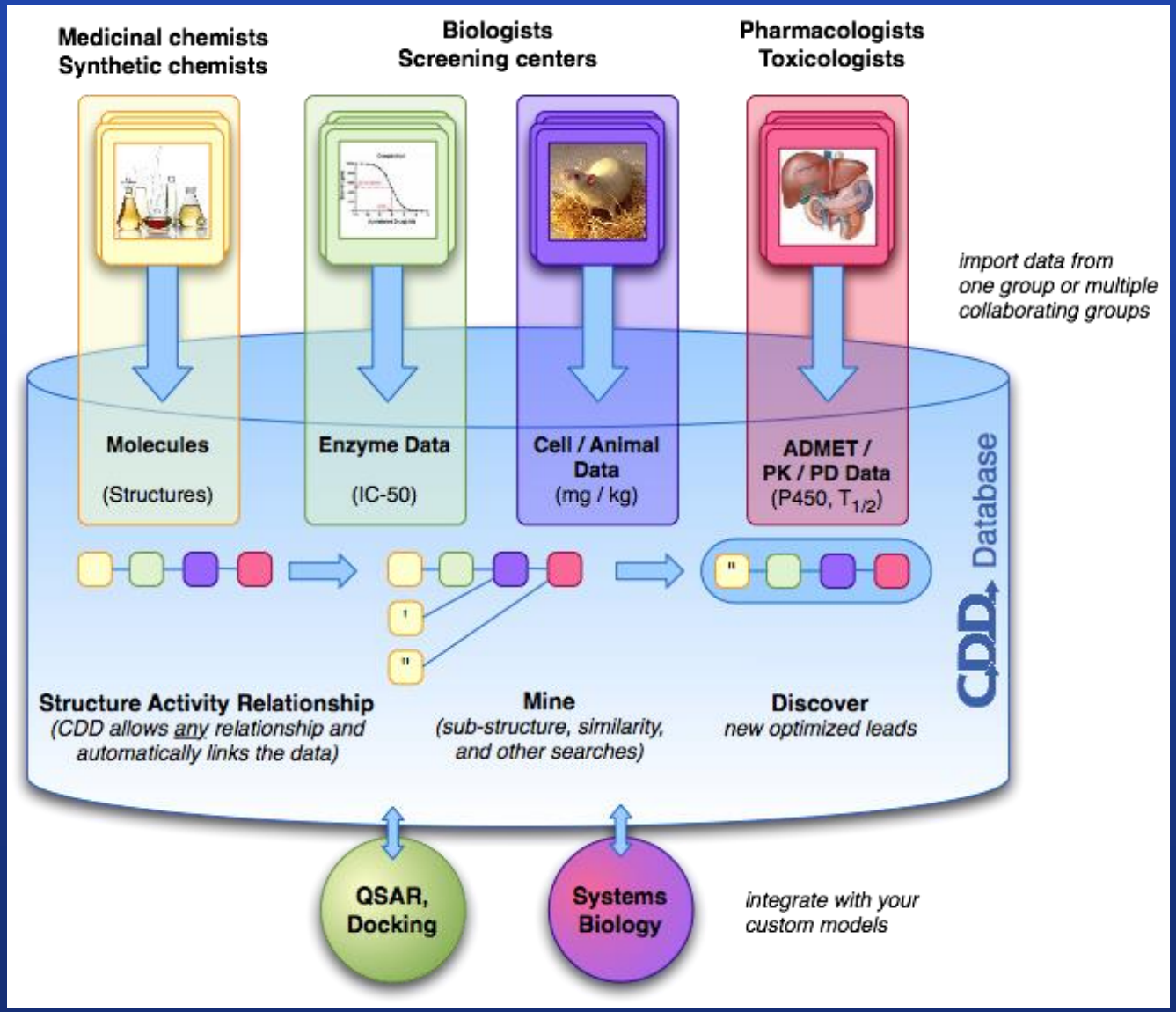


Collaborate: India CRO User Doesn't Even Know Other Projects Exist

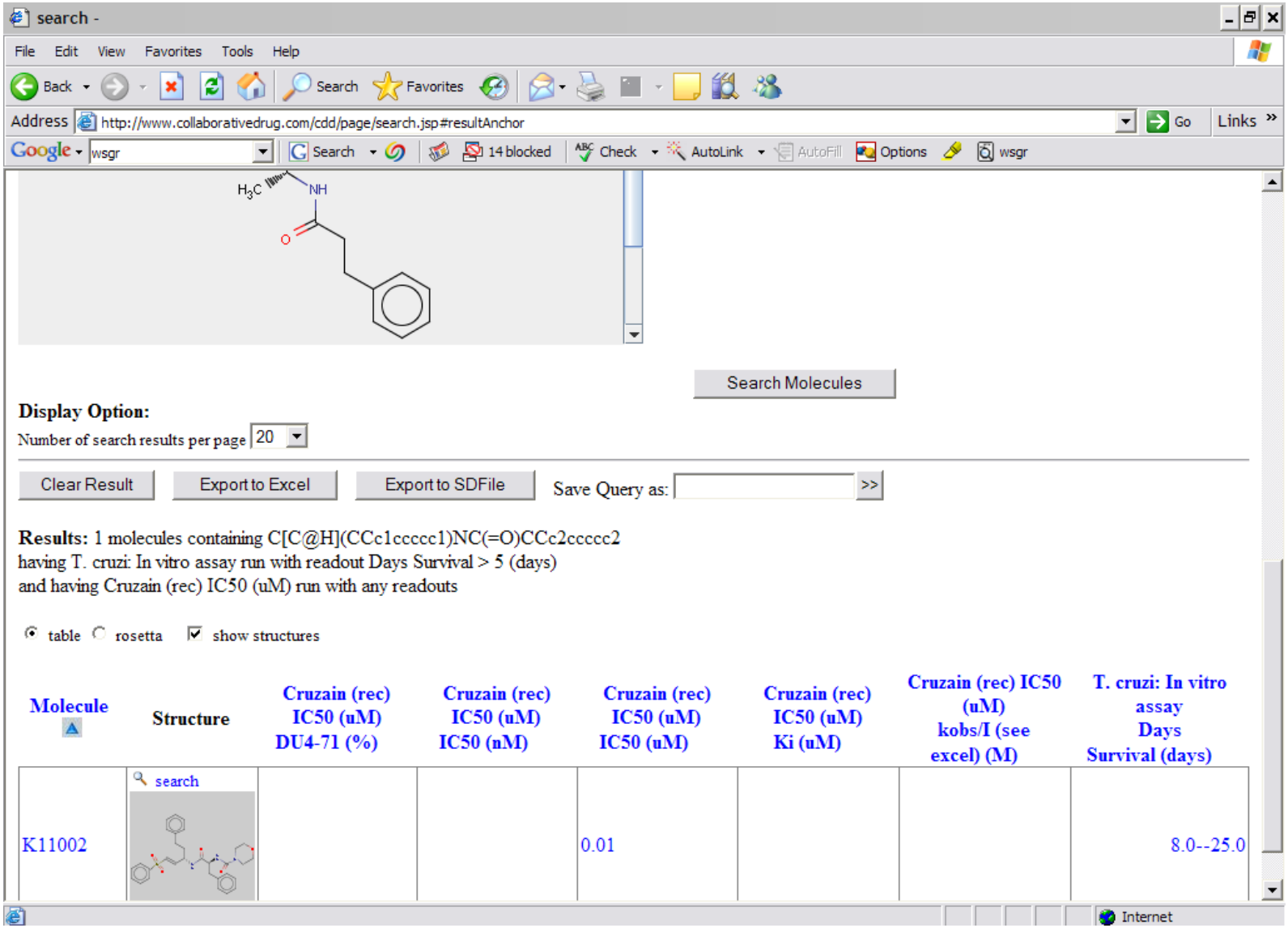


COLLABORATIVE DRUG DISCOVERY

CDD Vault for Heterogeneous Drug Discovery Data



Before:



CDD Vault® - After 10 Years

COLLABORATIVE DRUG DISCOVERY

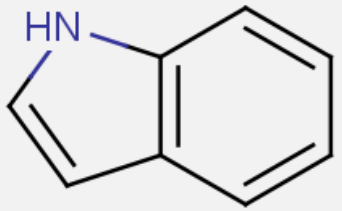
17 structures · Show 100 | Change display options · Plot results · Export results | Add results to project

