



Noteworthy recent enhancements and a preview of things to come

Kellan Gregory, Director of Product Management

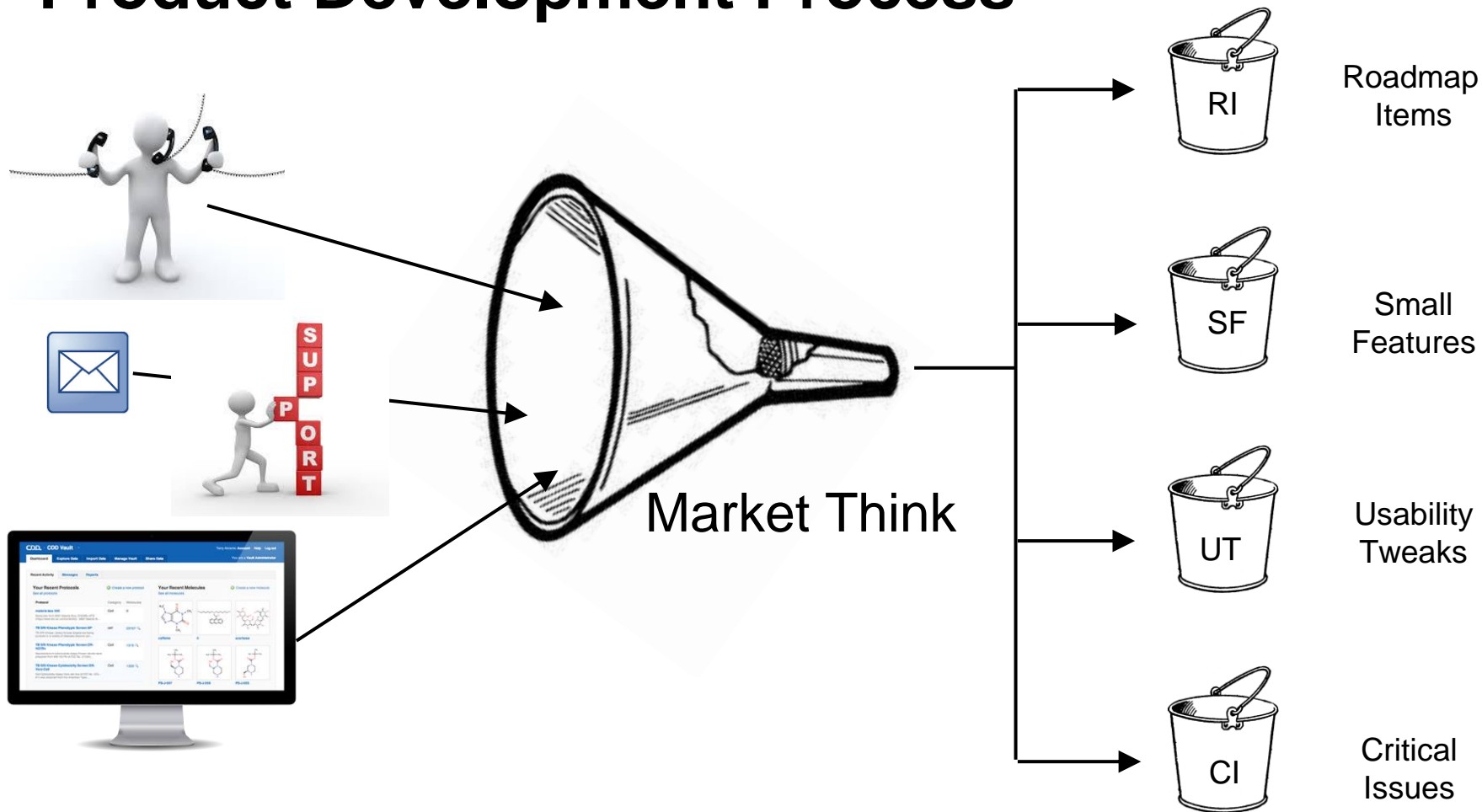
David Blondeau, Head of Software Development and Security Officer



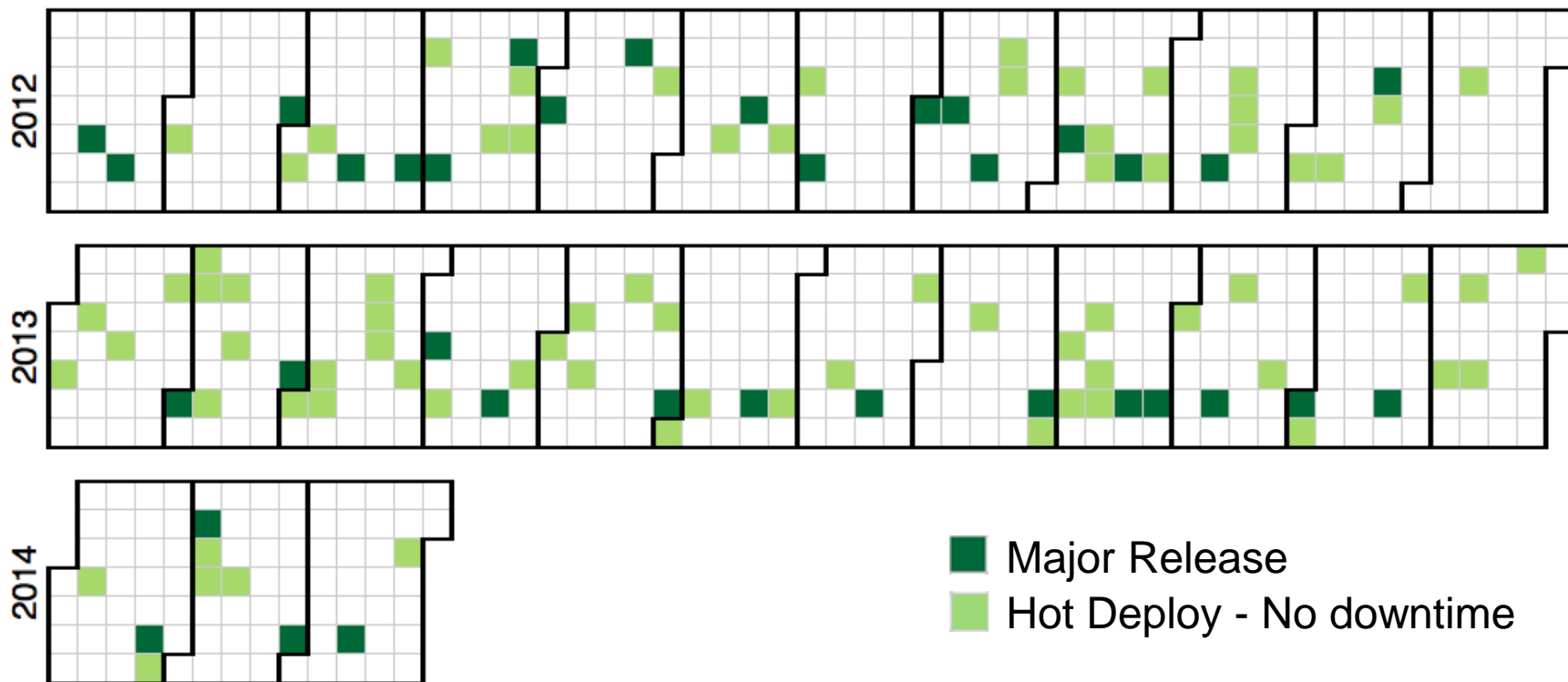
COLLABORATIVE
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CDD = Community Driven Development

