Collaborative Drug Discovery – UCSF 3rd Annual Community Meeting

Archive, Mine, and (selectively) Collaborate

COLLABORATIVE DRUG DISCOVERY

What if?

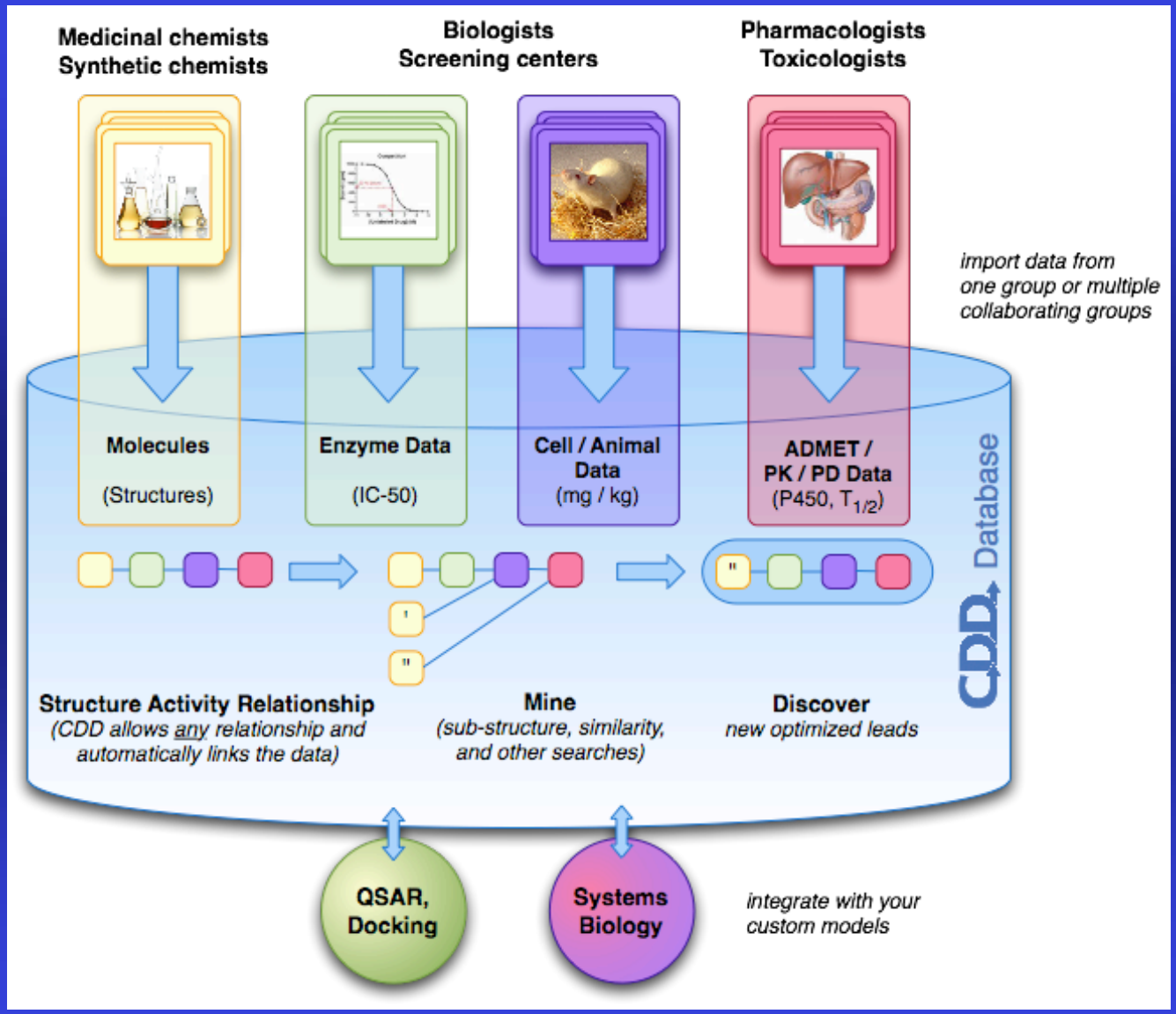
- Technology
- Collaborations

CDD Platform

- *Modules:*
  - **CDD Vault – Secure place for private data – private by default**
  - **CDD Collaborate – *Selectively* share subsets of data**
- *Datasets:*
  - **CDD Public – Expanding public data sets**
    - **Published compounds**
    - **Data from community members**
    - **Vendor libraries**
- **<u>Unique to CDD</u> – *Simultaneously* query your private data, collaborators' data, & public data**

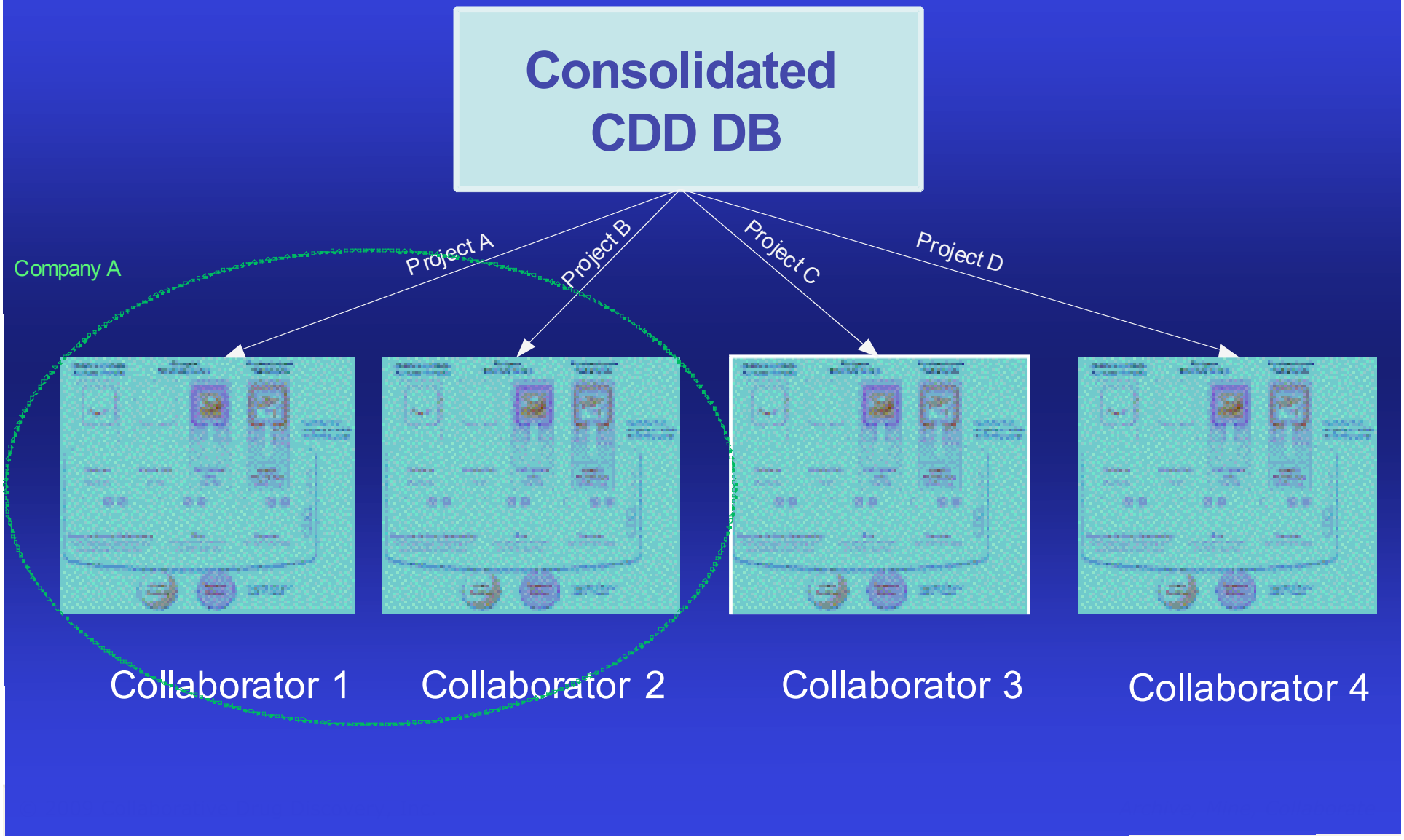
COLLABORATIVE DRUG DISCOVERY

CDD Database for Your Private Data



Collaborate Mode 1 – Big Pharma

with single login to multiple CROs/Biotech groups



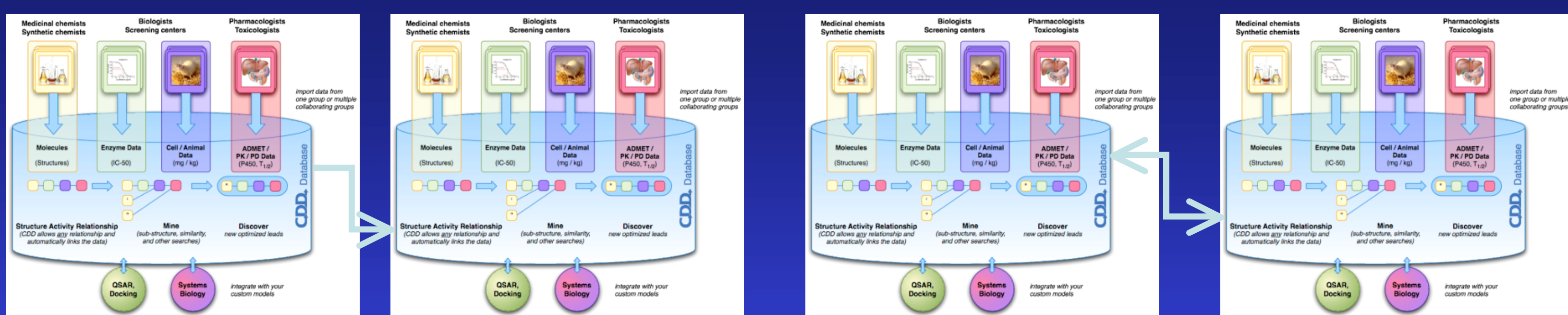
Collaborate Mode 2 – Academic + Foundations securely sharing <u>data subsets</u>

CDD DB
group 1

CDD DB
group 2

CDD DB
group 3

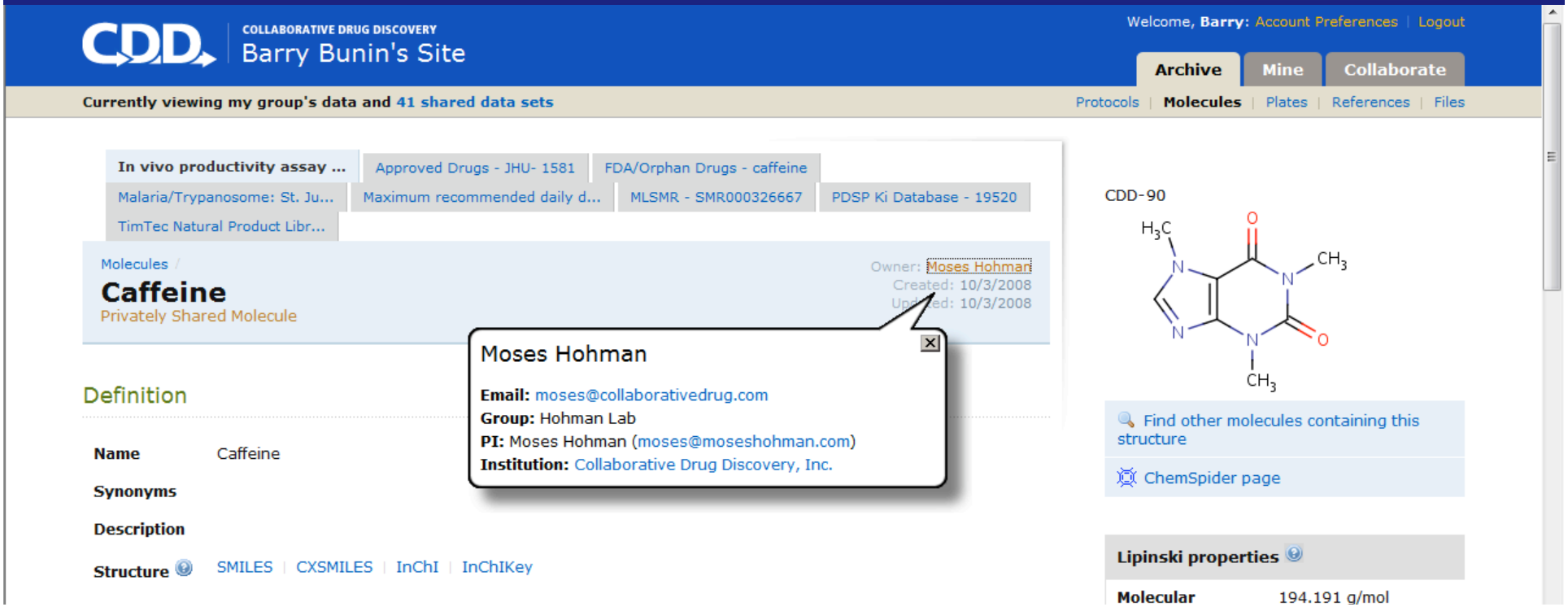
CDD DB
group 4



Use CDD Vault™, Collaborate™, Public™ for Global R&D Community

New Types of Offerings for a Rapidly Changing Industry

- CDD Community: tap into global R&D via “crowd-sourcing”
- CDD Alliance: better management of your collaborations
- CDD Customize: fast, good, and cost-effective = agile



CDD COLLABORATIVE DRUG DISCOVERY

CDD Public

CDD · Barry Bunin's Site

Barry Bunin: Your Account · Log out

Dashboard | Group Data | Import Data | Share Data 4

Currently using **Barry Bunin's Site** data and **2 shared data sets** Choose data sets ...

