

Explore Data

Search your data (or browse)

Current vault

Select another vault

Create new entity

- Molecule
- Project
- Protocol
- ELN Entry

Select project and/or Public Data to search

- Projects (3)
- CRO 1
- Project ABC
- Project XYZ
- Show/hide projects
- Public Data (0)

Search options

Browse/edit registered entities

Search within (or not) a protocol or category

Search by chemical properties

Launch Structure Editor to:

- Draw structure
- Paste smiles, mol, or IUPAC name
- Import file

Search results will match all criteria specified

Search within (or not) a collection

Add/remove a search term

Search molecule and batch fields

- Wildcard – asterisk (*)
 - Note: Wildcard must be at the end of the term, e.g. "ben*"
- Limits: 65000 characters and 5000 rows
- Retrieve all molecules – Any field & (Any Value) & leave the text box empty

Options

- (Any Value)
- has
 - Note: Only for numeric fields.
- from
- not
- (No Value)

Search

Explore Data

Search results

Export to Excel/CSV/SDF
Note: Use Excel for publication quality images.

Create Bayesian model
Note: Saved as a protocol

Select fields to display

Save search and report fields for future reference

Generate interactive visualizations
Note: Two numeric fields are required for the button to be enabled.

Sort on blue fields

Add results to collection

Flag outliers
Note: Calculations update automatically

Click to view molecule record

Click molecule to display light box to download structure formats and IUPAC name
Note: Molecule oriented based on how drawn in search

Flag outliers from curve and constrain fit parameters

10 Selected: Launch Vision Plot Export Add to collection Build model Flag outliers Customize your report Save this search

Chemical Properties Molecular weight (g/mol)

Inhibition Data Inhibition (%) Avg Inhibition (%) EC50 (uM)

Secondary CRC Assay Dose-response Plot

CDD-960611

DEMO-0007944
CDD New Demo Vault

12.33

6.54 ± 8.19 (n=2)

0.261

100
75
50
25
0
0.01 1
Concentration (uM)

% Inhibition (%)

Flag outliers & Override

Customize your report

Detail level: ? Summary Run/batch Details

Displayed readouts: ? Matching All

Dose-response plots scale: ? Per Run Per Molecule

Image size: Small Medium

Column widths: 25 characters

Set column width

Detail Level

- Summary - group data by molecule
- Run/batch - group data by run & batch
- Details - default - data not grouped

Displayed readouts

- Matching - default - only readouts that satisfy your search criteria
- All - every readout for each molecule

Structure Fields All None

Structure SMILES IUPAC

CDD Number InChI

CXSMILES (CDD Compatible) InChIKey

Reorder sections in report

Select fields to display

Single Point Screen

Secondary CRC Assay

Choose fields from additional protocols

Add Protocol: (select protocol)

Vision

Filters



Vision

Plots

The screenshot displays the CDD.VISION interface with two plots: a scatter plot of log P vs. Molecular weight (g/mol) and a histogram of CNS MPO score. The interface includes a table of molecules, a sidebar for plot management, and several callout boxes:

- Enlarge plot or table:** Points to the zoom-in icon in the top right of the plot area.
- Add selected molecules to collection:** Points to the '+' icon next to the 'Selected molecules 30 / 30' header.
- Select which plot to export:** Points to the 'Export' button in the 'Export Plots' section.
- Export PDF of a chart:** Points to the 'Download PDF' button in the 'Export Plots' section.
- Add a scatterplot or histogram to the display:** Points to the 'Add Scatterplot' and 'Add Histogram' buttons in the 'Plots' section. A note below these buttons states: "Note: Maximum of 4 plots".
- Drag to rearrange plots:** Points to the plot thumbnails in the 'Plots' section.

Axis and Legend Labels:

- X: Molecular weight (g/mol)
- Y: log P
- Color: Single Point Screen: Avg Inhibiti...
- Size: log D

Export Plots:

- Download your plots as
- Include the CDD logo on export
- Buttons: Export, Cancel, Download PDF

Plots:

- Drag the plots to reorder.
- Buttons: Add Scatterplot, Add Histogram

Molecule	Molecular weight (g/mol)	log P	H-bond donors	H-bond acceptors	Lipinski violations	log D	log S
<input checked="" type="checkbox"/> CDDAT-0003209	154.125	0.23	1	5	0	-3.01	1

COc1nc2c(nc(=O)O)c2n1

ELN

Search entries

The screenshot displays the ELN interface with a search bar and filter options. A search for "mice" is shown, resulting in 4 entries. The entry for "Squamous cell tumors" is highlighted, showing its details and chemical structures.