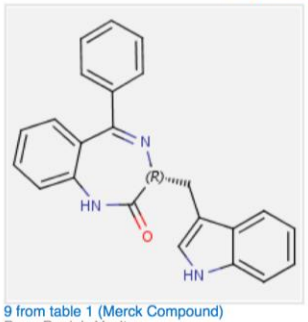
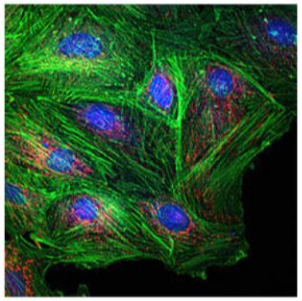
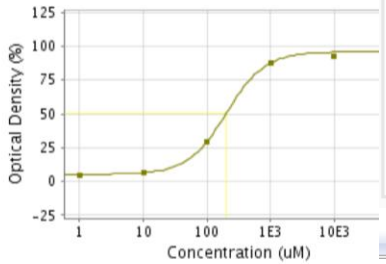
File format:
- XLS - Excel
- CSV - Comma-Separated Values
- SDF - Structure-Data File

Export or cancel

Structures

substructure similarity ≥ 70%



Select... all · none	Molecule	CCK-A Dose Response Curve: IC50 (uM)	Image	Dose-response Plot
✓	flag outliers  9 from table 1 (Merck Compound) Barry Bunin's Vault SMILES	201.42		 Flag outliers & Override

Protocols

CCK-A

- with run: (any run)
- with readout definition: IC50 (uM) < 10 uM
- and: show all

	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: -1.0
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: -1.0
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: -1.0
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: -1.0
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: -1.0
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: -1.0
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: -1.0
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: -1.0

Z'-factor: 0.969 (controls)

Z-factor: -1.928

Legend

- Positive control
- Negative control

Archive, Mine, Collaborate

CDD Vault - Made for the Internet Era

- 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
DISCOVERY

CDD Vault: Exciting Future Directions

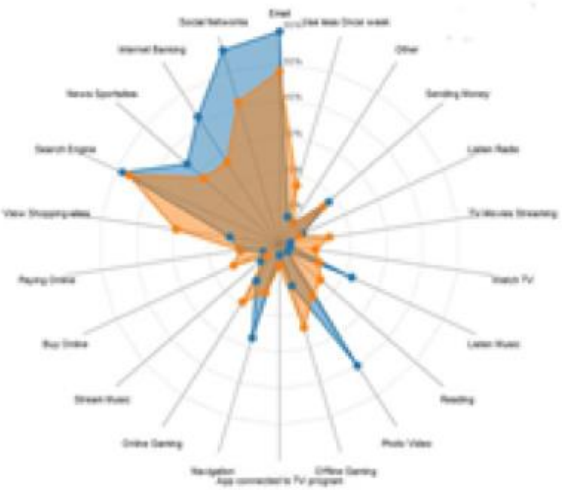
CDD Vision: New Calculations & Visualization Module in the CDD Vault

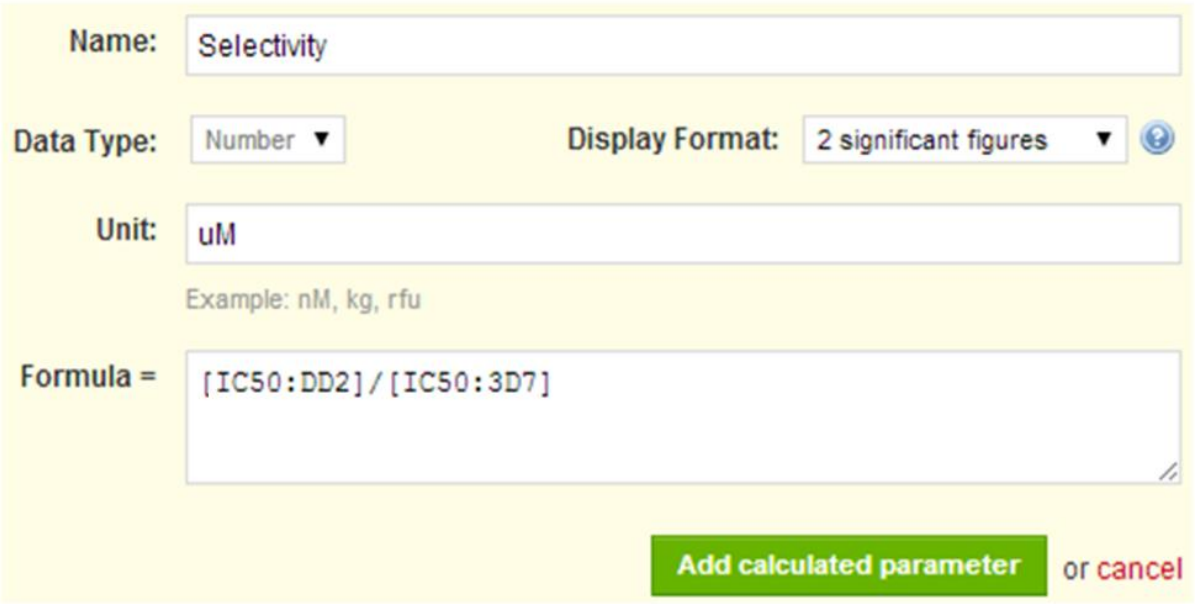
CDD Vision

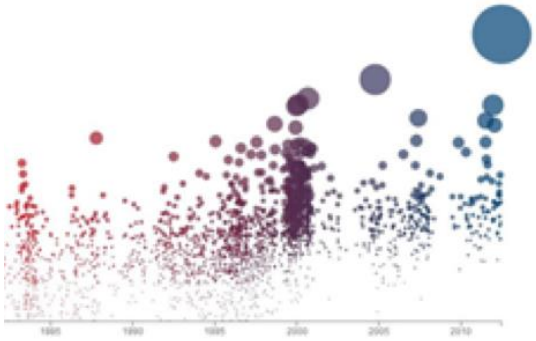
A powerful calculation and graphing extension to the CDD Vault