Product Development Process



100+ Updates in the last 2 years



Community Shout Outs

- Jim McKerrow
- Ken Duncan
- Fraser Glickman
- Jeff Blaney
- Enrique Michelotti

And many more that participated to contextual inquiry and usability testing sessions



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Recent Enhancements

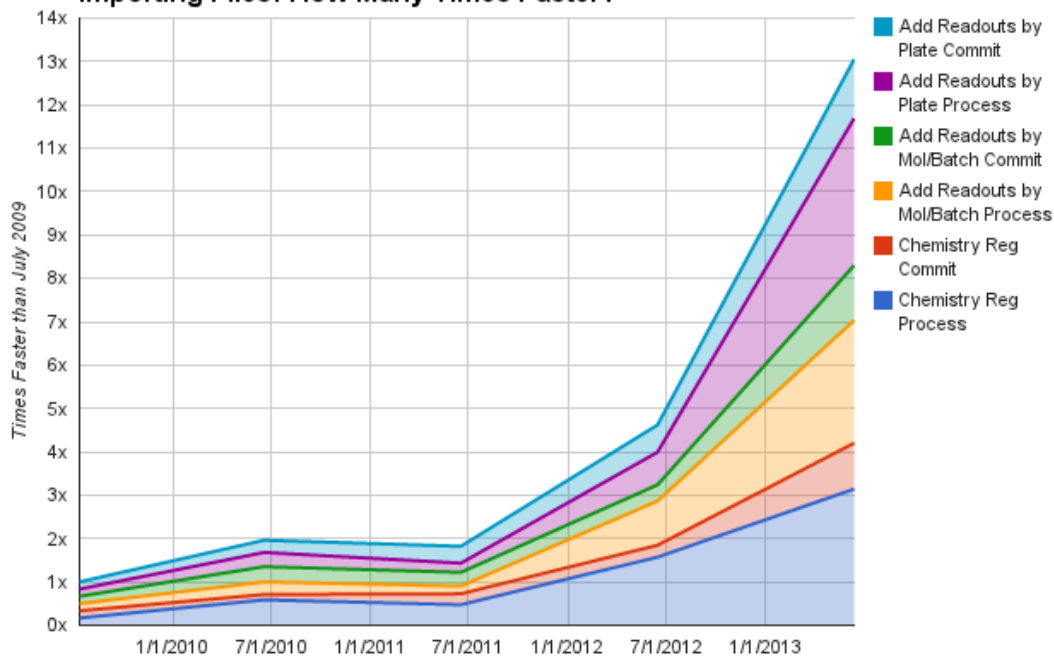
Faster Data Import

▶ Workbook4.csv	April 2, 2013	Awaiting confirmation
▶ Lesson2_CMPD_Library.csv	April 2, 2013	Awaiting confirmation
▶ Workbook12.csv	April 2, 2013	Queued (#1)

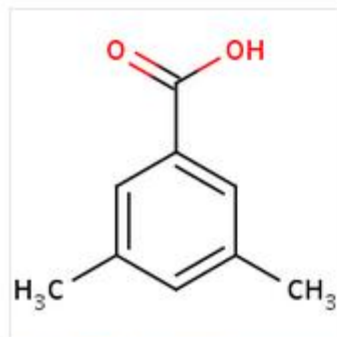
Your Current Imports:

Workbook4.csv *Processed (1 Error)* [Email me updates](#)
 Workbook12.csv *Queued (#1)* [Email me updates](#)
[click to view QC report](#)

Importing Files: How Many Times Faster?