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

Search references ... any field Go · Help · Add a new reference · Search and import from PubMed

1 Reference · Showing 20 per page Previous · Page 1 of 1 · Next

Reference Keywords

PUBLIC REFERENCE TB Efficacy Data from Published Literature

Synthesis and antitubercular activity of 7-(R)- and 7-(S)-methyl-2-nitro-6-(S)-(4-(trifluoromethoxy)benzyloxy)-6,7-dihydro-5H- imidazo[2,1-b][1,3]oxazines, analogues of PA-824.

Li, X.; Manjunatha, U. H.; Goodwin, M. B.; Knox, J. E.; Lipinski, C. A.; Keller, T. H.; Barry, C. E. 3rd; Dowd, C. S.

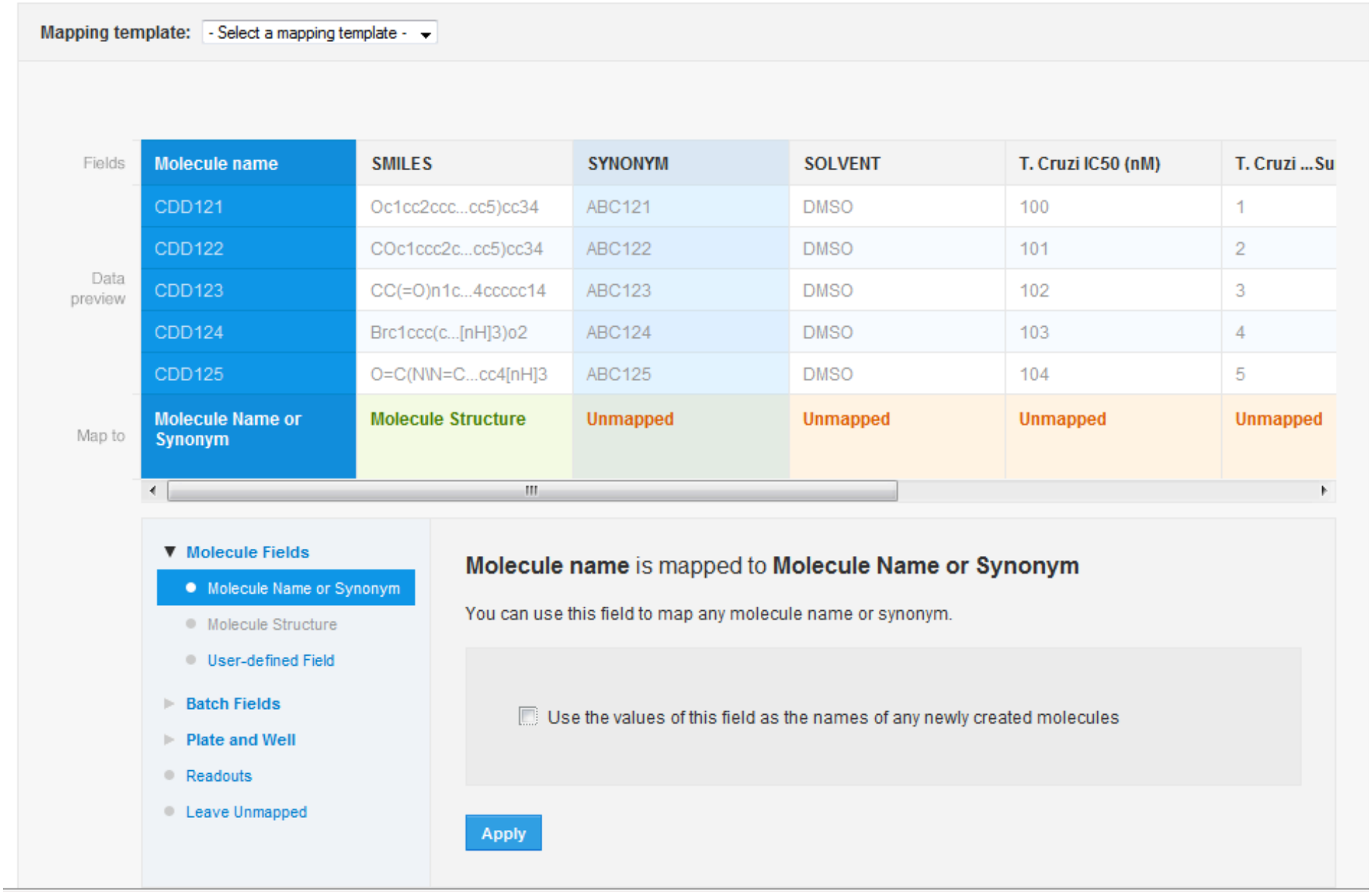
Bioorg Med Chem Lett (2008) Vol 18, No 7, pp 2256-2262

Abstract · Full text · View in PubMed

Previous · Page 1 of 1 · Next

21 Internet | Protected Mode: Off

Mapper Overhaul: Templates and Previews Simplify Archival

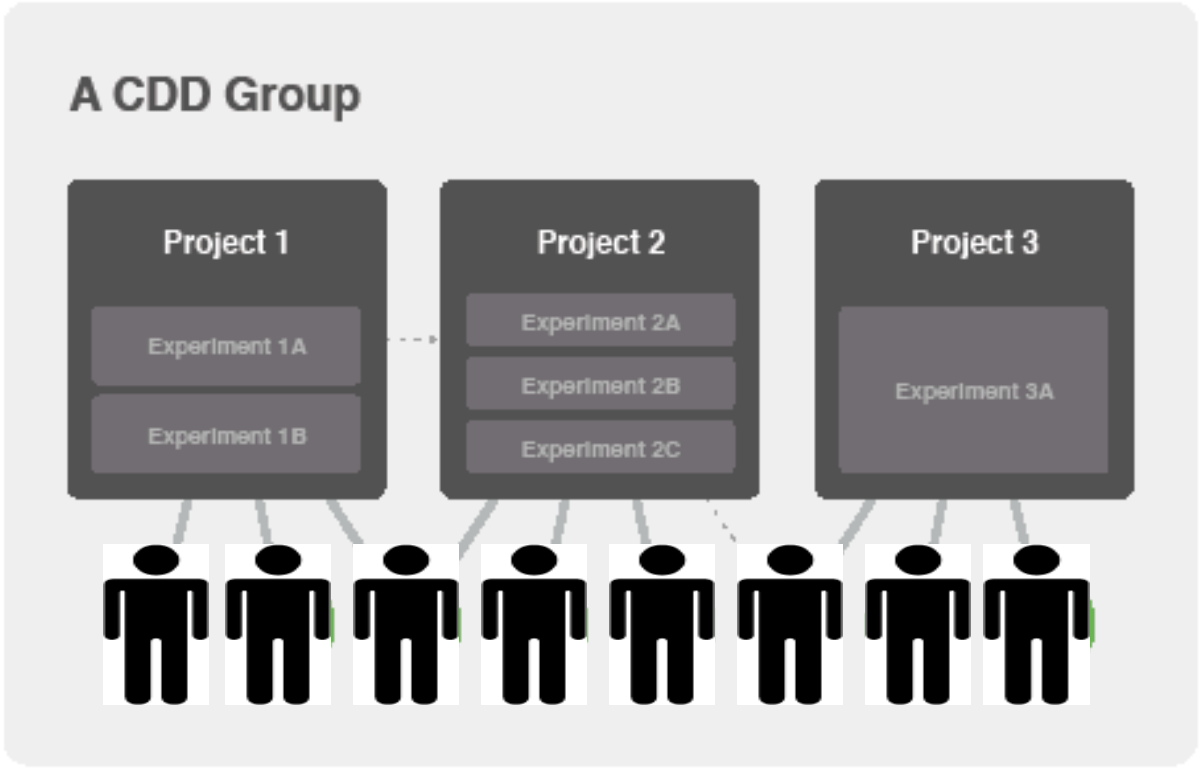


CDD "Top 10" Requests

- **Mapper Overhaul –** more intuitive to batch upload complex data, save mappings
- **Projects –** more advanced collaborative features beyond private-to-private data
  - Editable data
  - Refined data viewing selections
  - Multi-group functionality requested by screening centers, foundations, & biopharma
- **Configurable Terminology –**
  - Configure CDD w/ your own labels (alts to molecules, protocols…like objects, antibodies, sequences, screens, etc)
- **Advanced Filters & Alerts for Compound Liabilities**
  - Reactive Functionality likely to cause toxicity, alkylate DNA, BBB models, etc
  - What Lipinski calls Alerts (for example with Abbotts' ALERT SMARTS filters).

➢ NOTE: For each feature we do a "bang per buck" analysis, and truly agonize over which item is best to do first, given lots of competing requests