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

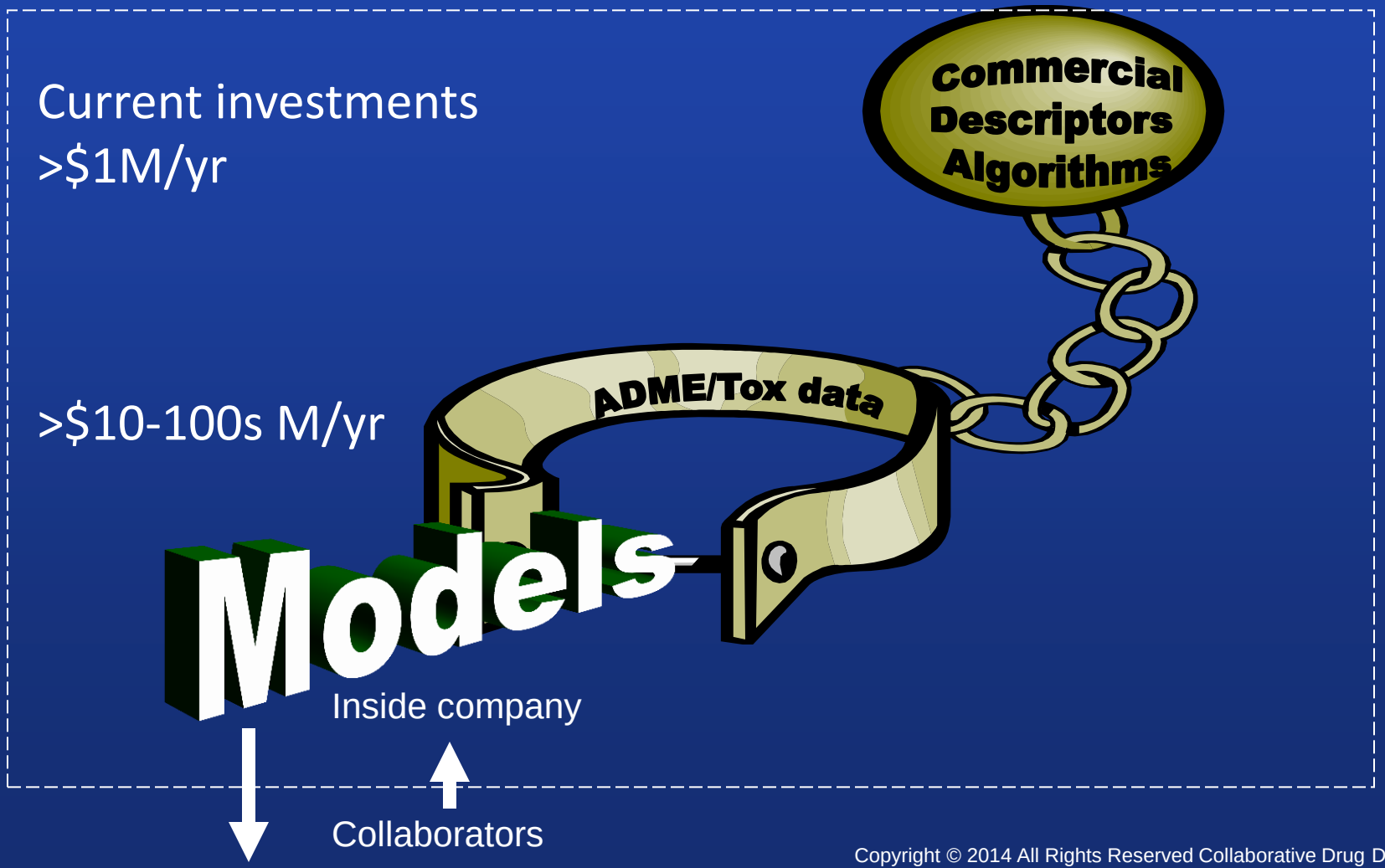






CDD Open Source Descriptors & Models: Extensions on Secure CDD Vault Collaborations

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



Build QSAR Models from Your Data

80 Selected: Plot · Export

Build a QSAR Model

Use all molecules from: Dose Response example

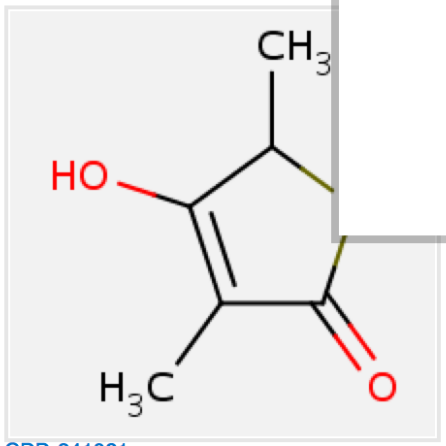
Active molecules: Your 80 selected results

Name: ABL Kinase Private Data QSAR Model

Project: Collaborative Drug Discovery, Inc.

Save or cancel

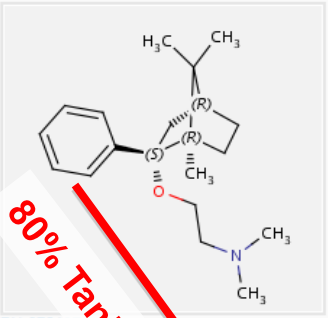
Select... all · none

Molecule	Plate Fields		Dose Response
	Name	Well	MIC99 (nM)
CDD-341021  CDD-341021 Collaborative Drug Discovery, Inc. CXSMILES (CDD Compatible)	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	

CDD Vault API Facilitates High Throughput Hypothesis Exploration

COLLABORATIVE DRUG DISCOVERY

6 Selected Results: Plot results · Export results · Add results to collection · Add results to project

Select... all · none	Molecule	Collections	NCATS Known Targets + ChemBL Predicted Targets: Predicted T...similarity)	Known Mechanism of action	Original de... indication	commercially available
✓	CDD-1351020 flag outliers  PH-67018	Malaria predictions Active, seans picks for further followup	GABA transporter 3 (CHEMBL5208) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5208			
			GABA transporter 2 (CHEMBL4889) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4889			
			Betaine transporter (CHEMBL3715) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3715			
			GABA transporter 1 (CHEMBL1903) https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1903			
				5-Hydroxytryptamine 2A/2C receptor (5-HT2A/2C) antagonist	Generalized anxiety disorder	
						yes
			tor (CHEMBL250) target/inspect/CHEMBL250			
			tor (CHEMBL4127) target/inspect/CHEMBL4127			
				Transient receptor potential cation channel vanilloid 1 (TRPV1) antagonist	Acute and chronic pain	

Original Target

80% Tanimoto Search

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EBI › Databases › Small Molecules › ChEMBL Database

ChEMBL

- ChEMBLdb
- Malaria Data
- ChEMBL-NTD
- Kinase SARfari
- GPCR SARfari
- DrugEBIlity
- 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

https://www.ebi.ac.uk/

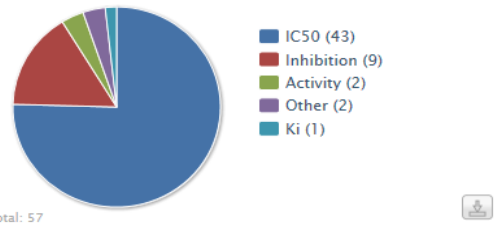
Target Report Card

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-symporter neurotransmitter betaine_gaba