Full Analytical Data Round Trip



CDD-61778 (See more data sources)

[Find molecules with this structure](#)

[View ChemSpider page](#)

[Add to a collection](#)

[Add a batch](#)

[Manage project access](#)

Overview Batches 1 Plates 0 Protocols 0 Collections 0 Projects 1

Batch

001

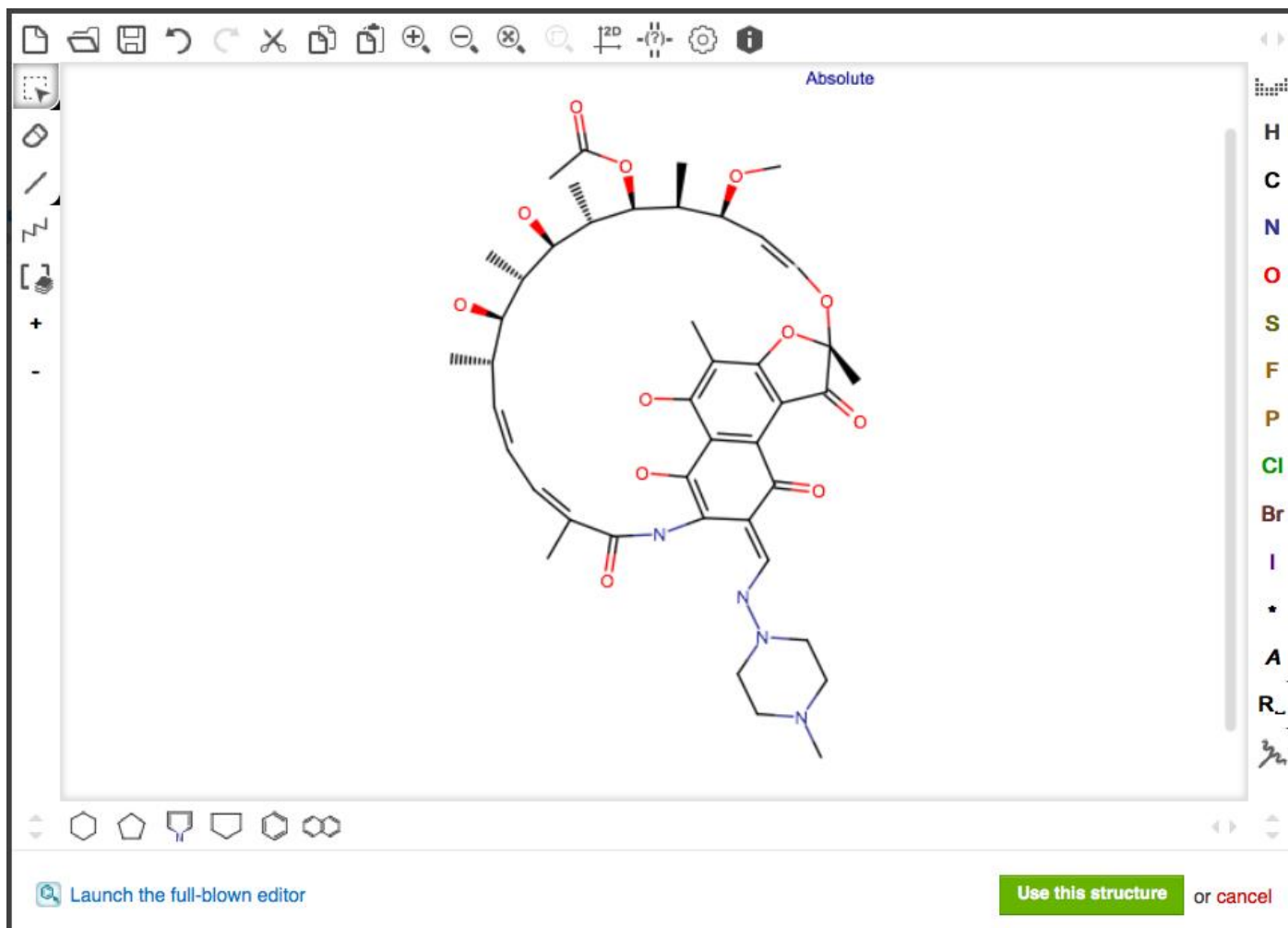
Salt: No Salt, free base or acid
 initial amount (mg): Solubility in DMSO:
 FW: 150.174 g/mol Date: 2013-10-10 Vendor ID:
 Barcode: 129472 Person: Terry Jones
 Lab Notebook #: CDD-0123 Vendor: CDD

NMR:

The NMR spectrum shows peaks at 12.6 ppm (carboxylic acid proton), 7.73 ppm (aromatic protons), 7.22 ppm (aromatic proton), 2.37 ppm (methyl protons), and 0 ppm (TMS). Integration values are shown below the peaks: 5.1, 9.8, 4.9, 30.3, and 0.8.

Select	Molecule *	v2 P. Falciperum IC50	Microscopy	File	Dose-response Plot
all - none	<p>flag outliers</p> <p>CDT-0000051 CDD Tutorial</p>	0.000000705		Data.txt	<p>Flag outliers & Override</p>

Fast Modern Structure Editor



Validating Dose-Response Curves

6 Plates		% Inhib (%) Z'-factor (controls)	IC50 (uM) Reference molecule intercept	IC90 (uM) Reference molecule intercept	% Inhib (%) Positive control mean
Protocol Averages:		0.87 ± 0.00 (n = 6 plates)	321.85 ± 328.37 (n = 6 plates)	2896.61 ± 2955.35 (n = 6 plates)	98.17 ± 2.14 (n = 6 plate)
Delete	Screen-01	0.87	962.00 (n = 1)	8657.99 (n = 1)	98.17 ± 2.14 (n = 6)
Delete	Screen-02	0.87	320.14 (n = 1)	2881.22 (n = 1)	98.17 ± 2.14 (n = 6)

Description: The Levenberg–Marquardt algorithm is used to fit a Hill equation to dose-response data.