CDD Projects – More Advanced Collaborate



Projects provide subdivisions of data and data privacy

Configurable Terminology: "User-Defined" Objects, Subjects, Molecules

CDD COLLABORATIVE DRUG DISCOVERY

CDD • Bunin Group

Barry Bunin: Admin · Your Account · Help · Log out

Dashboard | Group Data | Import Data | Share Data

Recent Activity | Messages 2 | Group Settings | People

Your Recent Screens

See all screens

Create a Screen

Screen	Type	Substances
Falcipain IC50	enzyme	80

Your Recent Substances

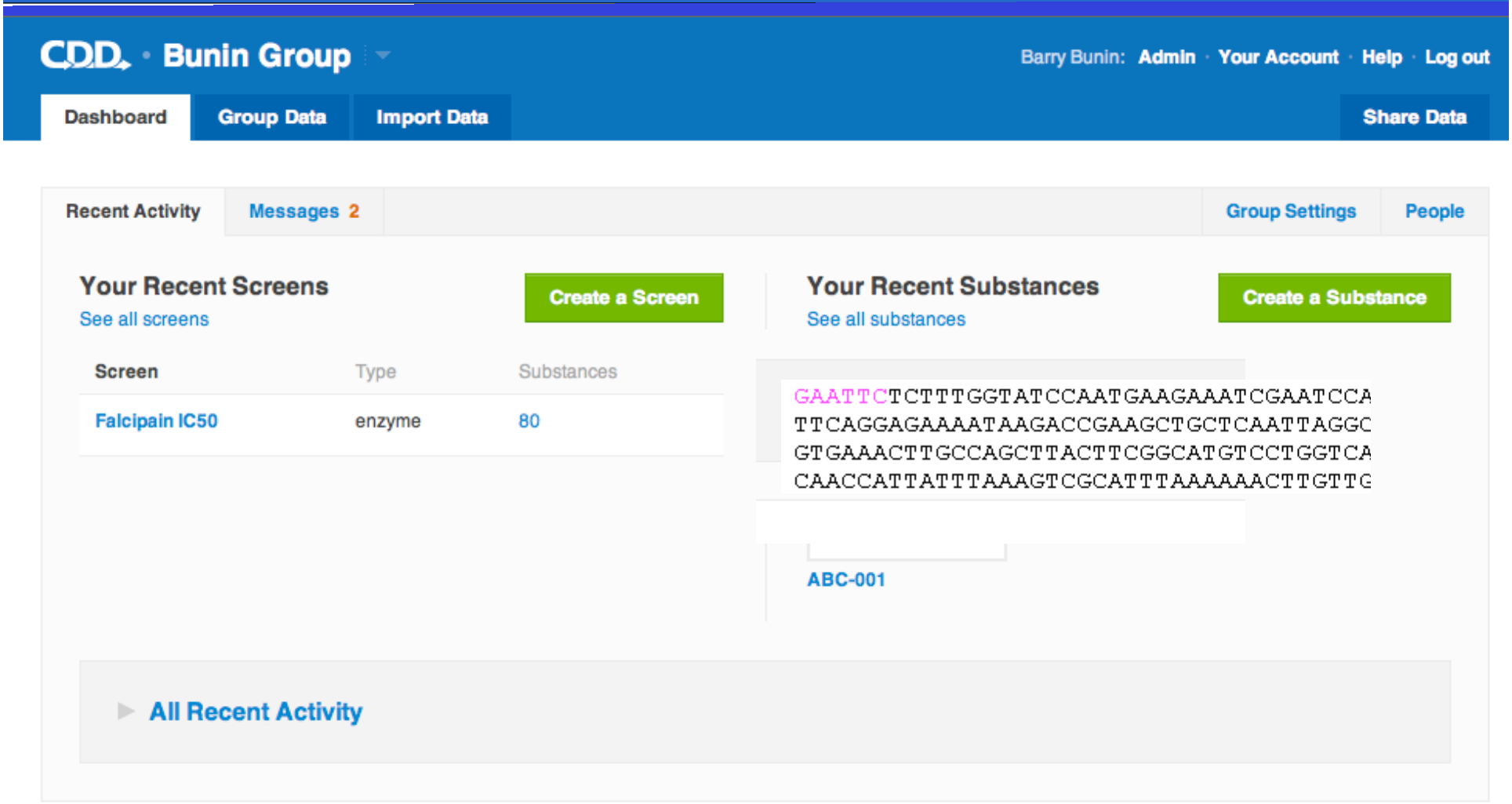
See all substances

Create a Substance

ABC-001

▶ All Recent Activity

Configurable Terminology: "User-Defined" Objects, Subjects, Biologicals



Drug Toxicity Alerts

CDD COLLABORATIVE DRUG DISCOVERY

Caffeine – Collaborative Drug Discovery

file:///Users/moses/code/design-svn/templates/molecule.html

Google

CDD · Lipinski Group

Chris Lipinski: Your Account · Help · Log out

Dashboard | Group Data | Import Data | Share Data

Currently using **Lipinski Group** data and **6 shared data sets** Choose data sets ...

Back to Dashboard

CAS 957217-65-1 PUBLIC MOLECULE

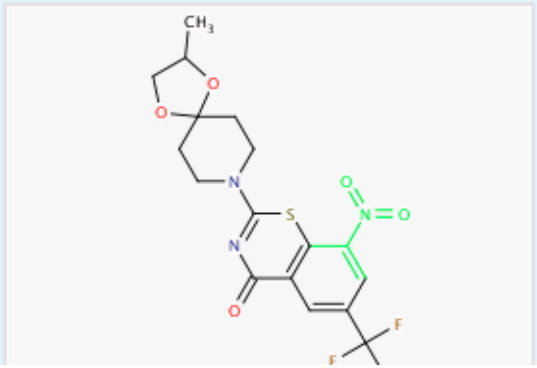
Available in 3 data sets. Now viewing:

TB MIC Prathipati NIAID – 37532

Overview | Batches 2 | Plates 1 | Protocols 3 | Associated Files 2 | Alerts 2

2 Alerts

Structure Match Preview



Alert

Abbott Alarm NMR failed

- csc
- Nc1cccc2aaaaa12

Pfizer Lint failed

- O~N(=O)-c(:*):* (aromatic NO2)

Implementing Toxic Functionality Alerts (see Lipinski's presentation)

- **Basic Capability = 2 FTE weeks**
  - Store list of SMARTS alerts with intuitive description
  - Associate list of alerts with structures
  - Set up alerts to be automatically run against new and existing structures
  - Display alerts
- **End User Flexibility = 1 FTE week**
- **Advanced Implementation = 3 FTE weeks**

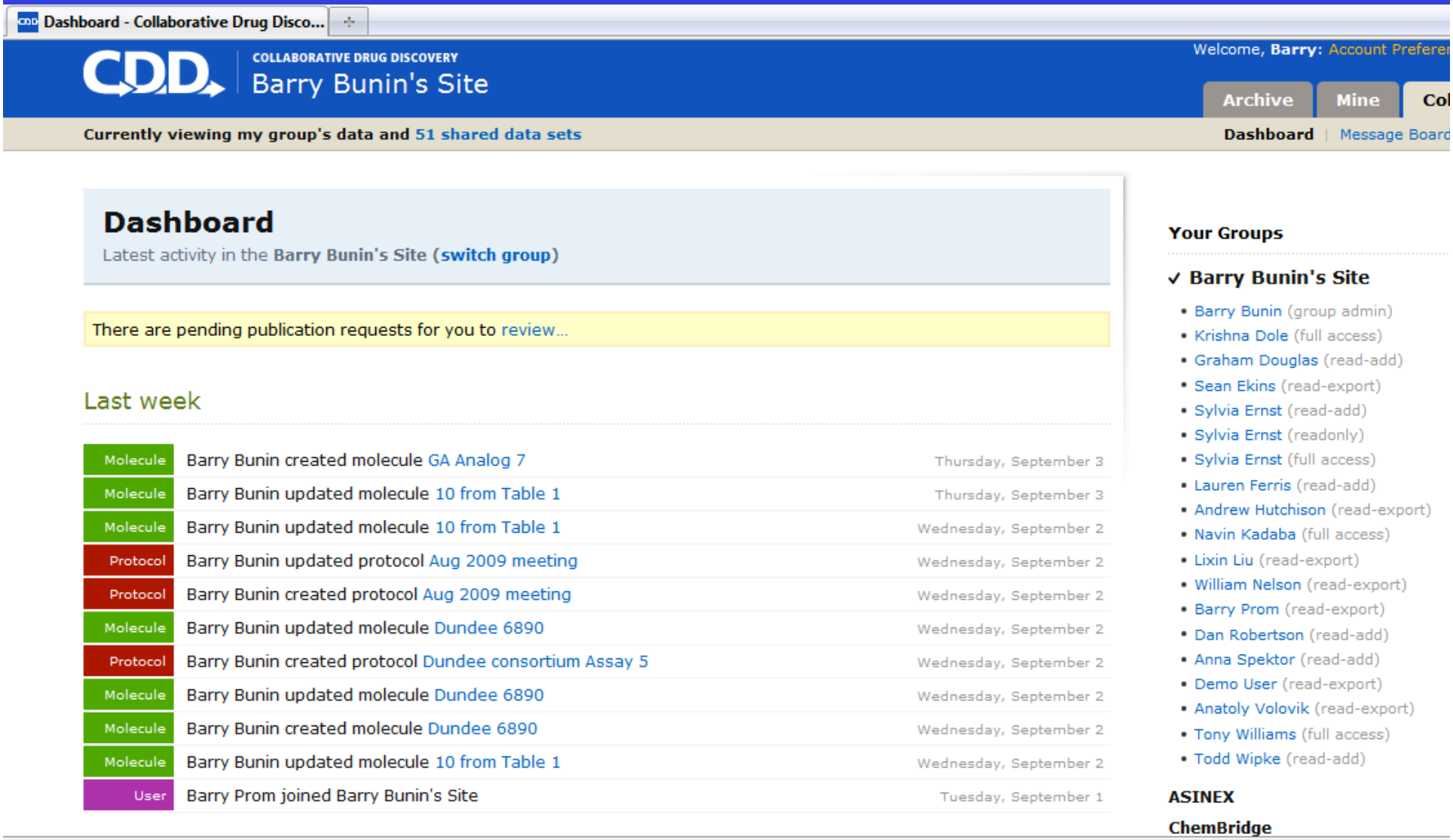
- NOTE: Generally any feature can have about 25% of unforeseen features

CDD "Top 10" Requests (cont.)

- **Advanced visualization tools –** for anything mined.
- **Mine page extensions –** e.g., more list logic on query results
- **Performance-Speed Optimization (mapper/slurper/mining)**
- **Processing data (averaging, SD, etc) and advanced calculations** – "Excel" manipulations
- **API –** program your own capabilities and integrate nicely with other technologies
- **Multi-group, Multi-dimensional MedChem Collaborations** –
  - Social Networking
  - Community of models to support complex, collaborative projects
- **Engage Big pharma**
  - Data, models, compounds, & capabilities
  - "Pre-competitive"

➢ Reminder: For each feature we do a "bang per buck" analysis

Collaborative Dashboard for Secure To-the-Minute Global R&D Tracking



CDD Search Results View

COLLABORATIVE DRUG DISCOVERY

Save this search...

Show first 1

Search Results

Display options | Export 9 res

9 matching results

Molecule	CCK-A Dose	IC50 (uM)	Dose-response Plot	CCK A receptor binding a	IC50 +/-
summary | details 10 from Table 1 Barry Bunin's Site SMILES | InChI		*2.51*	Mark outliers	0.12	+/- 0.02
				0.12	
summary | details					

Heat Maps, Controls, & Plate Statistics

	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

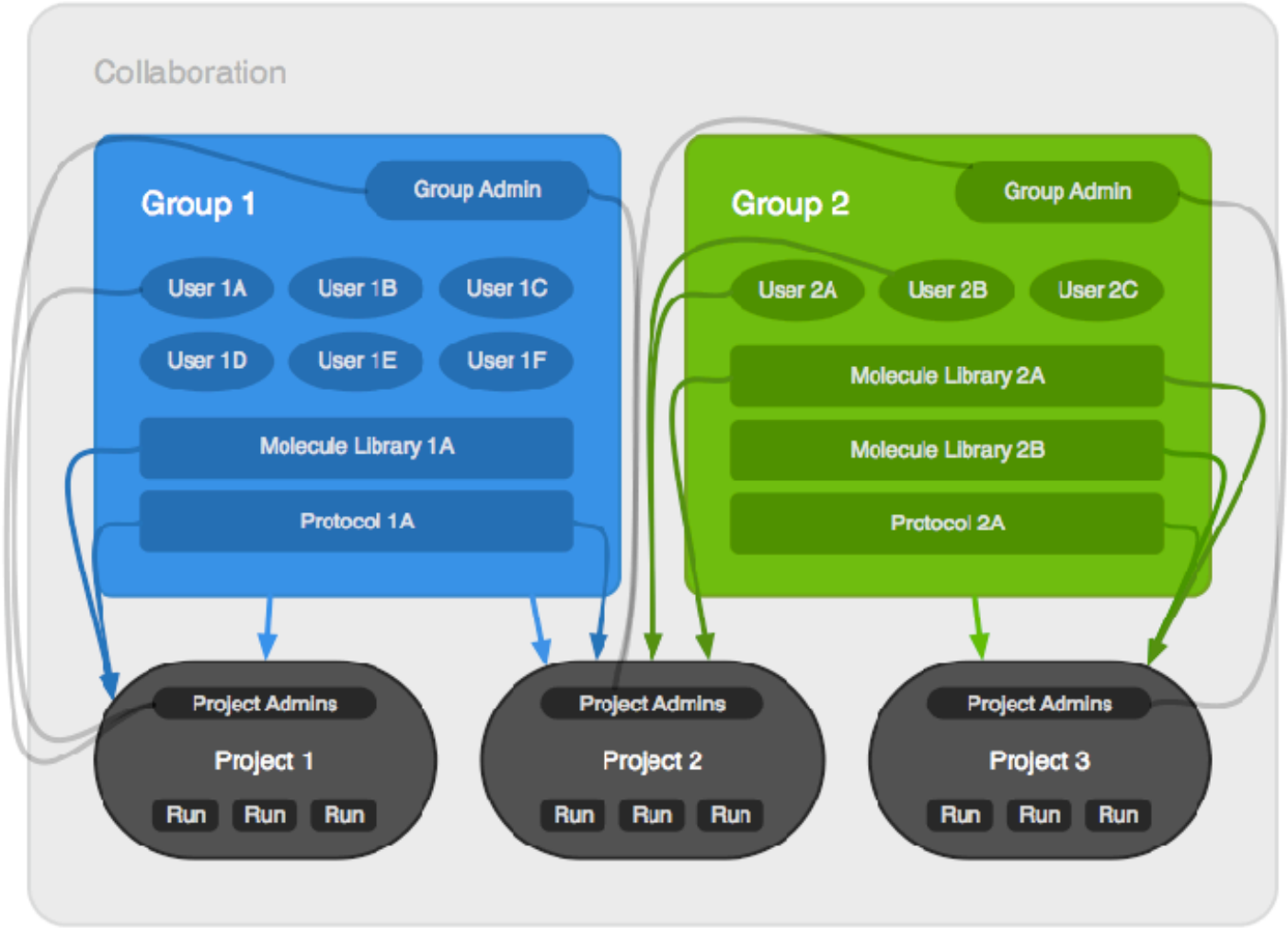
COLLABORATIVE DRUG DISCOVERY

What if?