Target Associated Bioactivities

ChEMBL Activity Types for Target CHEMBL3715



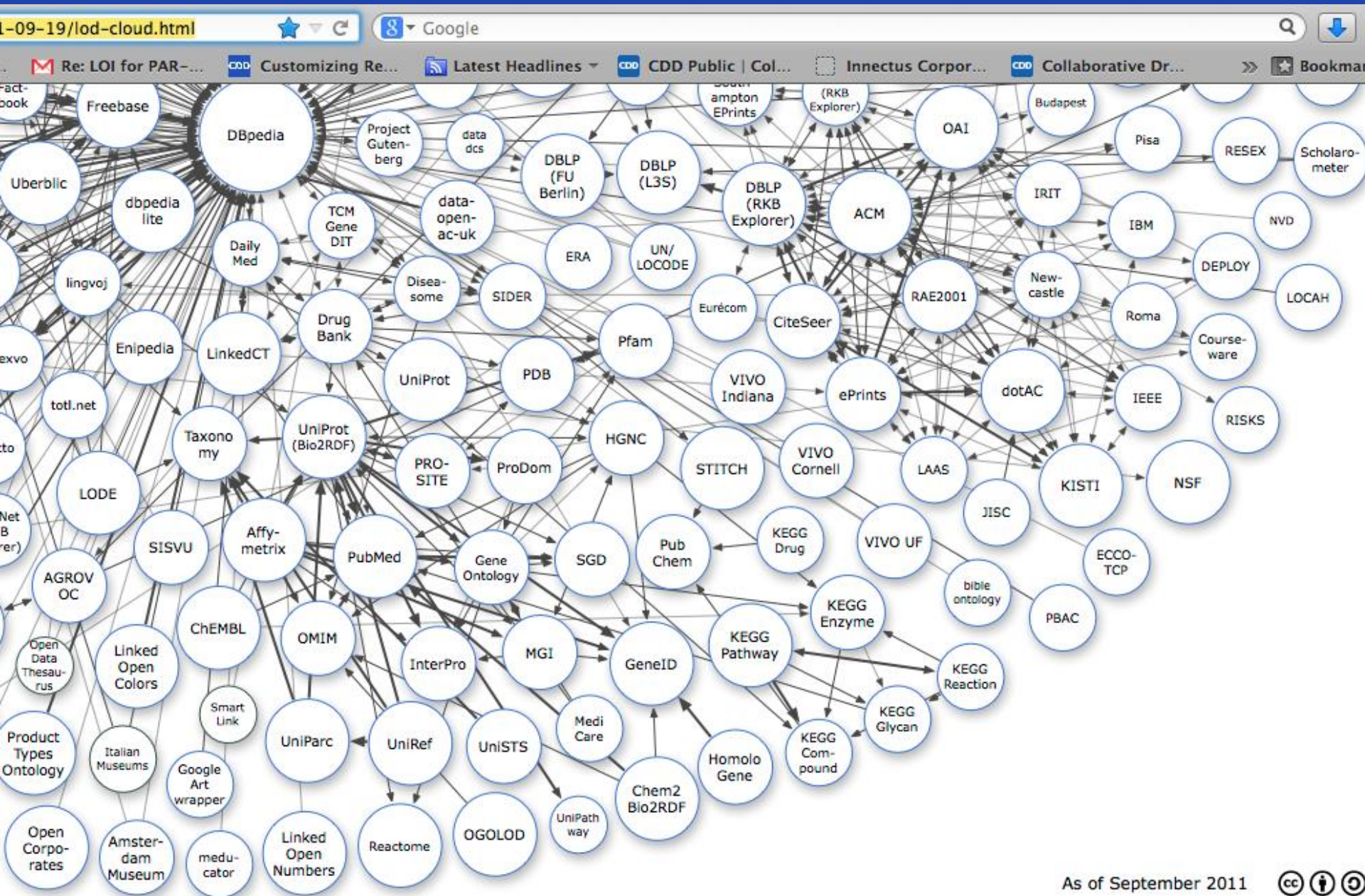
Total: 57

From:

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

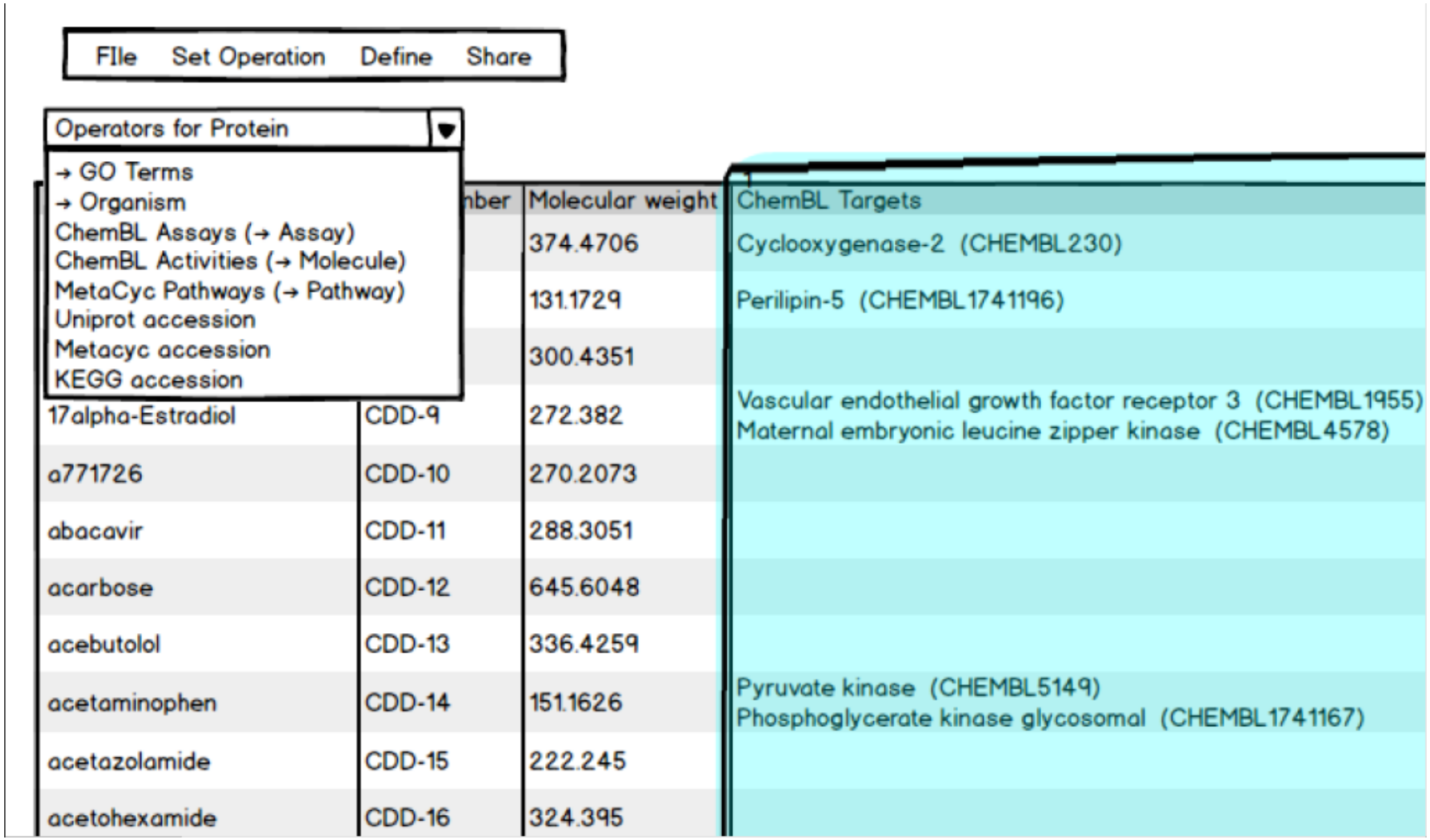
COLLABORATIVE DRUG DISCOVERY

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

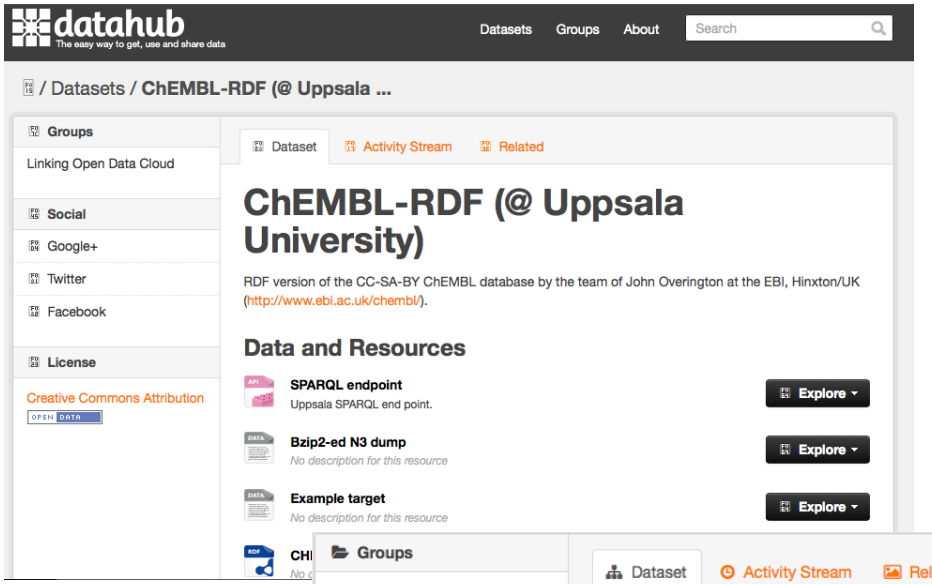


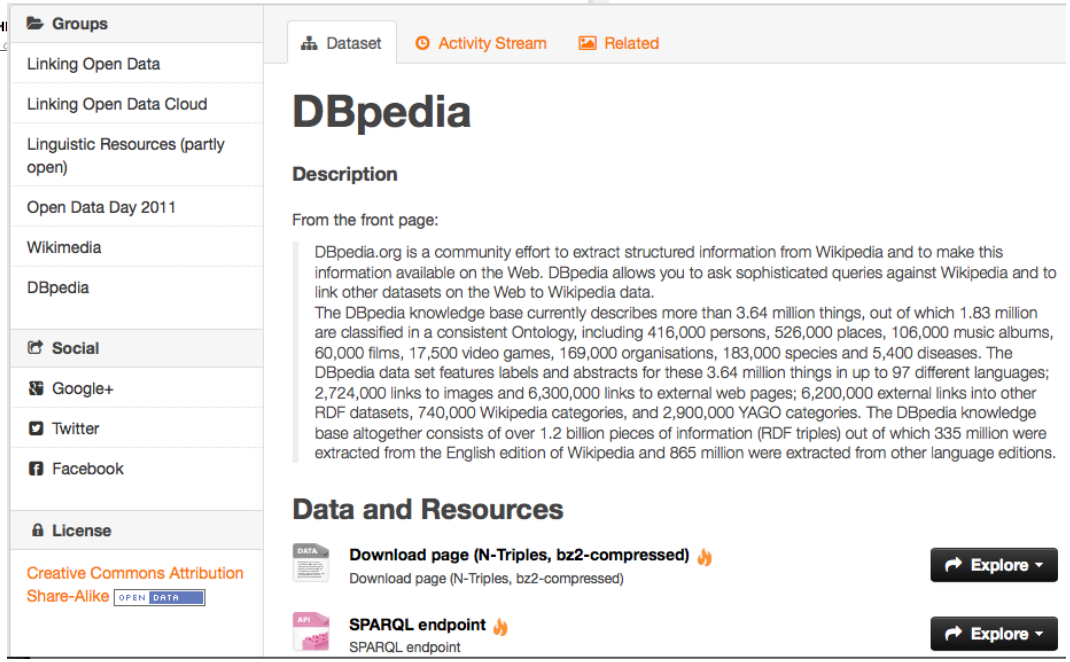
As of September 2011

CDD TraVerse™ ("Topic 1") – A Working Prototype: For People to Traverse All the Data

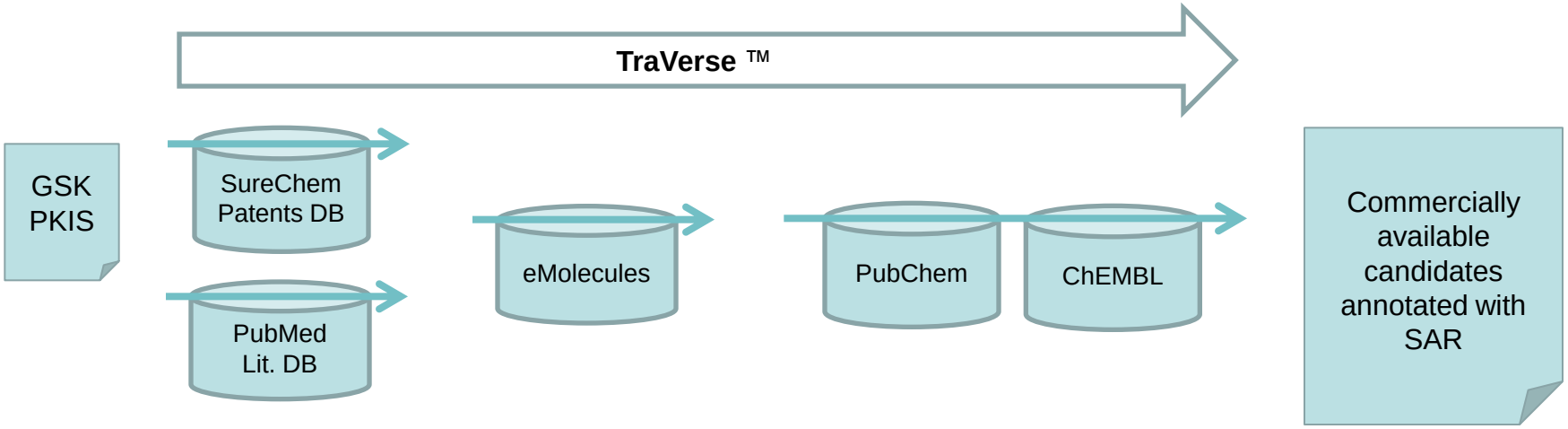


Data Already in the Prototype





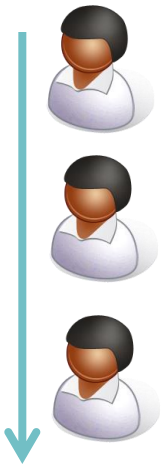
Example Use Case for TraVerse



"Look for interesting scaffolds and motifs"

"Reposition for neglected disease indications"

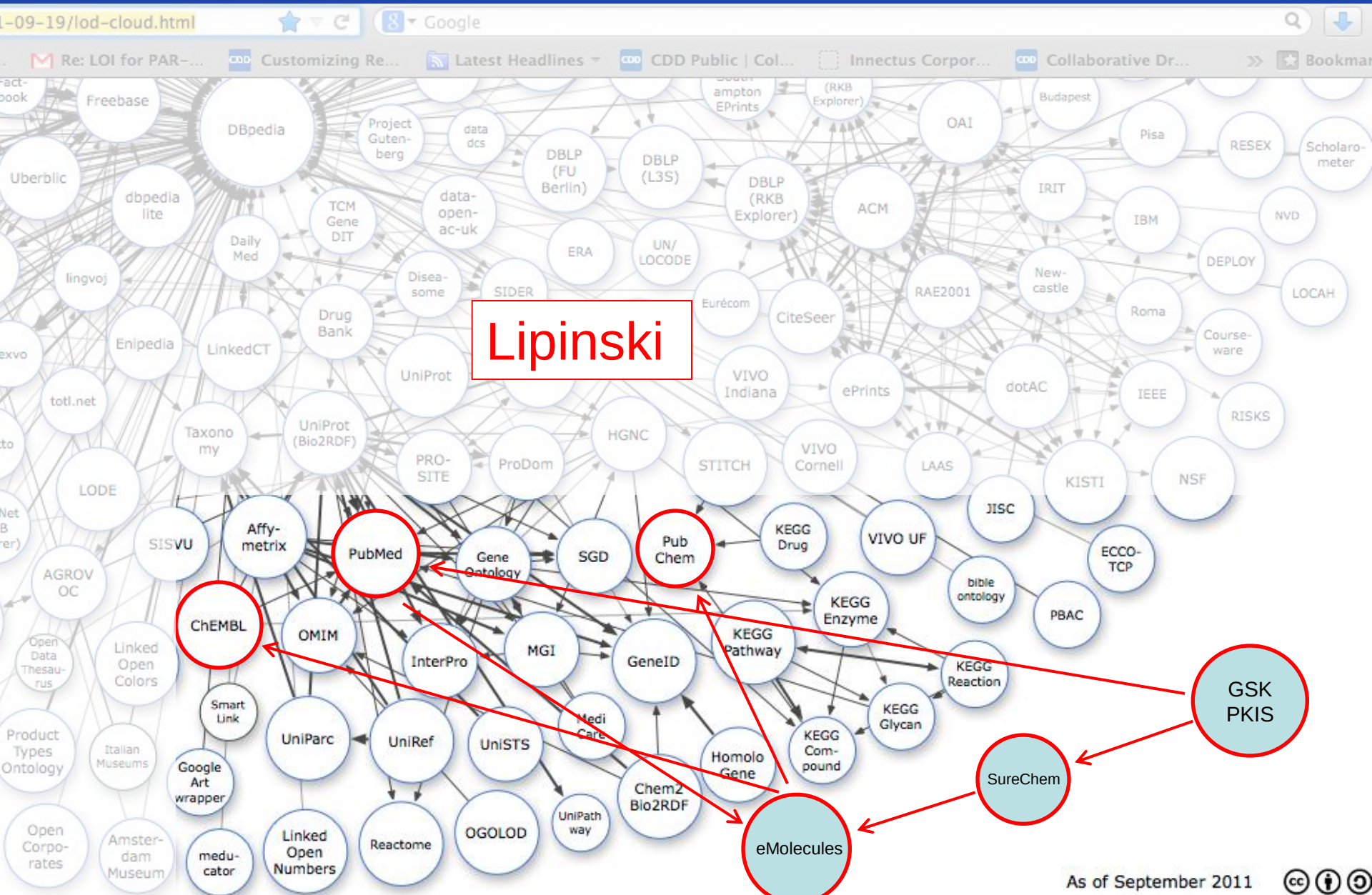
"Inexpensively test better informed hypothesis"