Fit Parameters: X: Unit:

Example: Concentration, Molar... Example: nM

Y: Unit:

Example: % Inhibition, RFU, raw data... Example: %

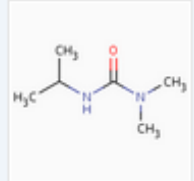
Normalization:

Type:

Name:

Subtract normalized value from 100% (e.g. for % Growth)

CDD Dose-response plot View plot Flag outliers & Override



ASCCDDPR-0000080

Assay & procedure: ABC-alpha2 Secondary

Run: Do Not Override
Cannot Be Calculated
✓ > 200 uM
< 1.00 uM

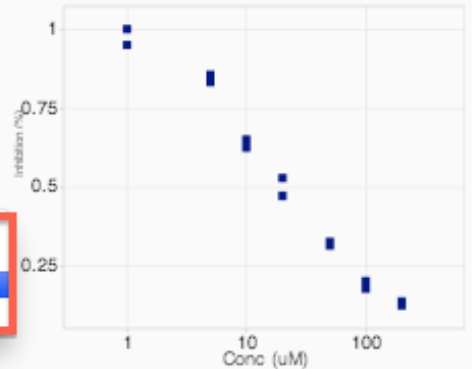
Batch:

IC50:

Min:

Max:

Hill slope:



Click points to mark outliers

Save Changes or cancel

[Reset Zoom](#) [Tips](#)

Reports and Alerts

[Dashboard](#)[Explore Data](#)[Import Data](#)[Manage Vault](#)You are a **Vault Administrator**[Recent Activity](#)[Messages](#)[Reports](#)Vault activity from to [Go](#)[Export report \(csv\)](#)

Project	New Batches	New Molecules	New Protocols	New Runs	New Readouts
CDD Tutorial	8	4	2	7	1,325
CRO Biology	0	0	0	1	0
CRO Chemistry	260	230	0	0	0
Total	266	231	2	8	1,325

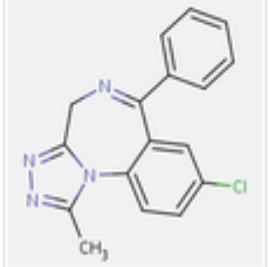
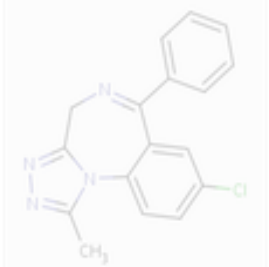
Notes: numbers are updated nightly; shared resources are only counted once for the totals, even if they occur in multiple projects.

CDD Weekly alerts for vault CDD Tutorial

BatchTerry Jones created batch [002](#) for molecule [CDT-0000004](#)[Manage your alerts.](#)

Collections

4 Selected Results: Plot results Export results Add results to collection

Select...	
all · none	Molecule [▲]
<input checked="" type="checkbox"/>	<p>CDD-30 <small>summary</small></p>  <p>CDT-0001297 CDD Tutorial</p>
<input type="checkbox"/>	<p>CDD-30 <small>summary</small></p>  <p>alprazolam Known drugs</p>

Add Selected Results To Collection ✕

Add to: New collection Existing collection

- There is already a collection with this name. Do you want to overwrite it?

Name:

Project: or private collection

Overwrite: Yes, overwrite existing collection

Save or cancel

CDD Vault Enterprise API

- Integrate CDD Vault with other data sources or internal tools
- Extend CDD Vault functionalities
- Read and Write - Fine grained and Bulk

The screenshot displays the CDD Vault Enterprise API user interface. At the top, a blue header bar contains the CDD logo and the text "Demo User" on the left, and an "Account" link on the right. Below the header, there are two navigation buttons: "Dashboard" and "Explore Data". The main content area has a tabbed interface with "Preferences" and "API Keys" tabs. The "API Keys" tab is active, showing the heading "Your API Keys". Below the heading is a table with columns for "Name", "Role", and "Token". At the bottom left of the table, there is a button labeled "Add a new key" with a green plus icon.