- Technology
- Collaborations

COLLABORATIVE DRUG DISCOVERY

Projects - complex



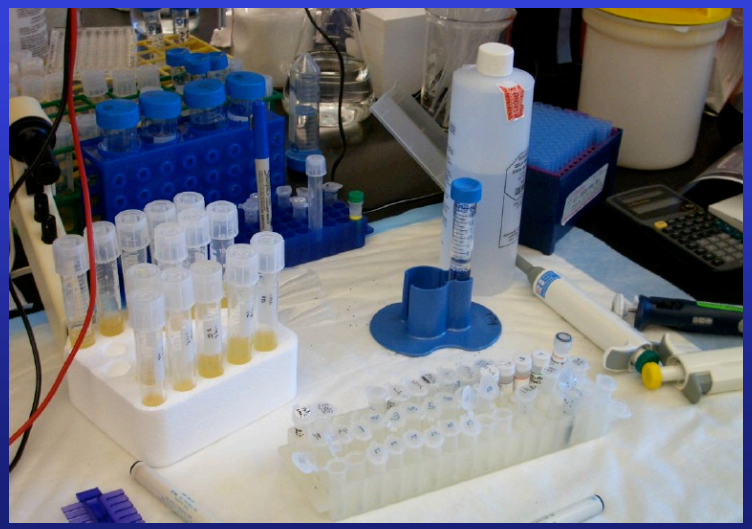
COLLABORATIVE DRUG DISCOVERY

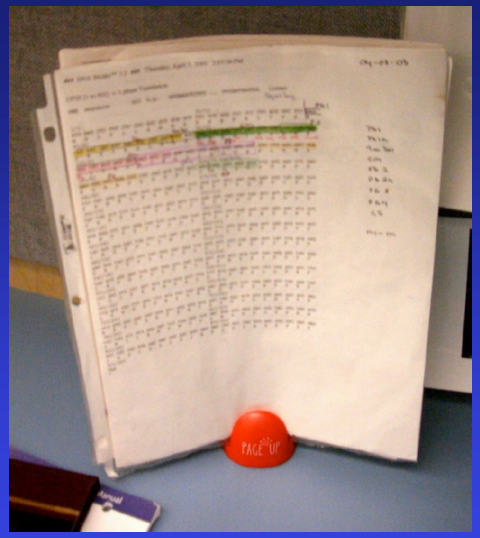
Who We Are

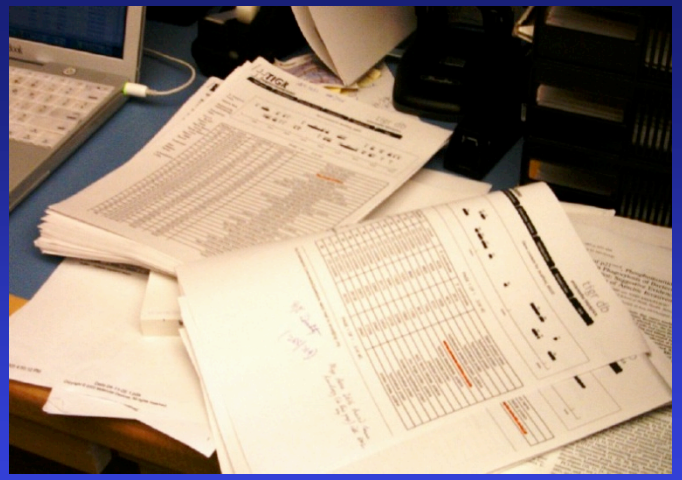
- **A private company, founded in 2004.**
- **Product: CDD database and custom services**
- **Working with thousands of leading researchers using CDD on six continents**
- **Provides secure "cloud-based" collaborative drug discovery embracing academic, non-profit, and for-profit company researchers (cultures) in invitation-only groups**
  - Affordable, easy-to-use, yet extremely powerful
- **SAB:**
  - Christopher Lipinski, PhD (ex Pfizer)
  - James McKerrow, MD PhD
  - David Roos, PhD
  - Adam Renslo, PhD
  - Wes Van Voorhis, MD PhD
  - Jim Wikel (ex Eli Lilly)

COLLABORATIVE
DRUG
DISCOVERY

Typical Lab:
The Data Explosion Problem

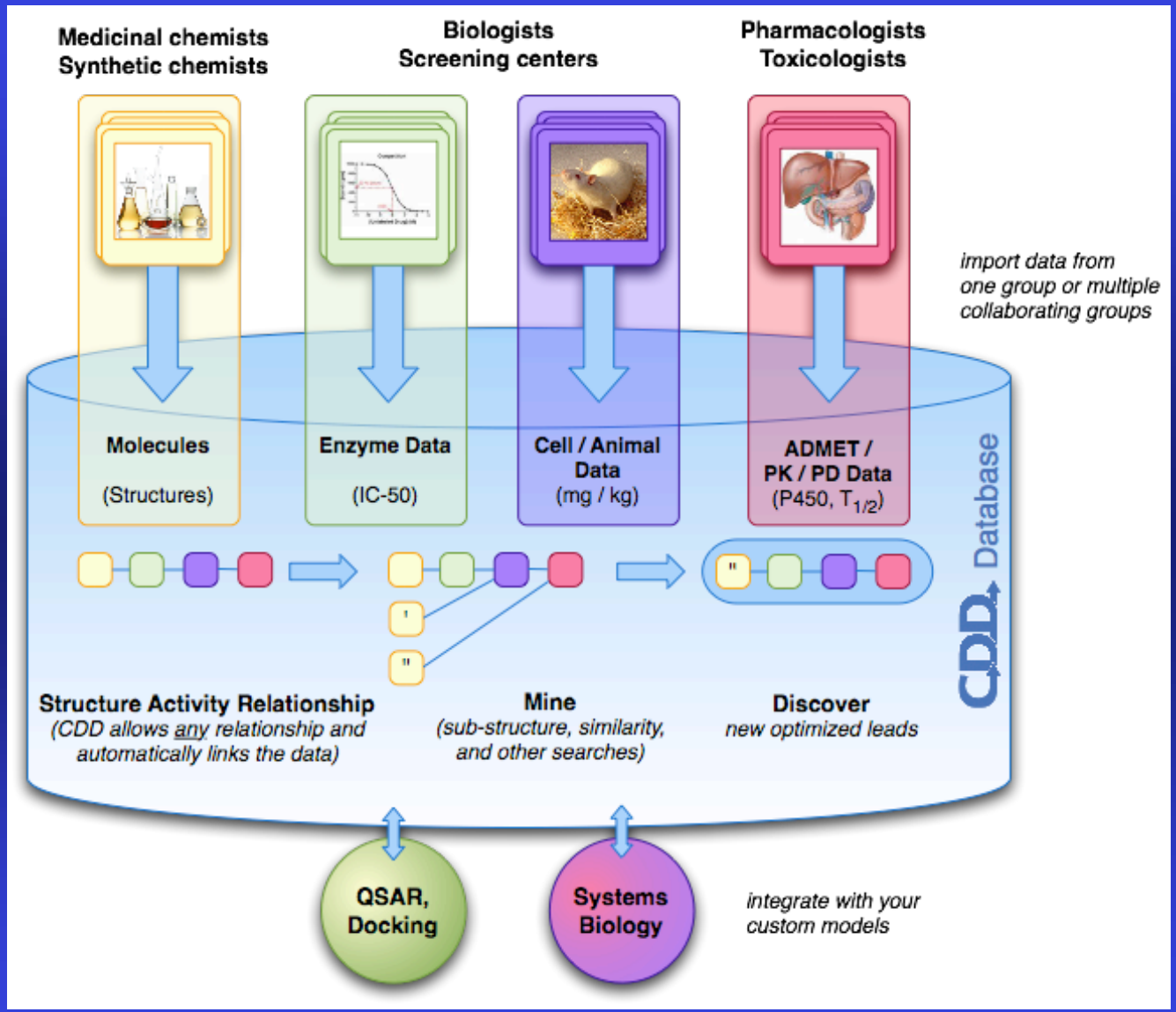






COLLABORATIVE DRUG DISCOVERY

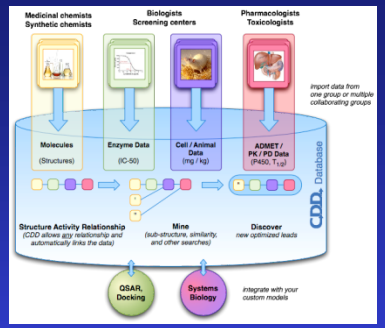
CDD Database for Your Private Data



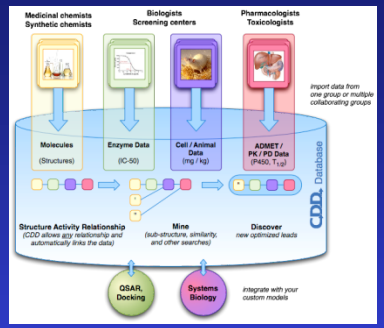
Collaborate Mode 1 – Big Pharma

with single login to multiple CROs/Biotech groups

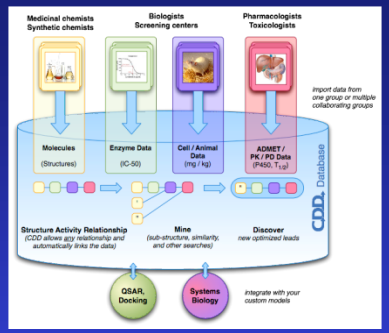
Consolidated CDD DB



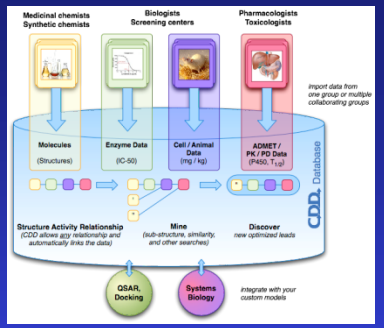
Collaborator 1



Collaborator 2



Collaborator 3



Collaborator 4

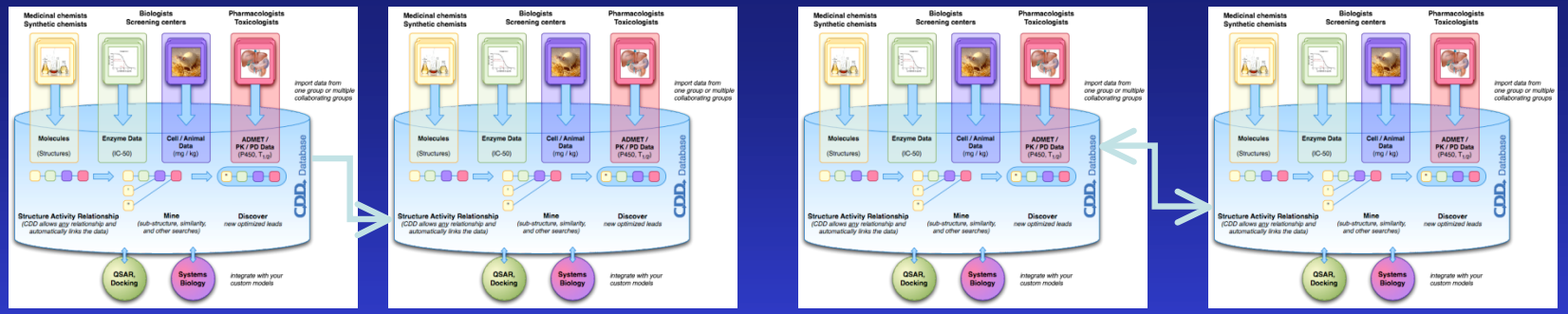
Collaborate Mode 2 – Academic + Foundations securely sharing data subsets

CDD DB group 1

CDD DB group 2

CDD DB group 3

CDD DB group 4



CDD database system

- Web based (log in securely into to your database from any computer).
- We host the server for you
- Highly secure, all traffic encrypted, server in a secure professionally hosted environment.