Search for term(s)

- Wildcard: *
- Use leading zeros for IDs
- Use double quotes for exact search

Search for substructure

Filter entries by

- Author
- Status

ELN entries associated with a project

- Click to open

Search terms appear in bold in context

Attached MS Office documents, PDF and text files are searched

ID	Title	Author	Modified	Created	Status
1186	Diels-Alder reaction of 1,3-butadiene ...	Heather Mattson Ar...	2018-11-27	2018-03-26	Open
3101	Analysis of 5-[2-chloro-5-(trifluoromet...	Heather Mattson Ar...	2018-11-02	2018-10-17	Open
2935	Coomassie Blue Analysis w				
1187	Principles of Early Drug Dis				
1367	Squamous cell tumors				
2202	Quinone methide synthesis				

Entries

Search: mice with structure

Filter By: 1 Author Any Status Showing 4 entries

ID	Title	Author	Modified	Created	Status
1367	Squamous cell tumors	Heather Mattson Ar...	2018-11-30	2018-04-26	Open

body: Procedure Monitored effect of HA-1 and HA-2 on squamous tumors in **mice**, Mus musculus. Results annotation - organism: mouse, **mice** C57BL/6xCBA/CaJ hybrid, house mouse, Mus muscaris

reference.pdf: findings in the Zmiz1 model, we examined squamous skin tumors from another tumor study in aging **mice** ...

2.1. **Mice** We studied cutaneous squamous tumors from two different genetically engineered mouse ... models. Zmiz1 Δ 1-185;K14-Cre double transgenic **mice** (Zmiz1) generated KAs as previous (B6.129S6-Rag2tm1Fwa N12; or Rag2 $^{-/-}$, Taconic, Hudson, NY, USA) and hetero the Zmiz1 (n = 33) and Rag-SB (n = 42) groups were examined for

molecule name: HADV-0000150

ClC1=CC=C(Cl)C=C1C1CCN(C1)C2CCO2

ELN

Create new entry

The screenshot shows the CDD Vault ELN interface. On the left is a navigation sidebar with options: Explore Data, ELN, Imp, + Create a new ..., Protocol, Molecule, Project, and ELN Entry. The main area displays the title "Synthesis of 2,2,2-trifluoroethyl (1S)-cyclohex-3-ene-1-carboxylate" and various metadata fields like Project (Project ABC), PI, Project code, Location (NA), Date, and File (Upload File). A rich text editor is visible with a toolbar and a "Saved" indicator. A chemical reaction scheme is shown at the bottom, depicting the synthesis of the product from 1,3-butadiene and 2,2,2-trifluoroethyl prop-2-enoate.

Annotations:

- Finalize entry once complete**: Points to the lock icon in the top toolbar.
- Duplicate an existing ELN entry**: Points to the duplicate icon in the top toolbar.
- Print entry to PDF**: Points to the printer icon in the top toolbar.
- Download attached files as .zip file**: Points to the download icon in the top toolbar.
- Select Create a new > ELN Entry**: Points to the "ELN Entry" option in the sidebar.
- Select project**: Points to the "Project ABC" selection in the sidebar.
- Begin Editing**: A green button in the sidebar.
- Title**: Points to the main title of the entry.
- Add metadata fields in Settings>Vault>ELN Fields**: Points to the metadata fields in the main area.
- Save status: auto-saves 8 times per second**: Points to the "Saved" indicator in the text editor.
- Elements**: A list of actions available in the text editor:
 - Insert a link
 - URL
 - CDD object
 - Attach file
 - Click icon
 - Drag and drop
 - Insert table
 - Click icon
 - Copy/paste from Excel
 - Insert structure
 - Insert assay annotation

ELN Elements

Links

Search for CDD object or paste URL

Insert CDD Objects:

- Molecules
- Protocols
- Protocol runs
- ELN entries

Display Options

- Text
- Caspase 12 Assay - 2018-08-10

Select display

- Custom text
 - URL entered if blank
- Default text
- Structure (molecules only)

Display in ELN Entry

Click link to go to object

Mouse over link to edit or attach Run Export (runs only)