CDD Vault Enterprise API Extensions



Excel



KNIME



PIPELINE®
PILOT

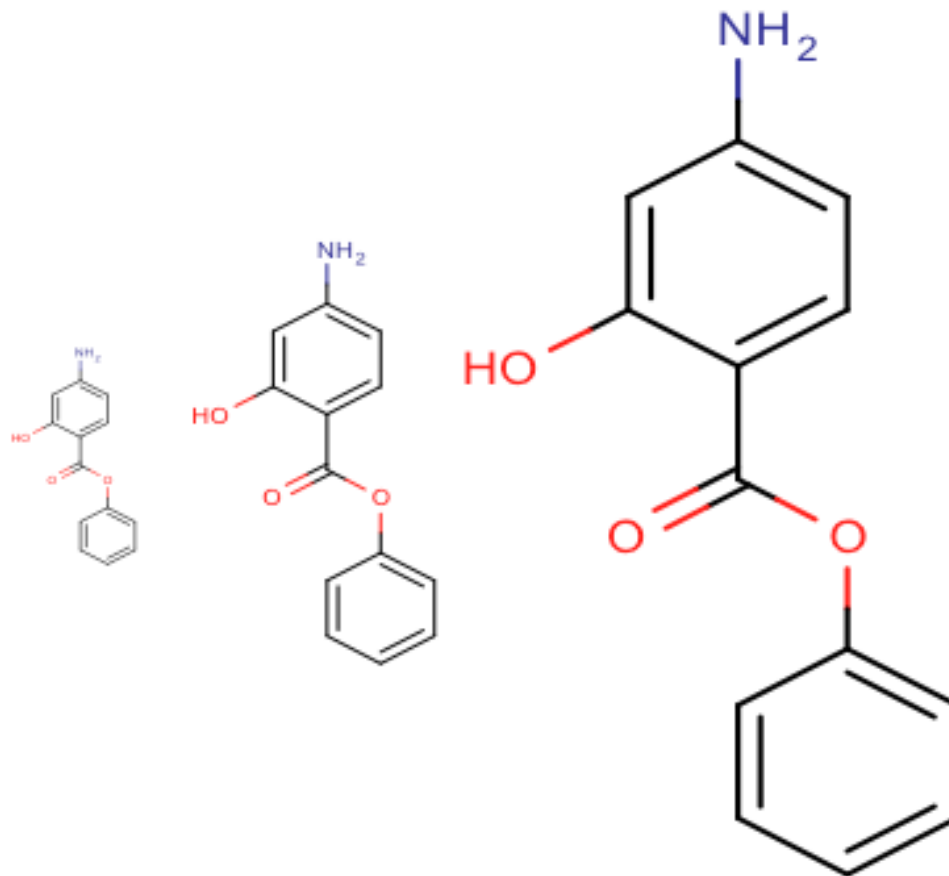
Configurable Batch Registration Rules

Name	Data Type	Must be Unique	This Field	
Batch Name			is auto-generated	Remove · Edit
Salt/Stoichiometric Ratio			is auto-generated	Remove · Edit
Formula Weight			is auto-calculated	Remove · Edit
<input type="text" value="External Identifier"/>	<input type="text" value="Text"/>	<input checked="" type="checkbox"/>	<input type="text" value="or Vendor is required"/>	Remove · Edit
<input type="text" value="Vendor"/>	<input type="text" value="Text"/>	<input type="checkbox"/>	<input type="text" value="or External Identifier is required"/>	Remove · Edit
<input type="text" value="Date"/>	<input type="text" value="Date"/>	<input type="checkbox"/>	<input type="text" value="is required"/>	Remove · Edit
<input type="text" value="Person"/>	<input type="text" value="Text"/>	<input type="checkbox"/>	<input type="text" value="is required"/>	Remove · Edit
<input type="text" value="Amount (mg)"/>	<input type="text" value="Number"/>	<input type="checkbox"/>	<input type="text" value="is optional"/>	Remove · Edit
<input type="text" value="Note"/>	<input type="text" value="Text"/>	<input type="checkbox"/>	<input type="text" value="is optional"/>	Remove · Edit
"State" will be removed (No batch data associated)				
<input type="text"/>	<input type="text" value="Text"/>	<input type="checkbox"/>	<input type="text" value="is optional"/>	Remove · Edit
+ Add a batch field				

Note: Uniqueness is compared across all batch fields within the vault.

[Update batch fields](#) or [cancel](#)

Scalable Images in Excel

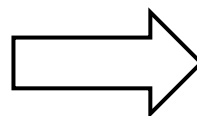


Preserve Molecule Orientation

```

-ChemAxon- 02240311302D
10 9 0 0 0 0 0 0 0 0999 v2000
-2.5000 0.4583 0.0000 S 0 0 3 0 0 0 0 0 0 0 0 0
0 0
-1.7917 0.0833 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
0 0
-0.3333 0.0833 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
0 0
-0.3333 -0.7917 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
0 0
0.3750 0.4583 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
0 0
1.1250 0.0833 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
0 0
0.3750 1.2917 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
0 0
-1.0417 0.4583 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
0 0
-3.2083 0.0833 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
0 0
-2.5000 1.2917 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
0 0
5 7 2 0 0 0 0 0
1 2 1 0 0 0 0 0
2 8 1 0 0 0 0 0
5 6 1 0 0 0 0 0
1 9 1 0 0 0 0 0
3 5 1 0 0 0 0 0
1 10 2 0 0 0 0 0
3 8 1 0 0 0 0 0
3 4 1 1 0 0 0
M END

```



Stay Up To Date





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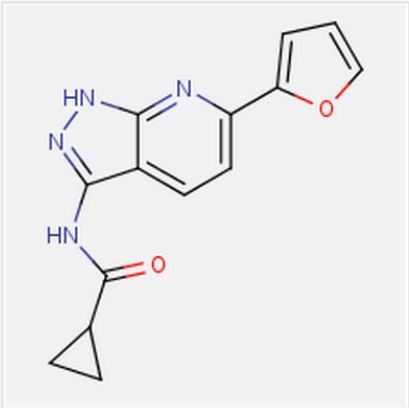
What's Next?

Protocol Conditions

Explore related assay protocols simultaneously...when only conditions differ

- Designate one or more readout definitions as Protocol Conditions
- Any calculation or post-processing activities will respect conditions
- Benefits:
 - Consolidate protocols for multiple strains & cell lines
 - Version tracking
 - Capture later stage data more effectively: number of compounds decrease but the number of conditions vary dramatically

Molecule	AKT1 Activity Value	AKT2 Activity Value	AKT3 Activity Value	
 <p>CHEMBL-162 CDD Vault</p>	flag outliers	20.0	6.5	5.0
		290.0	9.0	10.0
		460.0	44.0	10.0
		290.0	6.5	170.0
		1.5		0.64
		6.0		
		11.0		
		1.5		

Molecule	Kinase Assay						
	Target (short name)	Target (full name)	Species	Lab	Compound Co...ration (uM)	Inhibition (%)	
 <p>K2-0000001 Kinome2</p>	flag outliers	AKT1	Serine/threonine-protein kinase AKT	Homo sapiens	Nanosyn	0.10	-0.33
		AKT1	Serine/threonine-protein kinase AKT	Homo sapiens	Nanosyn	1.0	0.80
		AKT2	Serine/threonine-protein kinase AKT2	Homo sapiens	Nanosyn	0.10	0.45
		AKT2	Serine/threonine-protein kinase AKT2	Homo sapiens	Nanosyn	1.0	0.89
		AKT3	Serine/threonine-protein kinase AKT3	Homo sapiens	Nanosyn	0.10	0.35
		AKT3	Serine/threonine-protein kinase AKT3	Homo sapiens	Nanosyn	1.0	0.80

Self Administration

CDD · CDD Vault ▾
Simon Smith: [Account](#) · [Help](#) · [Log out](#)

Dashboard Explore Data Import Data Reports Manage Settings ✉
You are a **Vault Administrator**

Projects
Members

Go
➕ Add a member (licenses remaining: 3 read-only, 1 read/write)