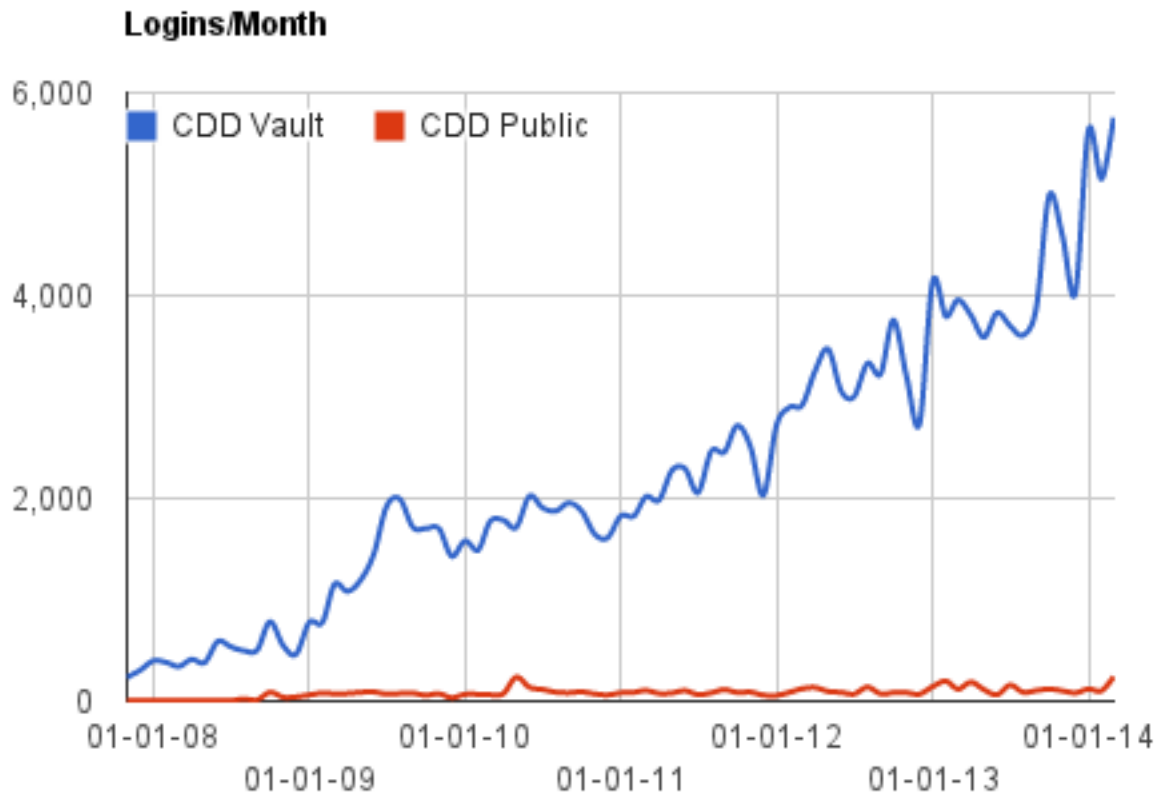
Better Drug Candidates

Dr. Christopher Lipinski
Retired Senior Research Fellow
Pfizer

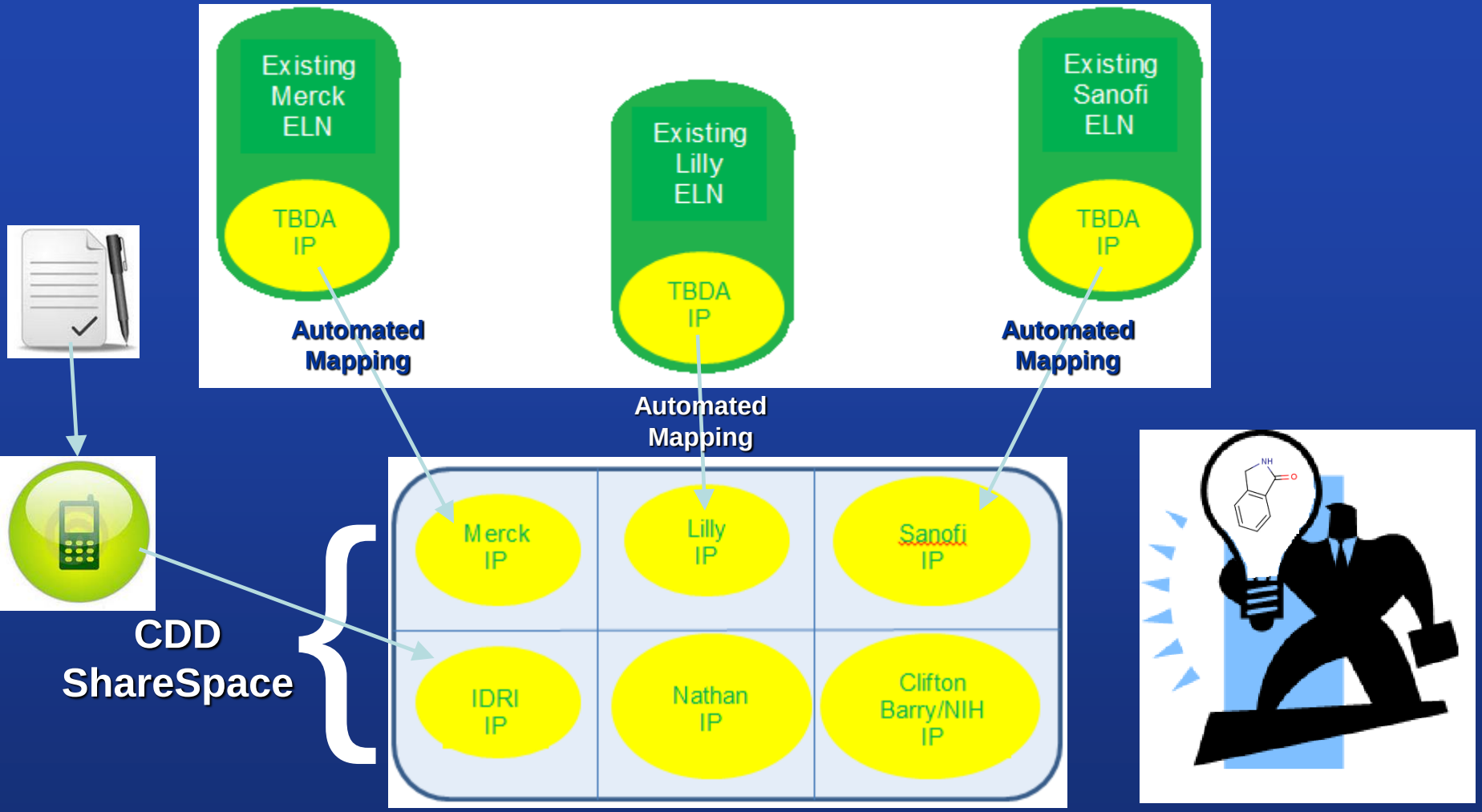
Lipinski Use Case for TraVerse



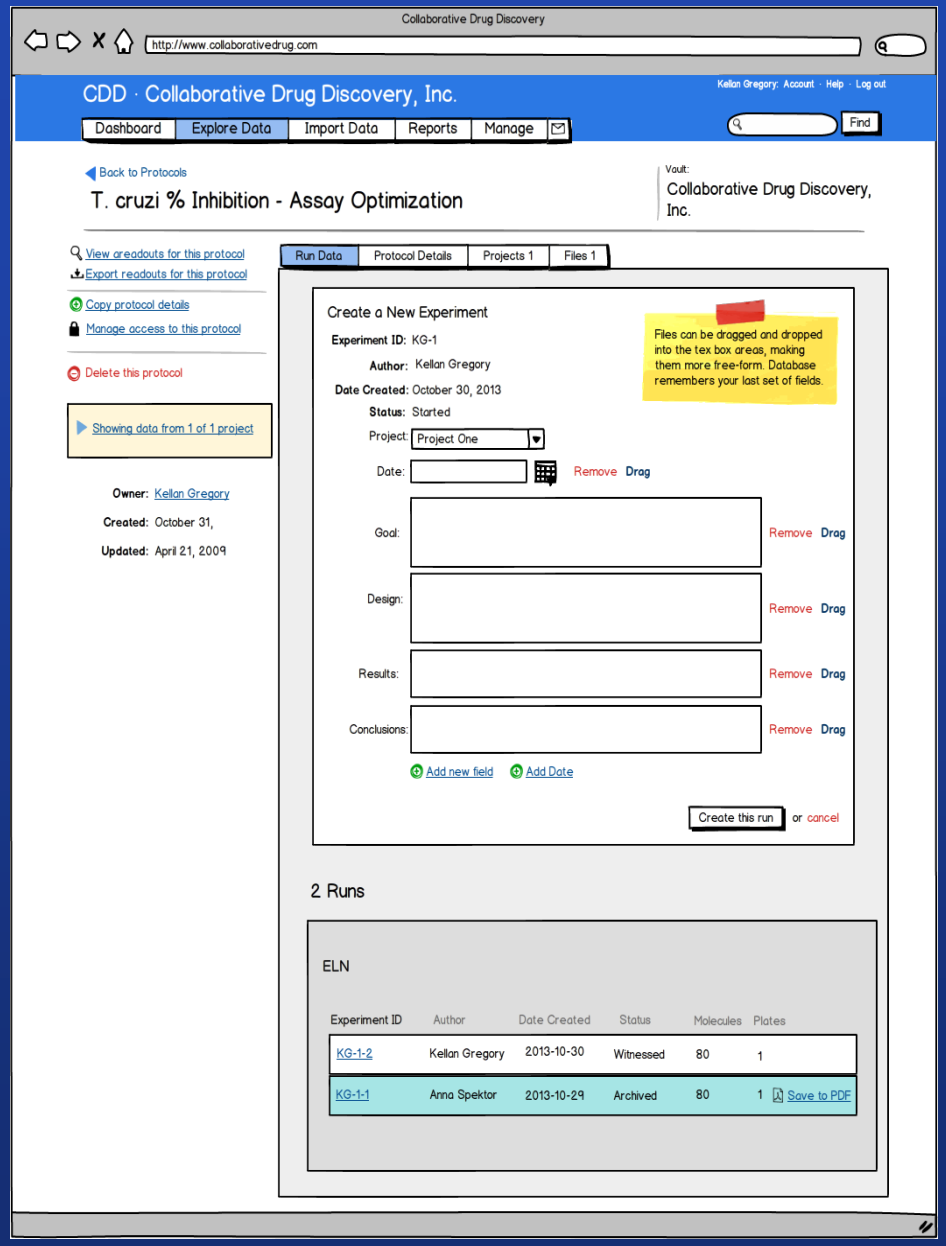