COLLABORATIVE
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DISCOVERY

Back pocket

Implementing Toxic Functionality Alerts (see Lipinski's presentation)

- **Basic Capability = 2 FTE weeks**
- **End User Flexibility = 1 FTE week**
- **Advanced Implementation = 3 FTE weeks**
- NOTE: Generally any feature can have about 25% of unforeseen features

Implementing Toxic Functionality Alerts (see Lipinski's presentation)

- **Basic Capability = 2 FTE weeks**
  - Store list of SMARTS alerts with the SMARTS, a name, and a text description (back end) - 1 point
  - Associate list of alerts that apply with structures - 1 point
  - Set up alerts to be automatically run when adding a new structure - 1 point
  - Run alerts against existing structures - 1 point
  - Ability to display alerts on the show molecule page - 2 points
- **End User Flexibility = 1 FTE week**
  - Allow super-users to manage this list - 2 points
  - Rerun alerts after they're changed against all structures - 1 point
- **Advanced Implementation = 3 FTE weeks**
  - Ability to display alerts in mine results - 3 points
  - Ability to mine by presence/absence of alerts in general - 2 points
  - Ability to mine by presence/absence of specific alerts - 3 points

➢ NOTE: Generally any feature can have about 25% of unforeseen features

Bunin Group

Dashboard | Group Data | Import Data | Share Data

Recent Activity | Messages 2 | Group Settings | People

Edit Group Settings

Group name: Bunin Group

Primary contact: Barry Bunin

Principal investigator:

Principal investigator email:

Institution:

Website URL:

External link setting:
- ○ Ban external links
- ◉ Allow external links
- ○ Allow external links and do not show a warning page

Experimental subject name: Substance

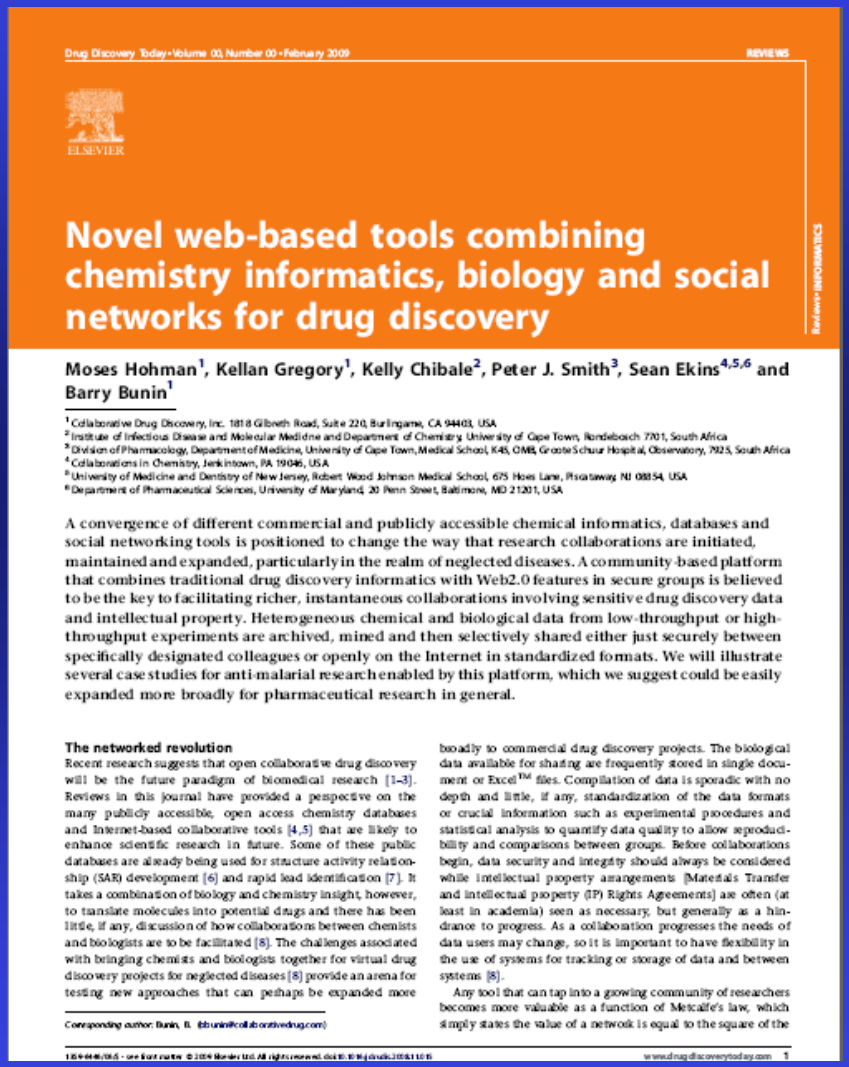
Experiment name: Screen

Run name: Test

Save changes or cancel

CDD Case Study Details

- **Published** Review in Drug Discovery Today 2009 (14: 261-270).



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]

[1] Collaborative Drug Discovery, Inc. 1818 Gilbreth Road, Suite 220, Burlingame, CA 94403, USA
[2] Institute of Infectious Disease and Molecular Medicine and Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa
[3] Division of Pharmacology, Department of Medicine, University of Cape Town, Medical School, K45, OMB, Groote Schuur Hospital, Observatory, 7925, South Africa
[4] Collaborations in Chemistry, Jenkintown, PA 19046, USA
[5] University of Medicine and Dentistry of New Jersey, Robert Wood Johnson Medical School, 675 Hoes Lane, Piscataway, NJ 08854, USA
[6] Department of Pharmaceutical Sciences, University of Maryland, 20 Penn Street, Baltimore, MD 21201, USA

A convergence of different commercial and publicly accessible chemical informatics, databases and social networking tools is positioned to change the way that research collaborations are initiated, maintained and expanded, particularly in the realm of neglected diseases. A community-based platform that combines traditional drug discovery informatics with Web2.0 features in secure groups is believed to be the key to facilitating richer, instantaneous collaborations involving sensitive drug discovery data and intellectual property. Heterogeneous chemical and biological data from low-throughput or high-throughput experiments are archived, mined and then selectively shared either just securely between specifically designated colleagues or openly on the Internet in standardized formats. We will illustrate several case studies for anti-malarial research enabled by this platform, which we suggest could be easily expanded more broadly for pharmaceutical research in general.

The networked revolution

Recent research suggests that open collaborative drug discovery will be the future paradigm of biomedical research [1–3]. Reviews in this journal have provided a perspective on the many publicly accessible, open access chemistry databases and Internet-based collaborative tools [4,5] that are likely to enhance scientific research in future. Some of these public databases are already being used for structure activity relationship (SAR) development [6] and rapid lead identification [7]. It takes a combination of biology and chemistry insight, however, to translate molecules into potential drugs and there has been little, if any, discussion of how collaborations between chemists and biologists are to be facilitated [8]. The challenges associated with bringing chemists and biologists together for virtual drug discovery projects for neglected diseases [8] provide an arena for testing new approaches that can perhaps be expanded more broadly to commercial drug discovery projects. The biological data available for sharing are frequently stored in single document or Excel™ files. Compilation of data is sporadic with no depth and little, if any, standardization of the data formats or crucial information such as experimental procedures and statistical analysis to quantify data quality to allow reproducibility and comparisons between groups. Before collaborations begin, data security and integrity should always be considered while intellectual property arrangements [Materials Transfer and Intellectual Property (IP) Rights Agreements] are often (at least in academia) seen as necessary, but generally as a hindrance to progress. As a collaboration progresses the needs of data users may change, so it is important to have flexibility in the use of systems for tracking or storage of data and between systems [8].

Any tool that can tap into a growing community of researchers becomes more valuable as a function of Metcalfe's law, which simply states the value of a network is equal to the square of the

Corresponding author: Bunin, B. (bbunin@collaborativedrug.com)

 doi:10.1016/j.drudis.2008.11.015

CDD Successfully Builds Collaborative Drug Discovery Communities

- Published Review in Drug Discovery Today 2009 (14: 261-270).
- $1.89M Tuberculosis B&MGF Project
- Thousands of scientists engaged:

Home /

Organizations that benefit from CDD

- ASINEX
- BioSeek, Inc.
- Broad Institute
- Cedars-Sinai Medical Center
- ChemBridge Corporation
- Columbia University
- Cornell University
- Drugs for Neglected Diseases initiative
- Fred Hutchinson Cancer Research Center
- Harvard University
- Indiana University
- Purdue University
- The Rockefeller University
- San Francisco VA Medical Center
- Scripps Research Institute
- Seattle Biomedical Research Institute
- Semafore Pharmaceuticals, Inc.
- St. Jude Children's Research Hospital
- Stanford University
- STATegics, Inc.
- TimTec, Inc.
- Torrey Pines Institute for Molecular Studies

Who Uses CDD?

Testimonials

"The CDD Database is an extremely elegant platform. I highly recommend it for anyone generating drug discovery data."

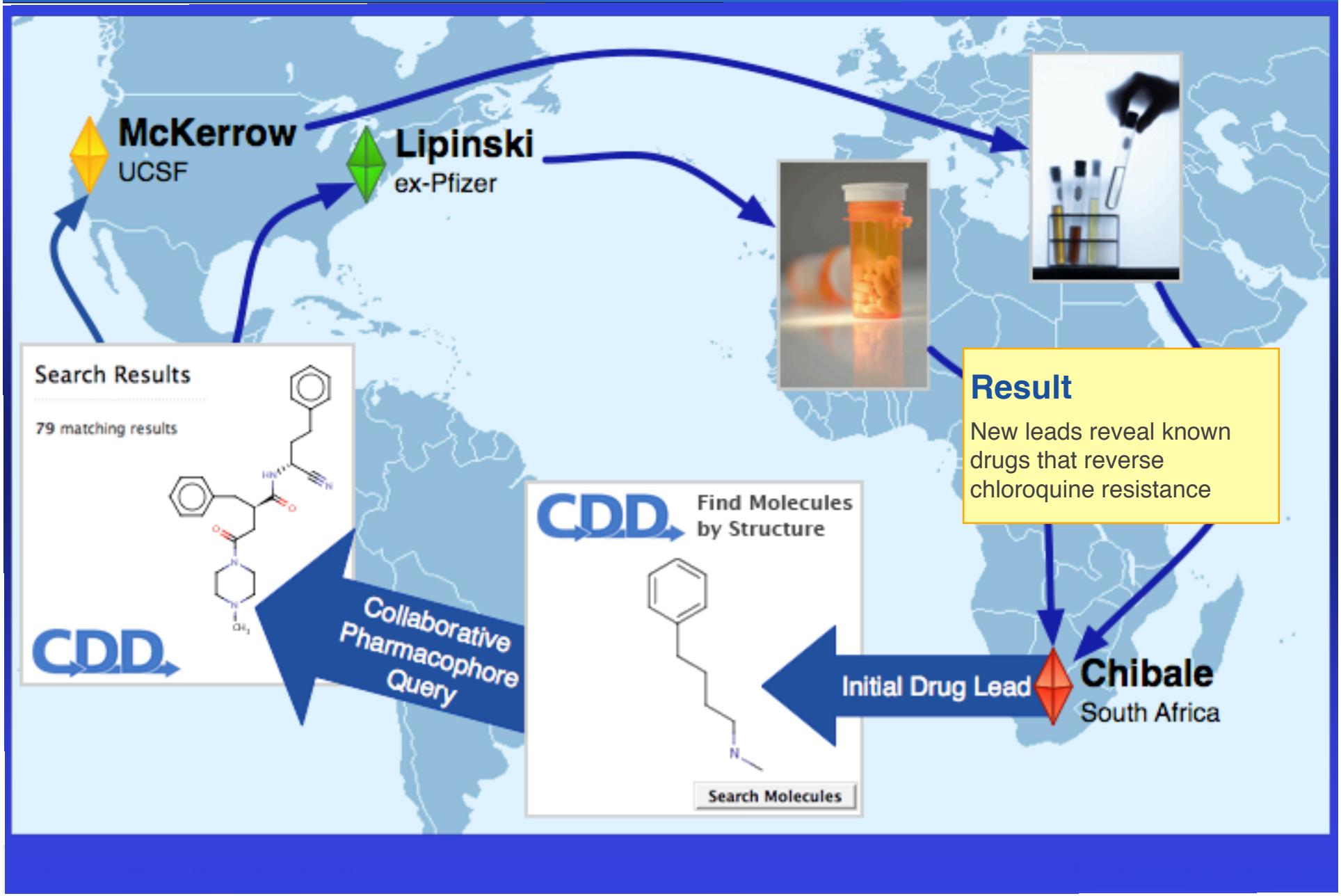
— Bryan Roth, M.D., Ph.D., University of