200 Members · Showing 10 per page Previous · Page 1 of 20 · Next

Member ↕	Role ↕	Projects ↕	Last Login ↕	
Randy Sabin CORE	Vault Admin	5	Today	Remove
Kay Skeens	Vault Admin	3	Yesterday	Remove
Luis Engel	Full Access	1	2 days ago	Remove
Rosalie Villalba	Read-Add	4	1 week ago	Remove
Sheila Metzger	Read Only	1	2 months ago	Remove
Eugene Sosa CORE	Vault Admin	1	1 year ago	Remove
Walter Espino	Full Access	2	2 years ago	Remove
Willie Villalobos DISABLED	Read-Add	1	3 years ago	Remove
Albert Glover	Full Access	3	Never	Remove
Terry Lujan INVITED	Vault Admin	0	Never	Remove

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Self Administration

CDD · CDD Vault ▾ Simon Smith: [Account](#) · [Help](#) · [Log out](#)

[Dashboard](#) [Explore Data](#) [Import Data](#) [Reports](#) **Manage** [Settings](#) [✉](#) You are a **Vault Administrator**

[◀ Back to Members](#)

Invite a New Member to Your Vault

New Member Details	Invitation Email Preview
<p>First Name: <input type="text"/></p> <p>Last Name: <input type="text"/></p> <p>Email: <input type="text"/></p> <p><small>The new member will receive an email invitation here.</small></p> <p>Access Role: <input type="text" value="Read Only"/></p> <p>Core Member: <input type="checkbox"/> Automatically add this member to new projects.</p> <p>Biologist: <input type="checkbox"/> Member cannot modify molecules and batches.</p> <p>Mask Structures: <input type="checkbox"/> Hide molecule structures from this member.</p> <p>Allow Downloads: <input type="checkbox"/> Allow member to download documents.</p> <p>Allow Export: <input type="checkbox"/> Allow member to export search results.</p>	<p>Hi [Name],</p> <p>Simon Smith has invited you to the CDD Vault vault on Collaborative Drug Discovery, a web application for intelligent data management and secure collaboration.</p> <p>Click this link to get started:</p> <p>https://app.collaborativedrug.com/invitation/adoifu29384723eijdf</p> <p>Simon also says:</p> <div style="border: 1px solid #ccc; padding: 5px; min-height: 80px;"><p>You can include a personal message here.</p></div>

[Send Invitation](#) or [cancel](#)

Self Administration

Welcome to CDD Vault

Mike Moore would like to collaborate with you using CDD Vault. Log in or create an account to accept the invitation and become a member of the CDD Vault vault.

Already a CDD Vault User?

Username:

Password:

[forgot your password?](#)

New to CDD Vault?

First Name:

Last Name:

Email:

This will be your username.

Password:

Password requirements go here.

By registering, you agree to abide by CDD's [Terms of Use](#)

If you do not know Mike Moore or do not want to become a member the CDD Vault vault, please disregard or [alert support](#)



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CDD VISION

Calculated Readout Definitions

Name:

Data Type: **Display Format:** ⓘ

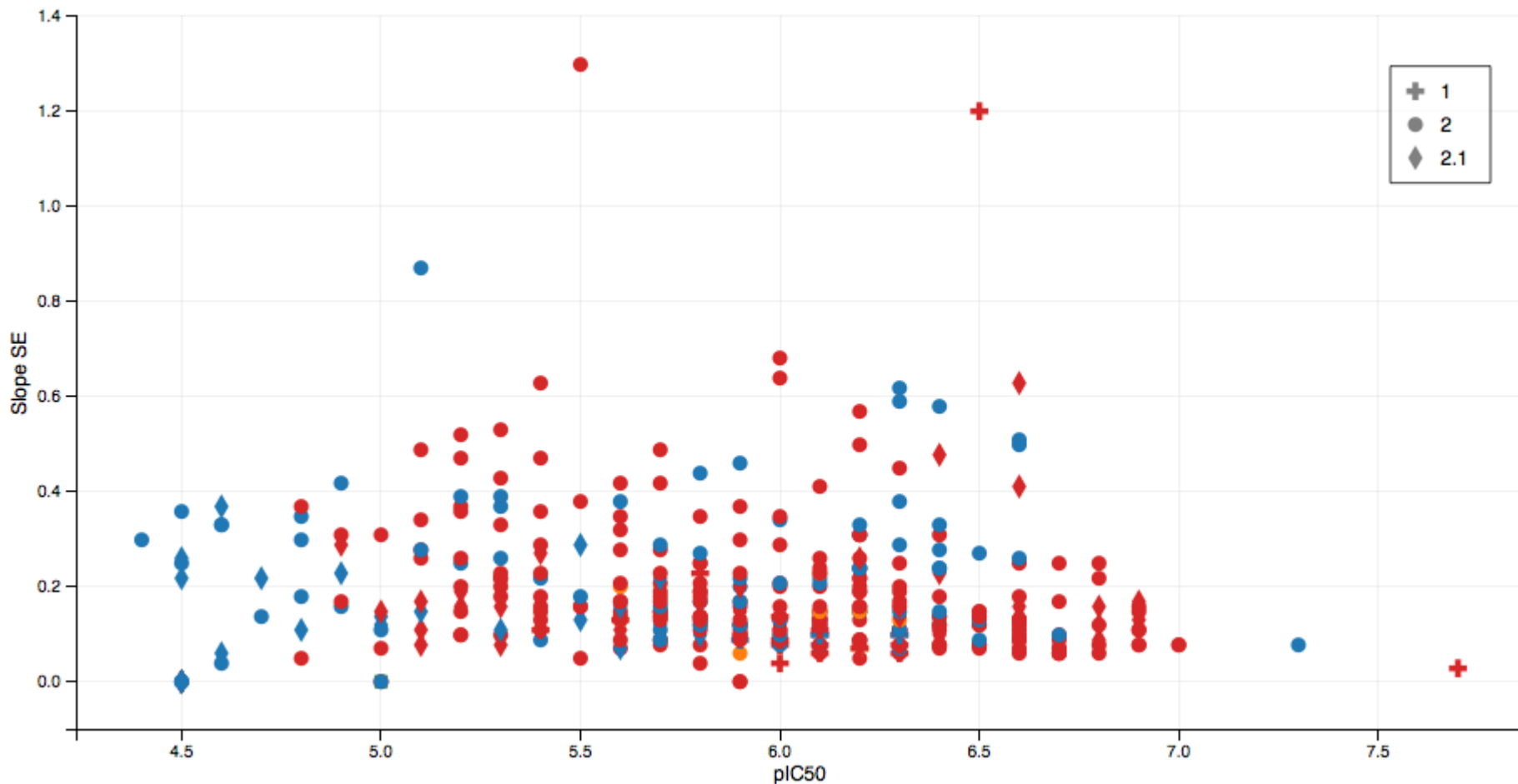
Unit:

Example: nM, kg, rfu

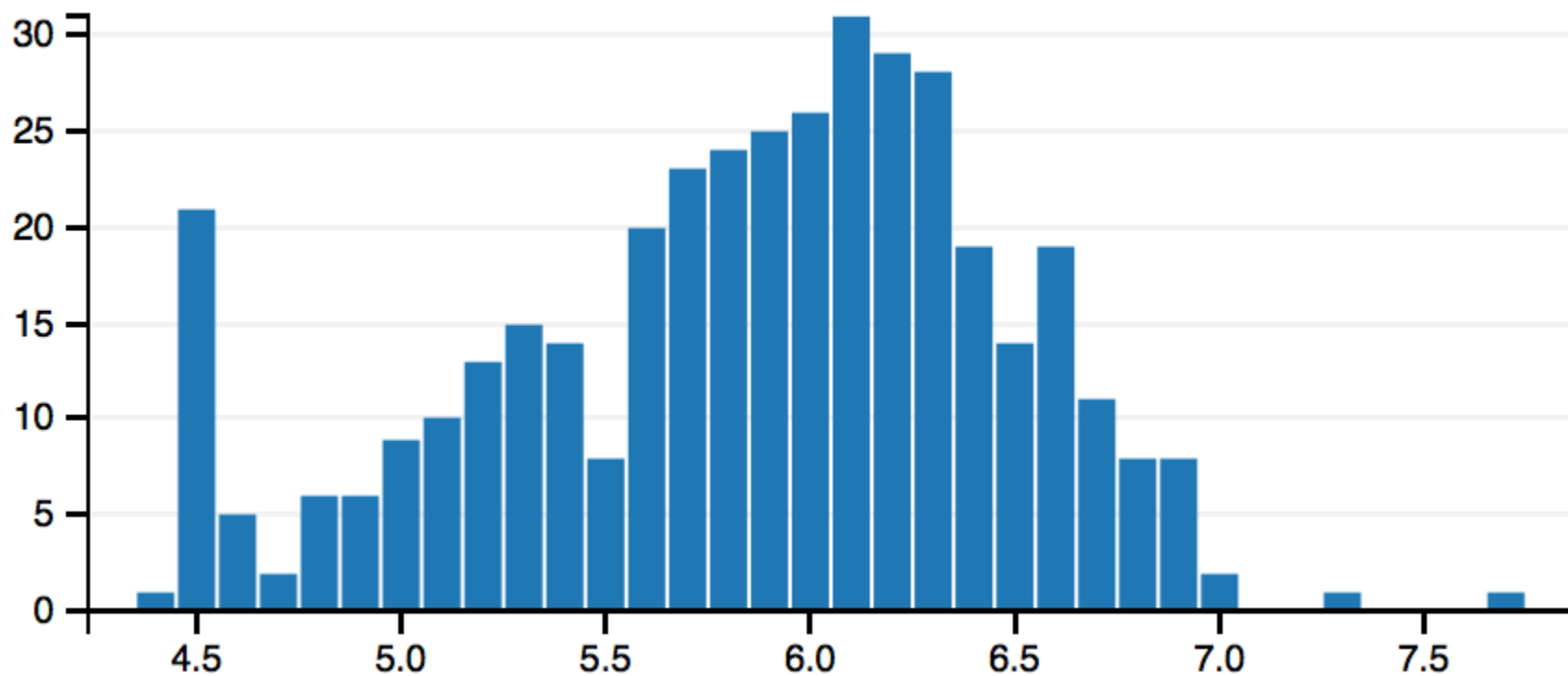
Formula =

Description:

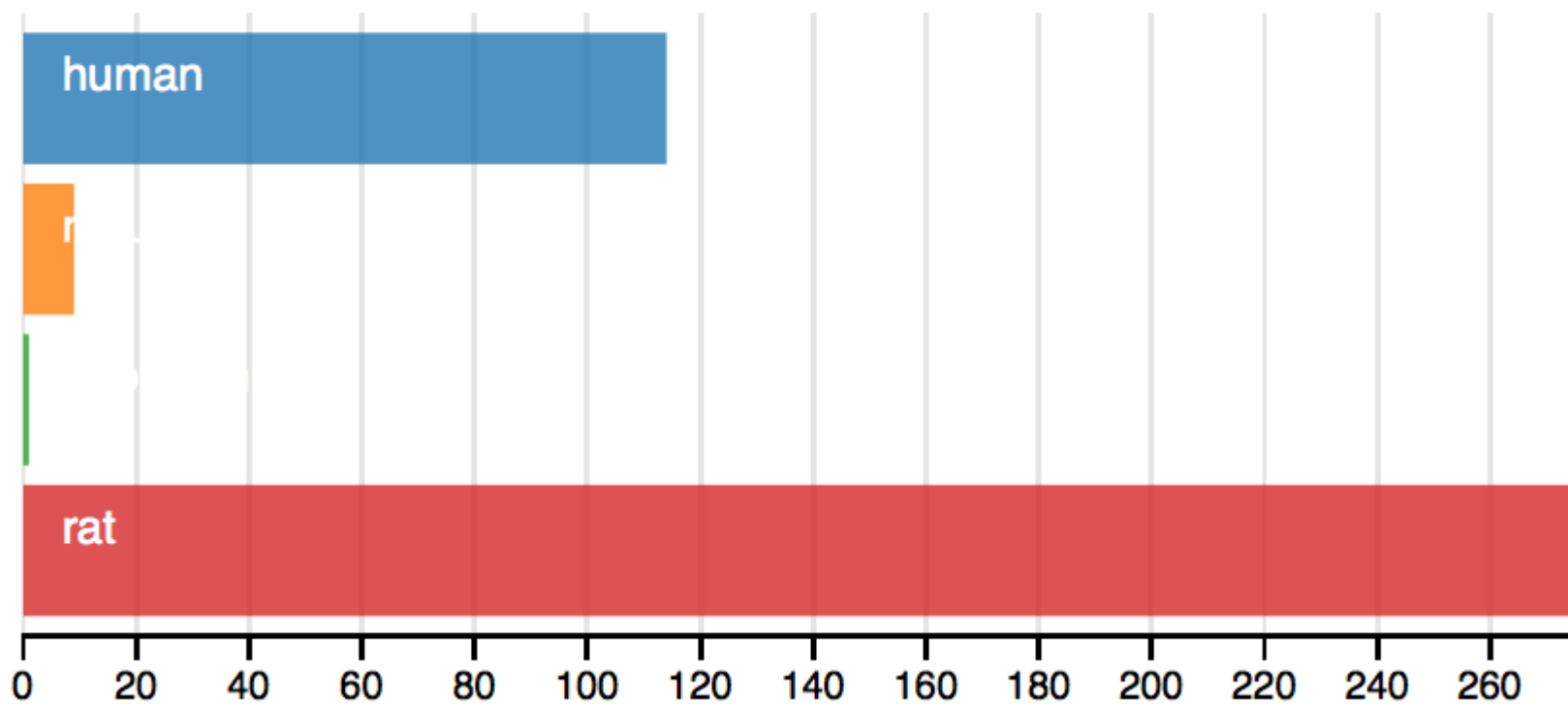
Visual Data Analysis



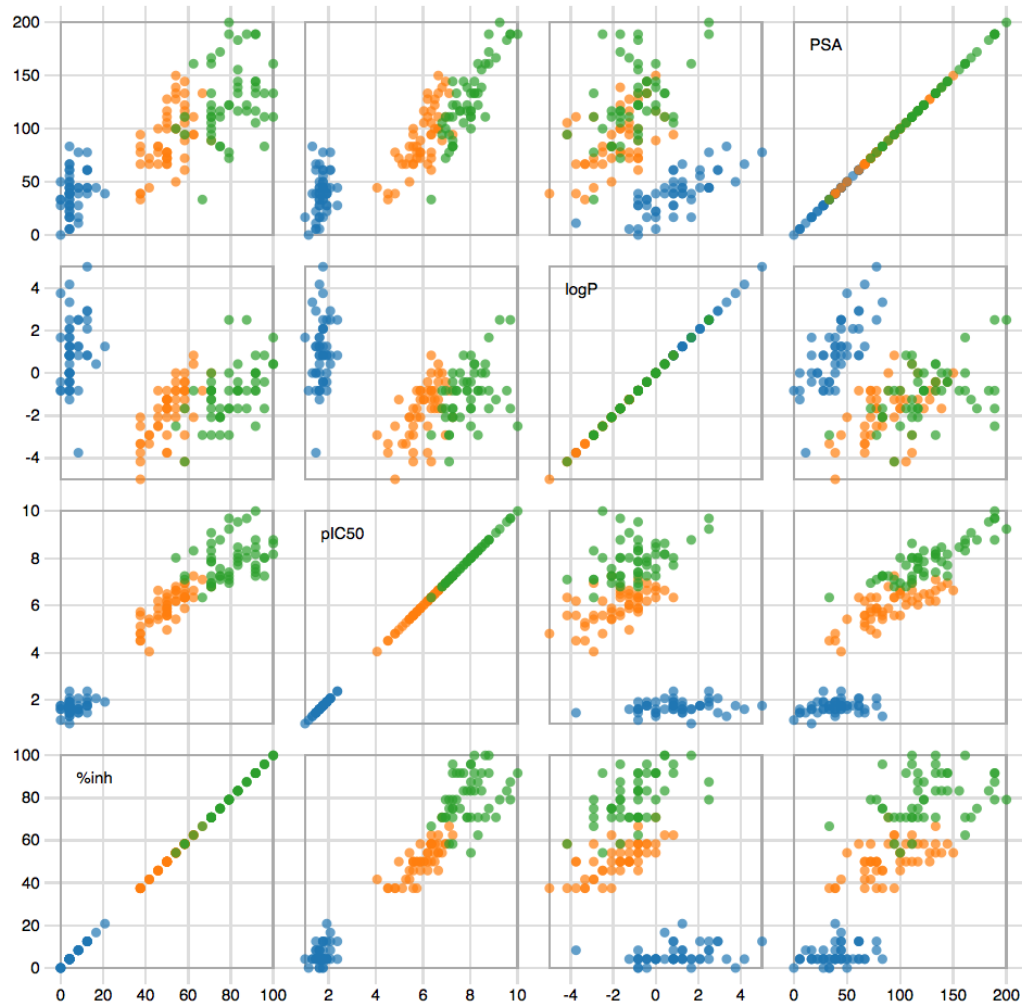
Visual Data Analysis



Visual Data Analysis



Visual Data Analysis





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DISCOVERY

Questions?

Feedback or Requests?

-
- Chat with us today
- Contact us anytime
 - Kellan: kellan@collaborativedrug.com
 - David: david@collaborativedrug.com
 - Support: support@collaborativedrug.com
 - Sales: info@collaborativedrug.com