CDD Public:
An Under Optimized Resource for Public Good

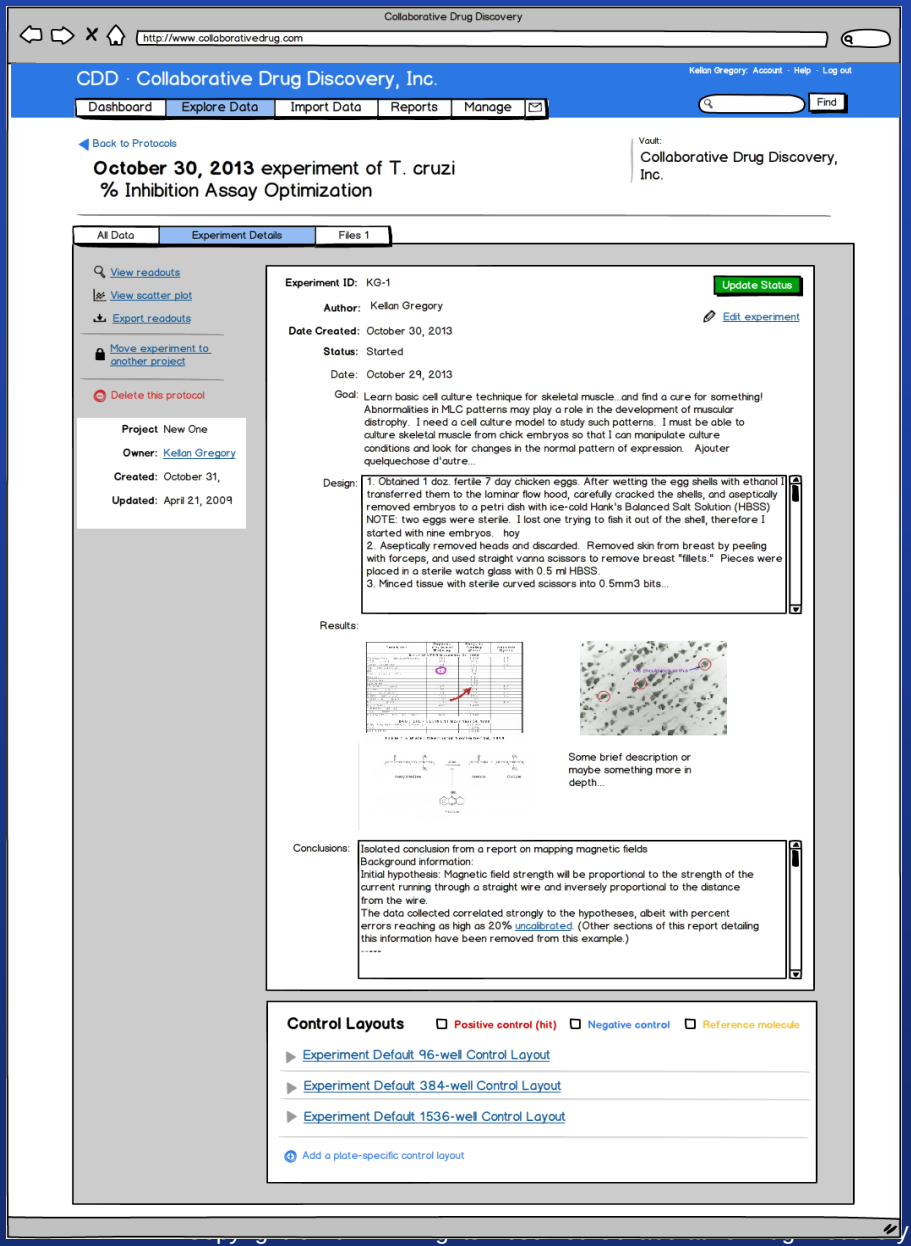


CDD ShareSpace

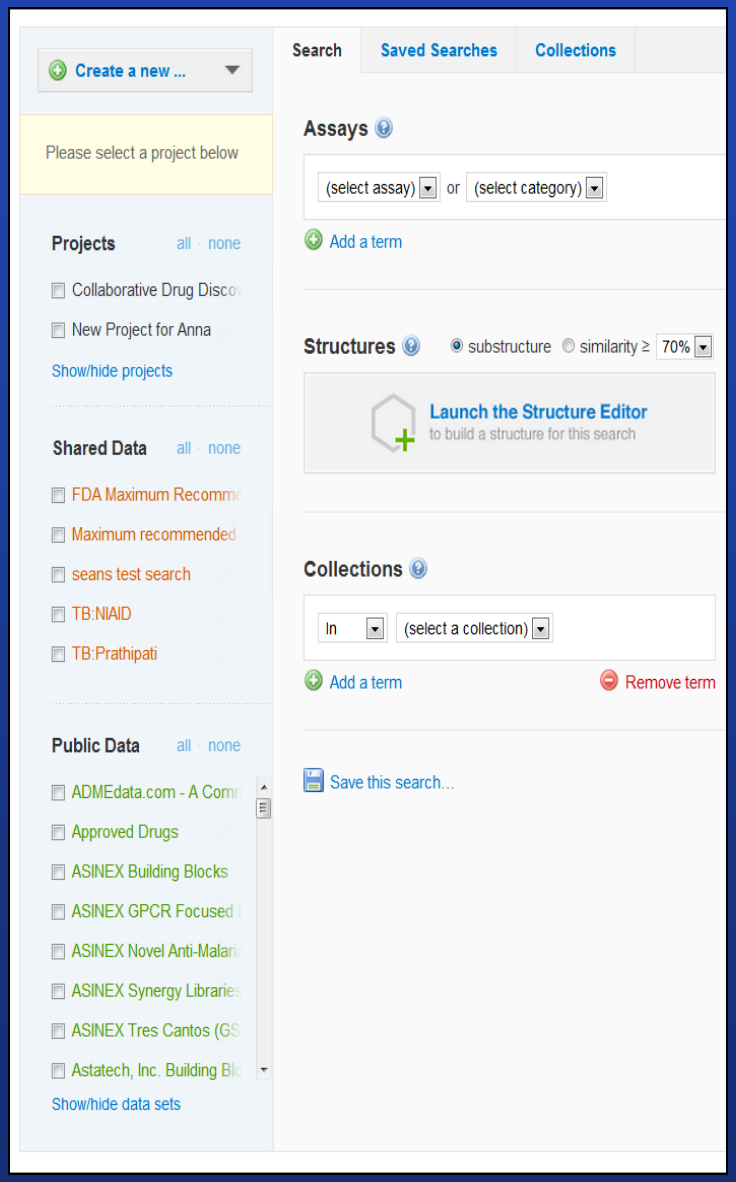


Collaborative CDD Vault ELN – Future Directions "Content Around Data"