Collaborative Drug Discovery

- **Archive**
  - Organize and upload your experimental data
- **Mine**
  - Analyze your data to suggest new drug candidates
- **Collaborate**
  - Keep your data 100% private,
  - Exchange confidentially with collaborators, *or*…
  - Share openly within the CDD community

CDD COLLABORATIVE DRUG DISCOVERY

Collaborate



CDD Database system

- CDD works right “out of the box”, no implementation hassle. Login & go.
- User can access (with Firefox browser) from Windows, Mac, even Linux/Unix
- A wide variety of data formats are supported including Chemical structure formats like SD format or SMILES. Files (images, pdf etc. can be associated to multiple entities)
- Easy to use - no special knowledge required; navigation with familiar web-browser tools like hyperlinks, tabs, dropdown menus etc.
- Different user privileges can be set according to your user structure.
- Supports Collaborations

COLLABORATIVE DRUG DISCOVERY

CDD Database system – Distributed Research

- Ability to tap into hundreds of external researchers data with no lengthy business/legal cycles
  - Save 6-12 months on a new discovery
- No need to “poke a hole” into your Firewall
- No need for users to have any IT expertise
- 3rd party for hosting – liability relief

CDD as collaboration platform

- You decide which data to share with whom
  (we currently manage this on our server via group management)
- Store and share protocols
- Via a unique identifier (e.g. a structure, a name, a unique label) teams from diverse disciplines as Chemistry, Toxicology, Assay design, animal studies etc. can share their data in real time.
- Collaborate across different organizations. Our technology and pricing enables and supports a variety of collaboration models.
- Publication mechanism: Specialized community data collections are available for no charge. Current collections – see next slide

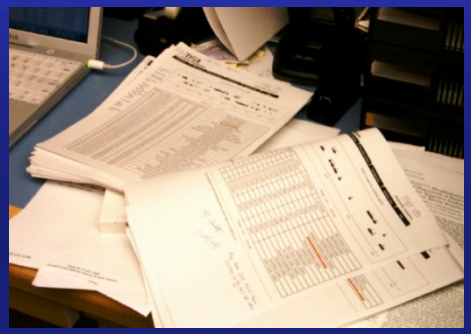
CDD database – more details

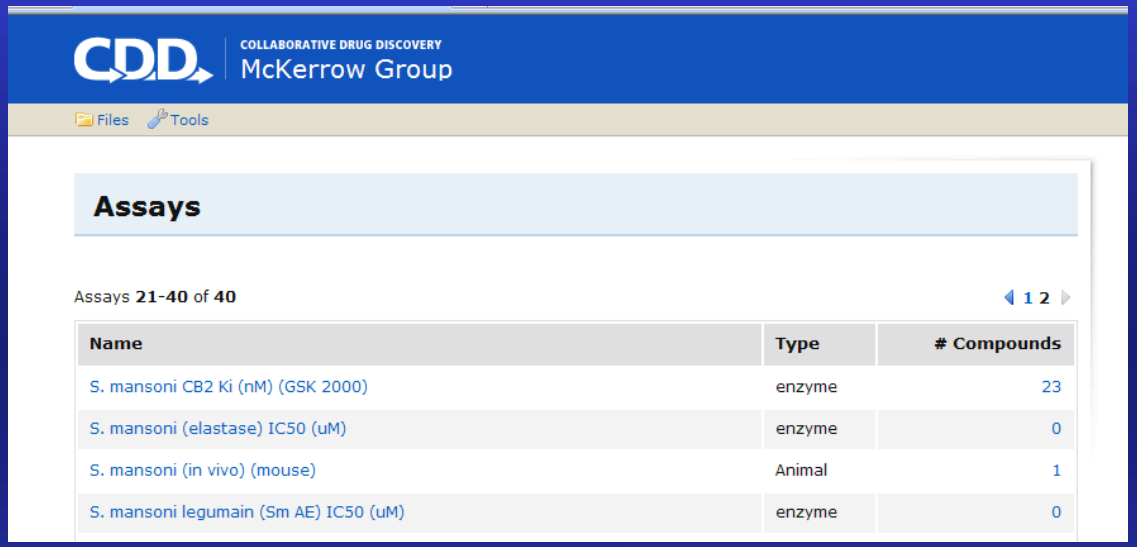
- Easy batch import of your data is supported by a mapper and slurper.
- Add molecules, analytical, or biological data manually, all required tools are integrated.
- Export your data with Chemical structures into Excel without the need for extra plugins or extra software.
- Chemical drawing tool integrated which is powerful and very easy to use.
- Plates, heatmaps, property calculations, 3D views and much more (similarity search by end of Jan/08)

CDD "Agile" Development Advantage

- Traditional software development life cycle (6-12 months)
- CDD Agile development includes automated testing:
  - Biweekly minor updates
  - Monthly major updates
- Recent examples:
  - Logins to multiple groups for screening centers
  - Dashboard for intra-group coordination
  - Customize mine results

Archive




COLLABORATIVE DRUG DISCOVERY
McKerrow Group
Files
Tools
Assays
Assays 21-40 of 40
1 2
Name
Type
Compounds
S. mansoni CB2 Ki (nM) (GSK 2000)
enzyme
23
S. mansoni (elastase) IC50 (uM)
enzyme
0
S. mansoni (in vivo) (mouse)
Animal
1
S. mansoni legumain (Sm AE) IC50 (uM)
enzyme
0

Molecules /

9 from Table 1 (Merck Compound)

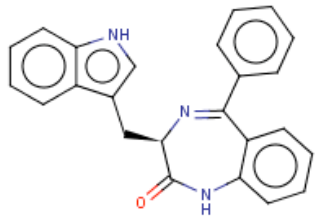
Owner: Barry Bunin
Created: 7/30/2007
Updated: 1/9/2008

Find other molecules containing this structure

Delete this molecule

Definition | Edit definition | Add synonym | Add user defined field

Name	9 from Table 1 (Merck Compound)
Synonyms	AA = R-Trp, RX = H
Description	Note - literature compound used as Internal Standard.
SMILES	O=C1Nc2ccccc2C(=N[C@@H]1Cc3c[nH]c4ccccc34)c5ccccc5
Solubility	10 uM



Molecular weight	365.427 g/mol
log P	5.0459
H-bond donors	2
H-bond acceptors	2
Lipinski Rule of 5	One violation 3 of 4 within desirable range

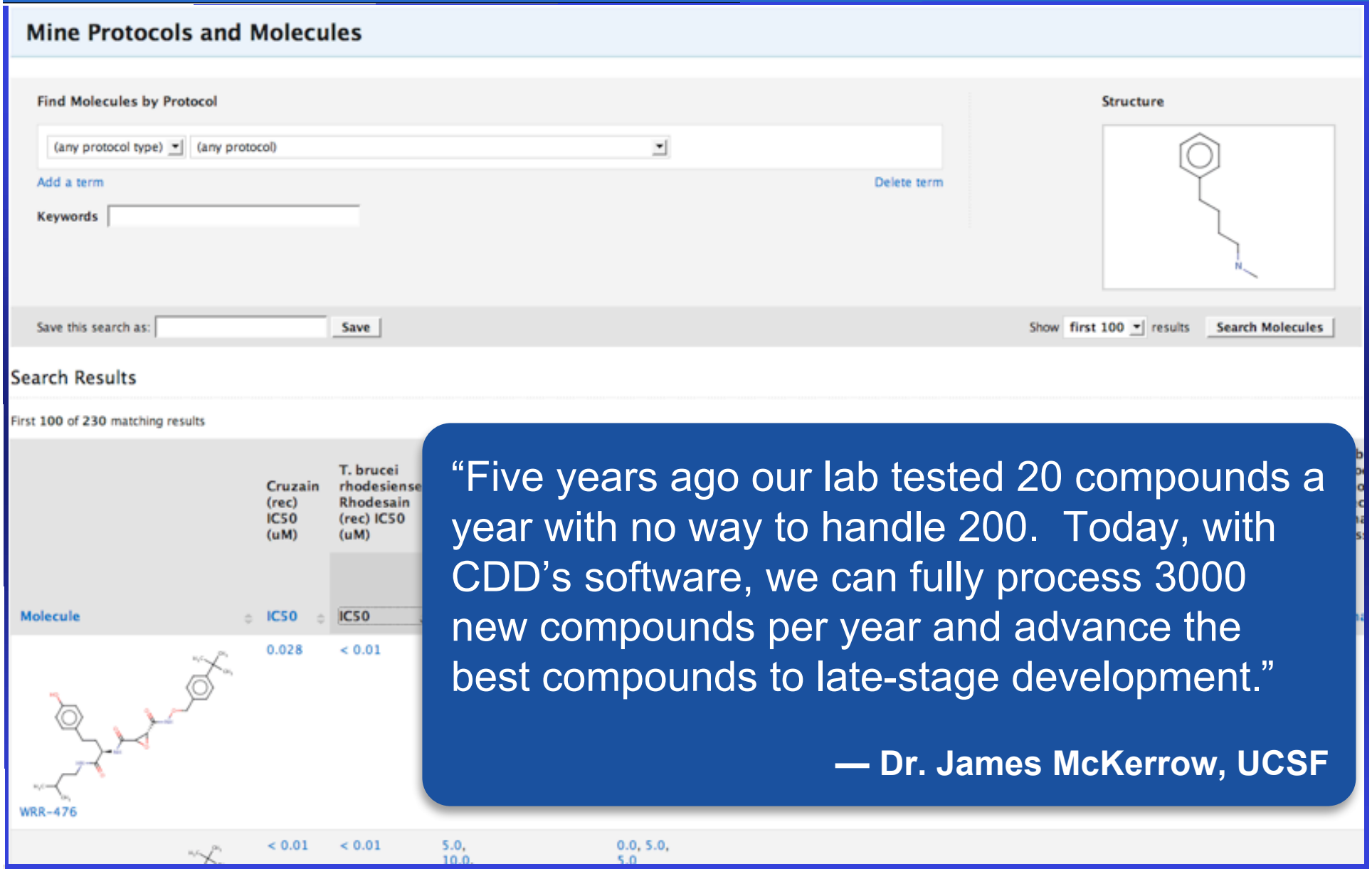
Formula	$C_{24}H_{19}N_3O$
pK_a	3.2221
Exact mass	365.153 g/mol
Atom count	47

Batches: 1 | Add a batch

Name	Date	Location	Who	Notes	#Protocols	Actions
1	2004-02-14	-20 Freezer	Barry	>99% Pure by HPLC 214 nM	0	

Plates: 1

Name	Size	Protocol Run
BAB-003	96	• CCK A receptor binding affinities



"Five years ago our lab tested 20 compounds a year with no way to handle 200. Today, with CDD's software, we can fully process 3000 new compounds per year and advance the best compounds to late-stage development."

— Dr. James McKerrow, UCSF

COLLABORATIVE DRUG DISCOVERY

CDD database – other benefits

- Low total cost of ownership: You do not need to buy and maintain your own server, run updates, have an IT specialist; minimal time for training; reasonable license fees. Lots of tools integrated which otherwise need to be purchased extra (structure editor, export with structures into regular Excel etc.).
- Superior customer support (support schedule including regular trainings and pings; collaboration support)
- Chemaxon tools integrated.
- New features added regularly and do not need to wait for a maintenance schedule.