“Projects Between Vaults” - Future Directions



- **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

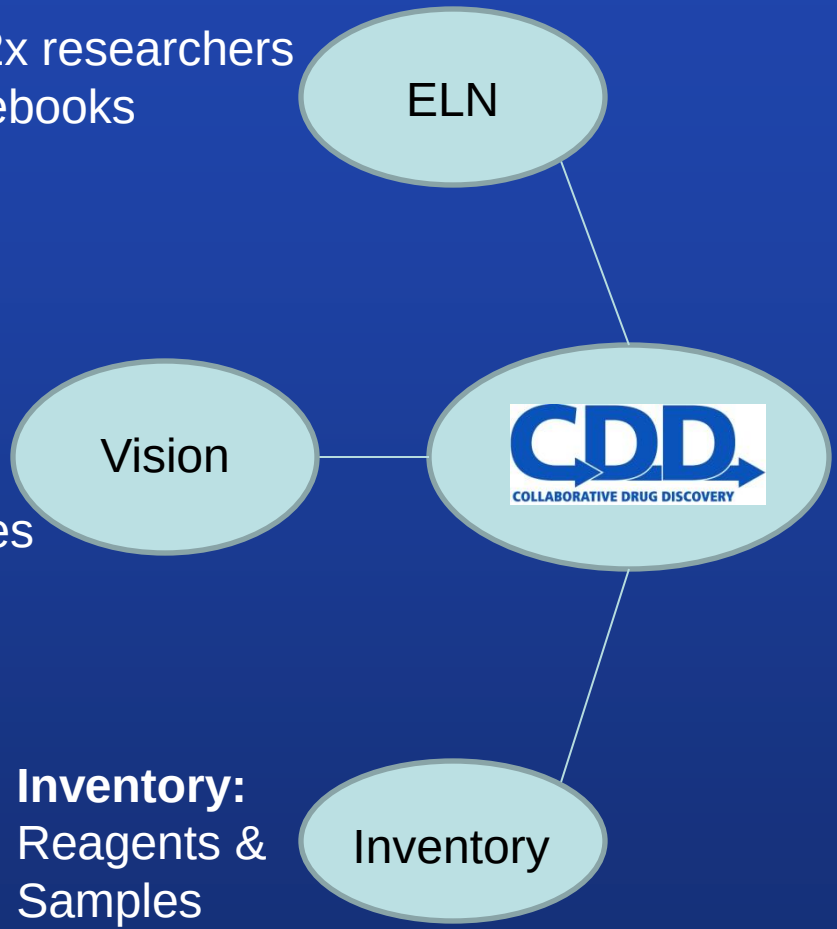
CDD Vault – Full Solution Roadmap for the Collaborative Drug Discovery Workspace

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

Establishing “Customer” Advisory Board (CAB)

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

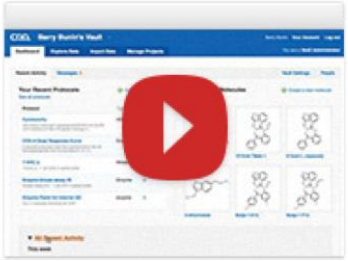
Case Studies

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.

CDD Vault – Technical Leadership

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.

CDD Vault – Technical Leadership

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
COLLABORATIVE DRUG DISCOVERY

User Login

Home | CDD Vault | Community | Blog | About Us

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 ›

Acetylon Pharmaceuticals Inc | BROAD INSTITUTE | Lilly | JOHNS HOPKINS UNIVERSITY | MIT | NOVARTIS ›

CDD “Rule of 10”

GSK Open Malaria SAR in CDD Vault

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

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)

Commercial Collaboration Case Study: Cash Conscientious Harvard Spinout

CDD Vault Case Studies

Acetylon Pharmaceuticals

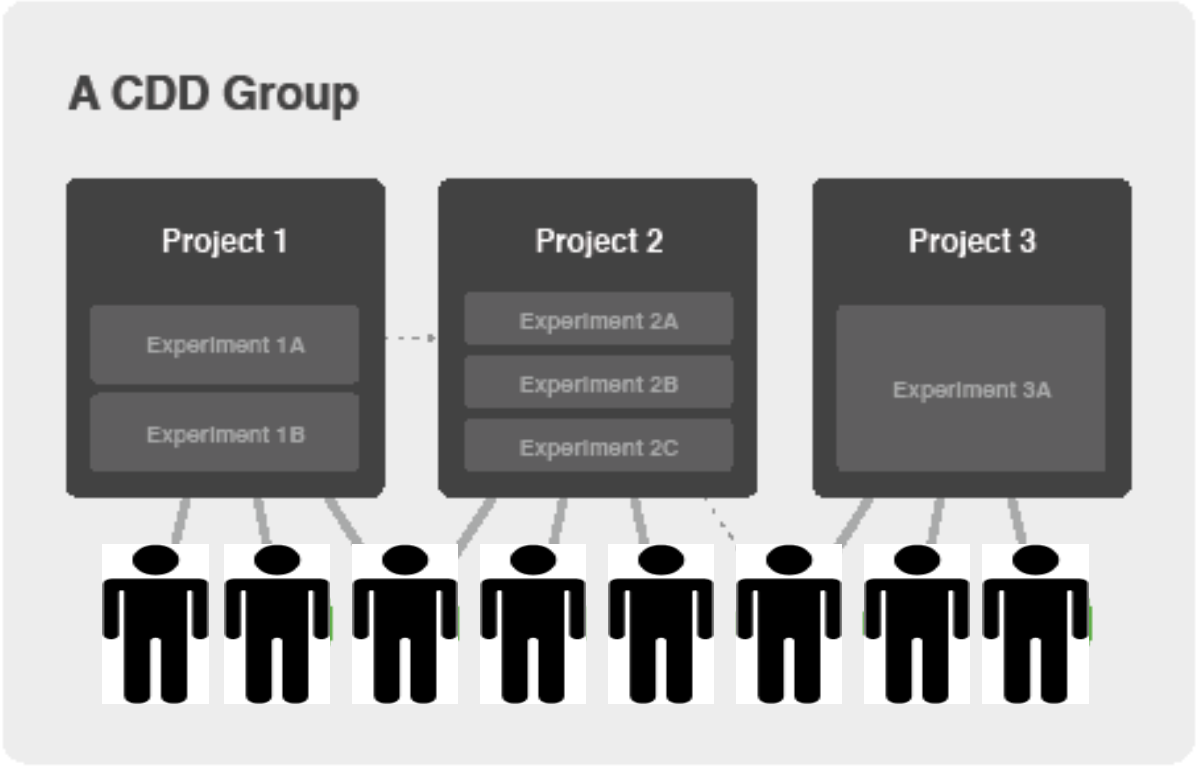
This Harvard spinout company uses CDD Vault to manage both academic-industry and China CRO collaborations. After becoming a customer in 2009, they have grown to a dozen CDD Vault users presently, all while filing for an IND for their HDAC inhibitor and raising $27M in a Series-B financing in the meantime.

Acetylon Pharmaceuticals, Inc.

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

CDD Projects:
Advanced Collaboration in Natural Workflows



Projects provide subdivisions of data and data privacy

10 Year Summary

- 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"**

Behind Firewall

Both hosted and behind firewall options

Run QSAR Models on Your Data

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.