COLLABORATIVE DRUG DISCOVERY

Testimonials

- "Five years ago our lab tested 20 compounds a year with no way to handle 200. Today, with CDD's software, we can fully process 3,000 new compounds per year and advance the best compounds to late-stage development."
  - James McKerrow, MD, PhD, UCSF
- "One of the biggest barriers for academic drug discovery is the poor access to chemical data represented in an intelligent format. CDD presents data and associated tools that capture the relationship between chemical structure and biological activity. Structure-Activity Relationship (SAR) data substantially improve the distributed drug discovery process."
  - Christopher Lipinski, PhD, Pfizer, Retired
- "It's a great tool for mining and sharing data with collaborators. I've used a couple of other programs, but they don't put everything together so intuitively."
  - Mary Lynn Baniecki, PhD, Clardy Laboratory, Harvard Medical School
- "I was very impressed by the system's simplicity, responsiveness and functionality. It certainly looks better than anything I've seen so far."
  - Wayne Best, PhD
- "The CDD Database is an extremely elegant platform. I highly recommend it for anyone generating drug discovery data."
  - Bryan Roth, MD, PhD, University of North Carolina

COLLABORATIVE DRUG DISCOVERY

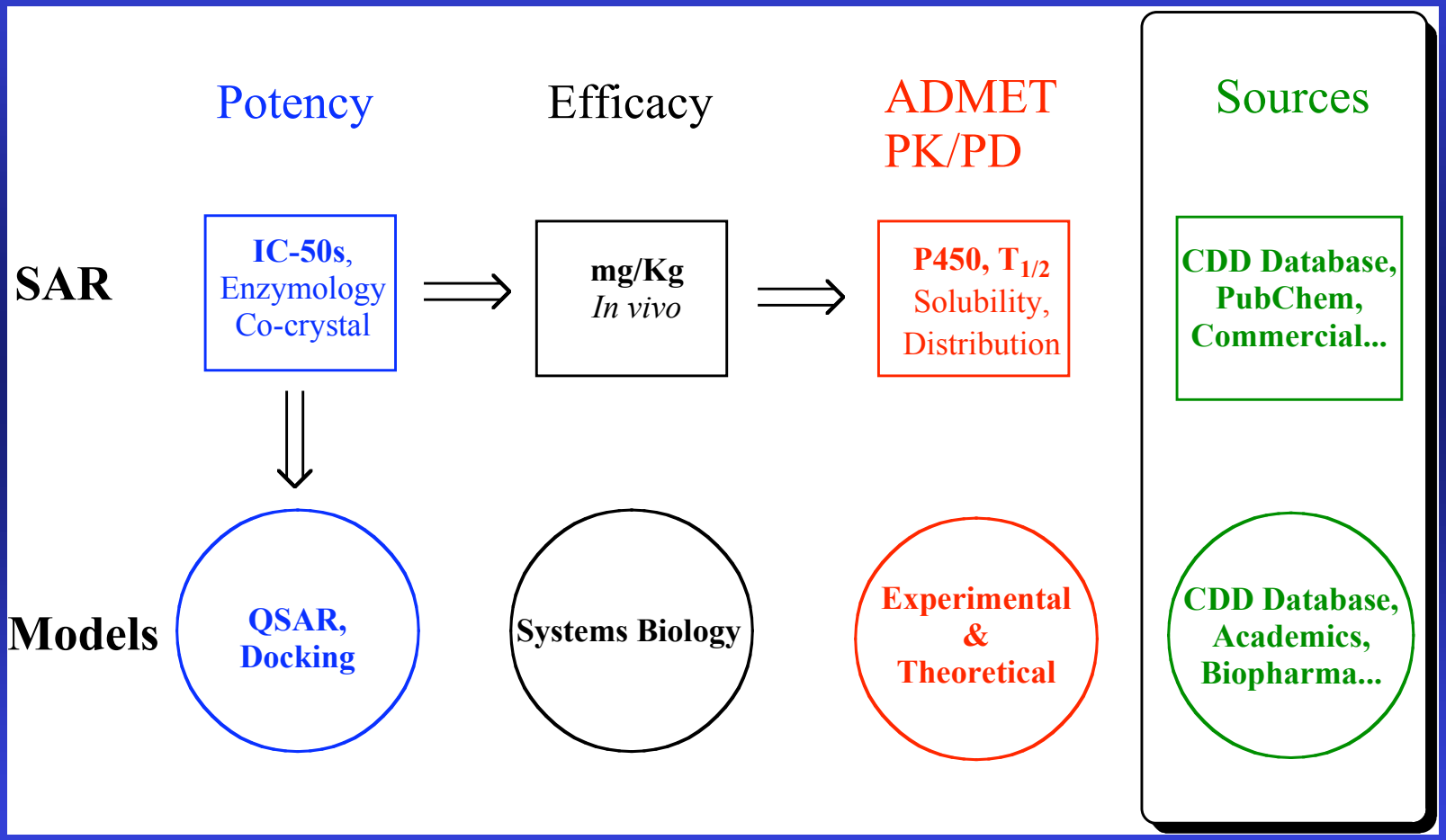
CDD Current Community & Strategic Relationships

- ASINEX, Inc.
- Broad Institute
- Cedars-Sinai Medical Center
- Columbia University
- Cornell University
- Drugs for Neglected Diseases initiative
- Fred Hutchinson CRC
- Gates Foundation (BMGF)
- Harvard University
- Indiana University–Purdue University Indianapolis
- Johns Hopkins
- Louisiana State University
- Marine Biological Laboratory
- MIT
- Myelin Repair Foundation
- Purdue University
- San Francisco VA Medical Center
- Seattle Biomedical Research Institute
- Semafore Pharmaceuticals, Inc.
- Stanford University
- St. Jude Children's Research Hospital
- SureChem
- TimTec, Inc.
- UCSF General Hospital
- University of California, Berkeley
- University of California, Los Angeles
- University of California, San Francisco
- University of California, Santa Cruz
- University of Cape Town
- University of Mississippi
- University of North Carolina
- University of Pennsylvania
- University of Sydney
- University of Texas
- University of Washington

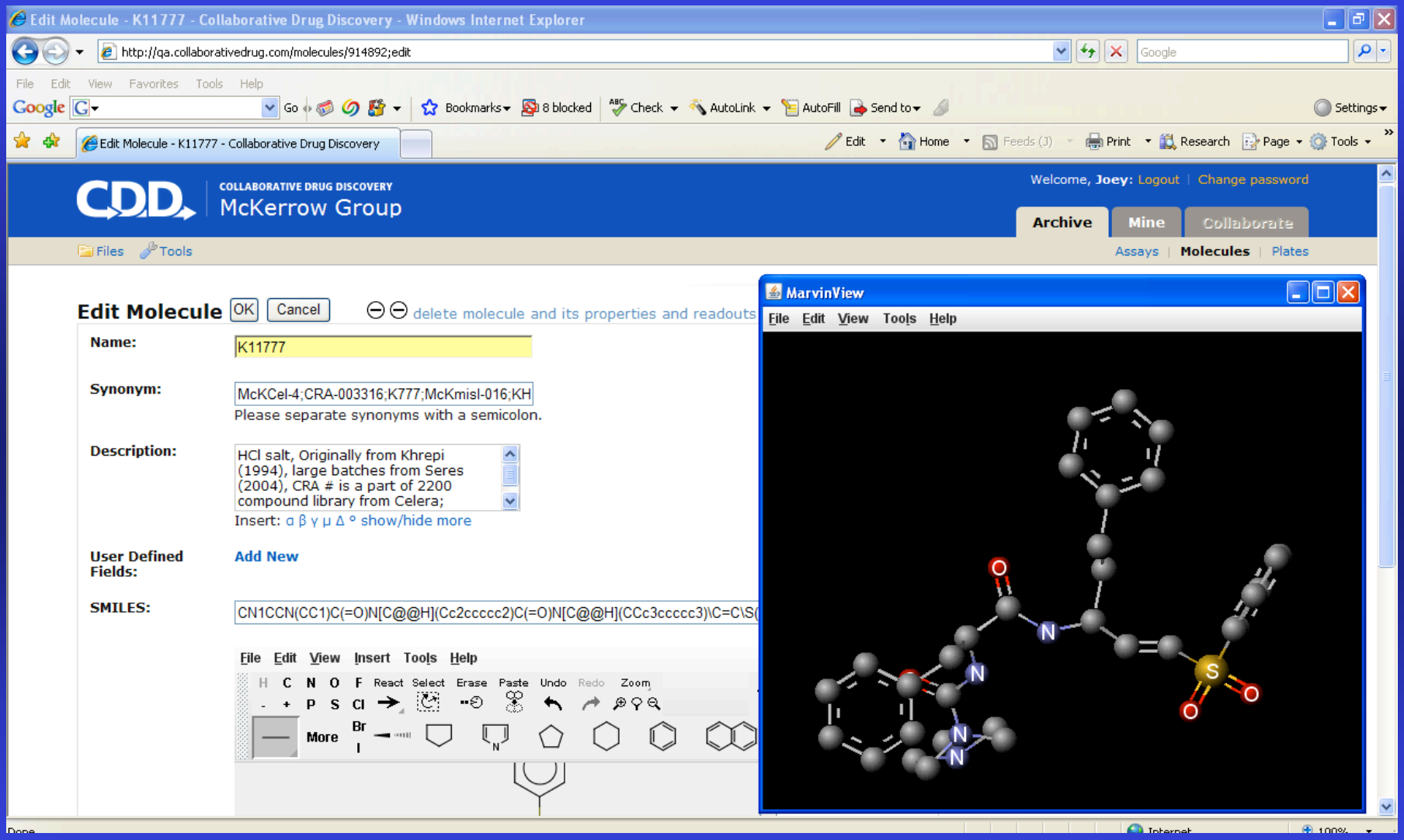
- All at: www.collaborativedrug.com/who

COLLABORATIVE DRUG DISCOVERY

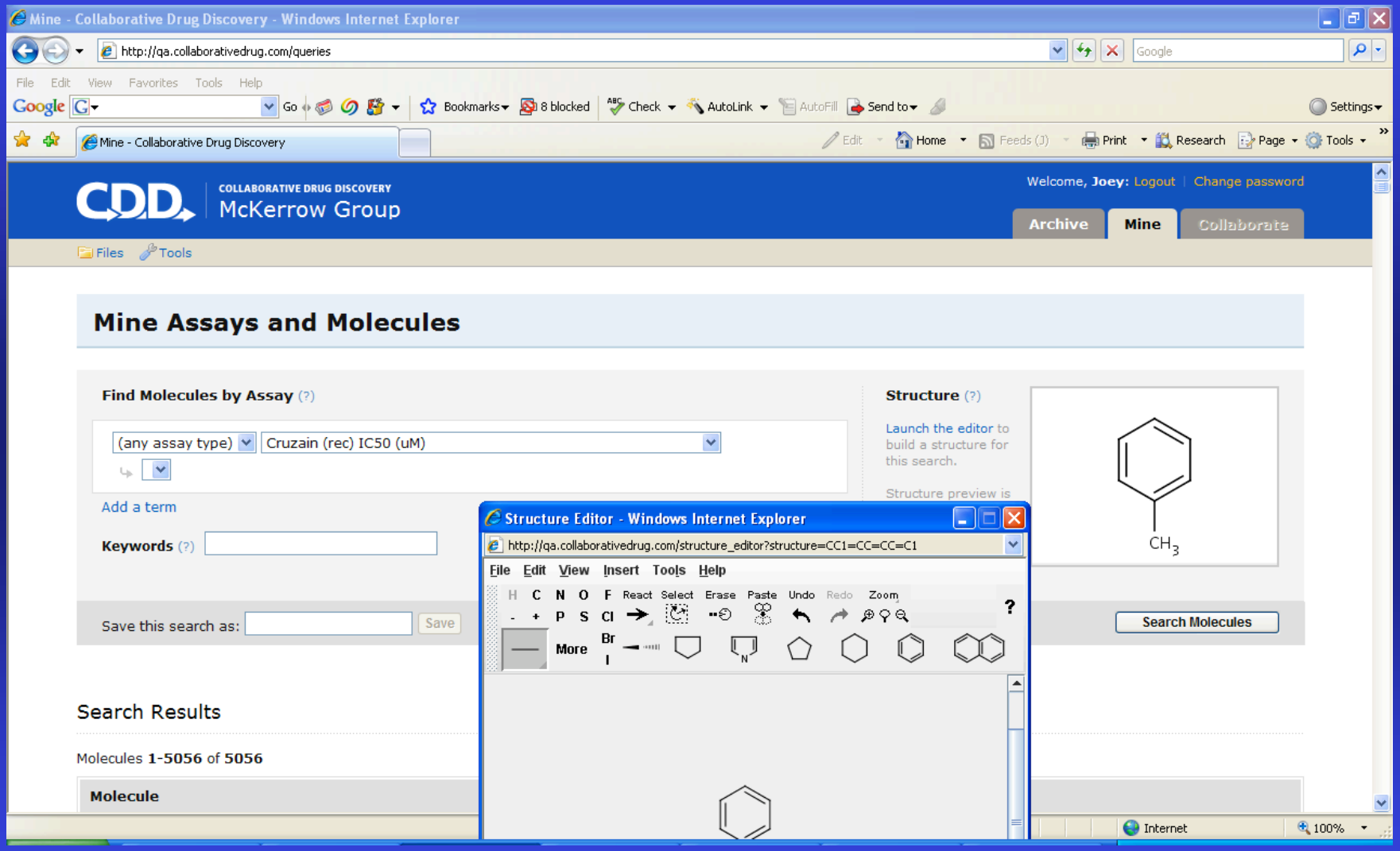
Archive Preclinical SAR (with any *Relationship*)



CDD COLLABORATIVE DRUG DISCOVERY



COLLABORATIVE DRUG DISCOVERY



COLLABORATIVE DRUG DISCOVERY

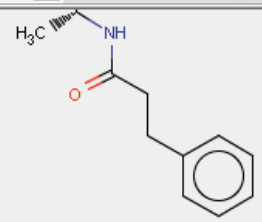
search -

File Edit View Favorites Tools Help

Back Search Favorites

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

Google wsgr Search 14 blocked Check AutoLink AutoFill Options wsgr



Search Molecules

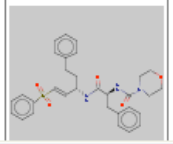
Display Option:

Number of search results per page 20

Clear Result | Export to Excel | Export to SDFile | 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

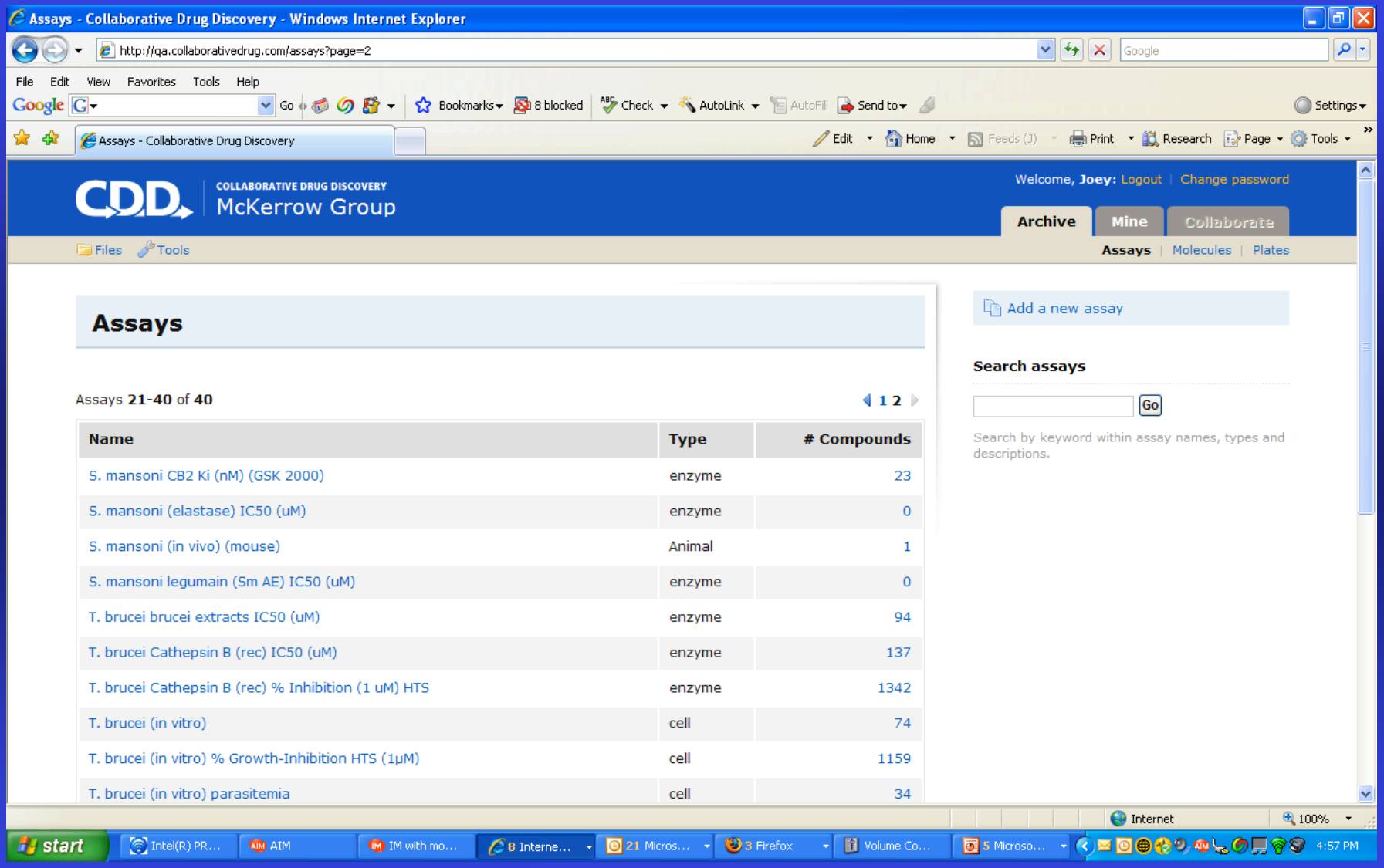
Molecule	Structure	Cruzain (rec) IC50 (uM) DU4-71 (%)	Cruzain (rec) IC50 (uM) IC50 (nM)	Cruzain (rec) IC50 (uM) IC50 (uM)	Cruzain (rec) IC50 (uM) Ki (uM)	Cruzain (rec) IC50 (uM) kobs/I (see excel) (M)	T. cruzi: In vitro assay Days Survival (days)
K11002	search 			0.01			8.0--25.0

Internet

CDD – Community Open Access Data

1. **Dr. Christopher Lipinski**
   Chemoinformatics data on FDA and Orphan approved drugs
2. **Prof. Roos (U. Penn)**
   Modern Malaria literature data linked to genes
3. **Prof. Gelb (UW)**
   Modern Malaria literature data linked to assays
4. **Prof. Guy (St. Jude CRH)**
   >15,000 Army Malaria screening data dating back to WW-II after escrow period
5. **Prof. McKerrow (UCSF)**
   "Open-Content" Drug discovery – T. Brucei, T. Cruzi, S. Mansoni, Leishmania, P. falciparum

COLLABORATIVE DRUG DISCOVERY



CDD COLLABORATIVE DRUG DISCOVERY

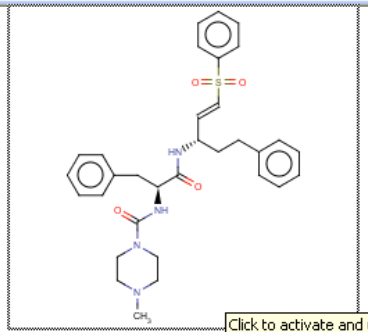
K11777 - Collaborative Drug Discovery - Windows Internet Explorer

http://qa.collaborativedrug.com/molecules/914892

File Edit View Favorites Tools Help

K11777 - Collaborative Drug Discovery

Name	K11777
Synonyms	McKCel-4;CRA-003316;K777;McKmisI-016;KH11777
Description	HCl salt, Originally from Khrepi (1994), large batches from Seres (2004), CRA # is a part of 2200 compound library from Celera; Delivered=Celera 2006
SMILES	CN1CCN(CC1)C(=O)N[C@@H](Cc2ccccc2)C(=O)N[C@@H](CCc3ccccc3)\C=C\S(=O)(=O)c4ccccc4



Double-click image above to see alternate views

Batches: 3

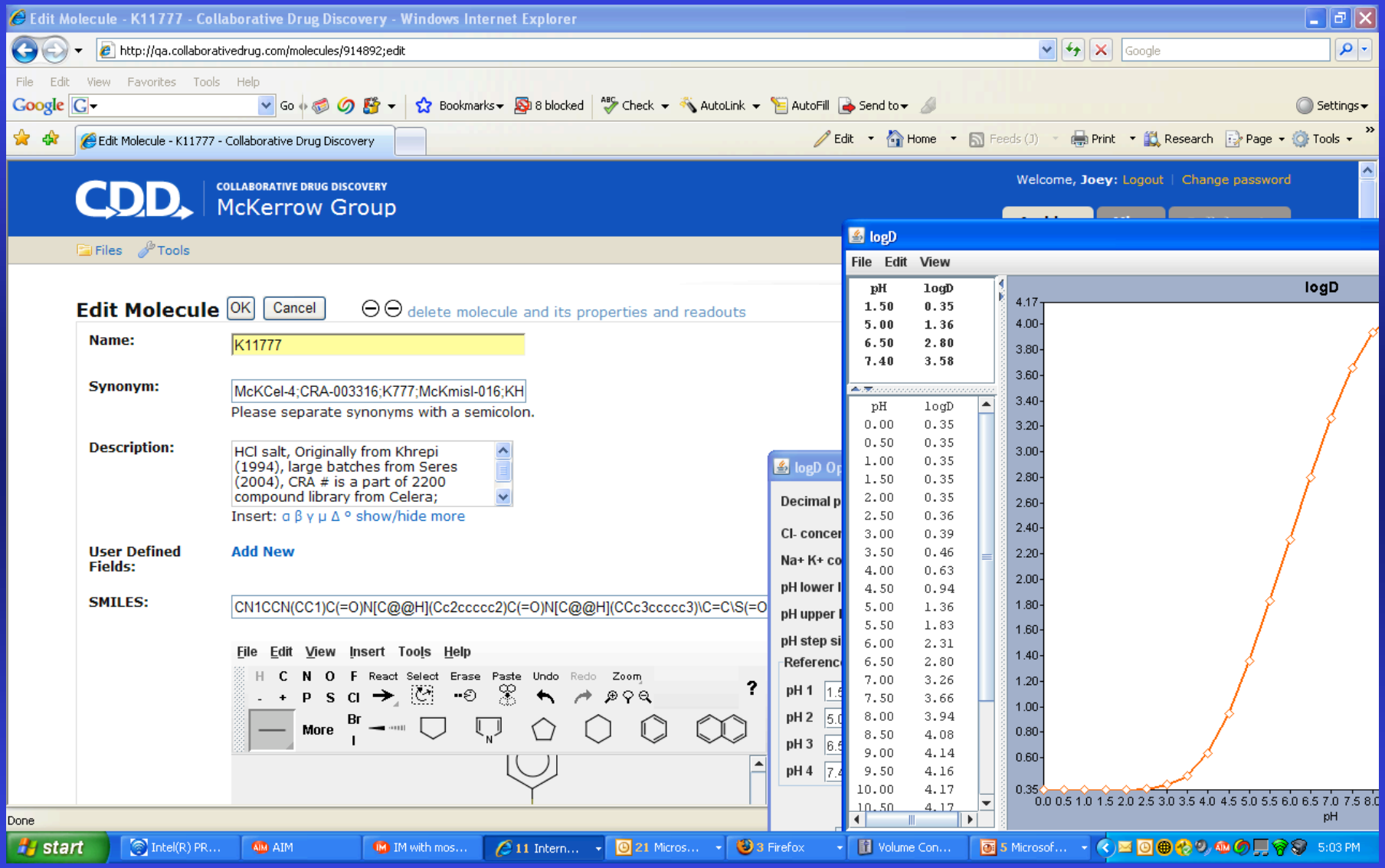
Name	Date	Location	Who	Notes	#Assays
	2006-05-24				8
Batch-01					2
BATCH-1	2006-05-25				1

Plates: 0

Assays: 12

Assay Name	Run Date	Readout	Value
Cruzain (rec) IC50 (uM)	2005-02-17	IC50 (uM)	0.1
T. cruzi: In vitro assay	2005-04-04	Days survival minus control (days)	

CDD COLLABORATIVE DRUG DISCOVERY



CDD database system: Security overview

- *CDD encrypts all traffic between a user's web browser and our servers once the user has logged in.*
- *CDD does thorough automated testing of our application code, including security tests to make sure one group cannot access another group's private data.*
- *CDD uses two levels of firewalling ("defense in depth"), hardware and software, for each sensitive server in our server environment.*
- *CDD encrypts all database and customer file backups using public key cryptography, and the private keys are backed up securely.*
- *CDD stores user passwords in our database using strong, one-way encryption hashes.*
- *CDD stays current with all security updates to our system software, firmware and operating systems.*
- *CDD uses Linux systems in production.*
- *A number of application security enhancements around password security are being made mandatory.*
- *Access to production servers and superuser accounts is limited and audited within CDD.*