Attached Run Export

Active hyperlinks

<https://www.ncbi.nlm.nih.gov/pubmed/28203483>

File Attachments

Image files and first page of PDF files rendered

PDB files rendered in an interactive viewer

- Drag to rotate
- Shift + drag to zoom

Additional file types appear as links

Import data from CSV or SDF files

View imported data

Assay results

betaLactams.sdf

Inhibition Data.csv

Import File

Explore imported data

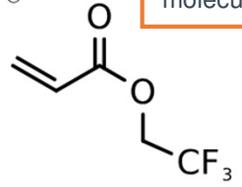
Molecules and Reactions



Registration number link added to drawn structures already registered

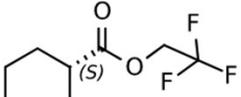
HADV-0035551

Register molecule

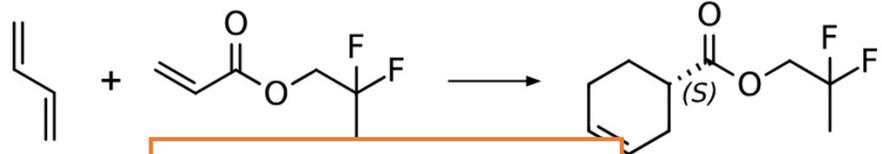


Only displayed molecules are substructure searchable

Link to registered molecule record



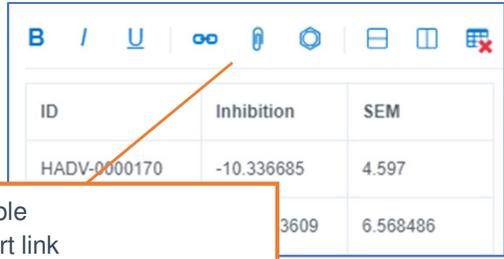
HADV-0000170 (003)



Attach CDX or CDXML files from ChemDraw to add reaction and stoichiometry table

Reactants				
Formula	C4H6	C6H8F2O2	Formula	C10H14F2O2
MW	54.09	150.12	MW	204.22
Limiting?	Yes	No	Equivalents	

Tables



B / **U** | **∞** | **🔒** | **⚙️** | **📄** | **🗑️**

ID	Inhibition	SEM
HADV-0000170	-10.336685	4.597
	3609	6.568486

Edit Table
 • Insert link
 • Insert file
 • Insert structure
 • Insert/delete row or column
 • Delete table

Assay Annotation

In ELN Entry

Assay Annotation

This is an assay to identify potential treatments for an unknown disease, by investigating the biological pro target from **Mus musculus**.

This is a **ADMET/functional/plasma stability assay** in , using , w physical detection method, using an unknown detection instrument

Target

Bioassay Type	Mode Of Action
- ADMET	- inhibition
- functional	

Method

Bioassay	Assay Cell Line
- plasma stability assay	- 184B5 cell

Auto-generated text from annotations

Summary of annotations



Dialog

TARGET METHOD

bioassay type

ADMET functional

Mode Of Action (click to see prop)

Proposals

inhibition

activation

Start typing to select desired value

Note: Add custom annotations by typing desired value

Proposals are above dotted line

Import Data

Choose file

Explore Data ELN **Import Data** Reports Settings Heather Arnaiz

Step 1: Choose Data File Step 2: Map Fields Step 3: Commit Data

Files Templates **View saved mapping templates**

Choose a file to upload: Secondary CRC Assay.zip Project: Internal data

Select file and project to import data

Uploaded Files Show files being imported and: Files you uploaded All files

Filename	Date	Status	
▶ Secondary CRC Assay.zip	January 23, 2018	Partially mapped	Continue mapping
▶ Secondary CRC Assay.zip	December 14, 2017	Imported	Explore data Report Import again

Revisit previous imports

Revisit previous imports

View imported data in table

View import data report

Map fields

Step 1: Choose Data File Step 2: Map Fields Step 3: Commit Data

File: Secondary CRC Assay.zip

Add readouts (protocol data) only Update existing molecules Register new molecules / batches with structures

Add data to existing molecules

	A	B	C	D	E	F
1	Molecule Name	Plate	Well	Conc (uM)	Raw (RLU)	Microscopy
2	Sample-10-001	Sample PL_20151108	A10	0.01	2.67E+03	Microscopy/mag
3	Sample-10-001	Sample PL_20151108	B10	0.03	2.84E+03	
4	Sample-10-001	Sample PL_20151108	C10	0.1	2.04E+03	

Map fields
Note: System will map columns with similar names to fields

Molecule Fields

- Molecule Name or Synonym
- Structure
- User-defined Field
- Batch Fields
- Plate and Well
- Readouts (Protocol Data)
- Do not Import

Molecule Name is mapped to Molecule Name or Synonym

You can use this field to map any molecule name or synonym.

Optional prefix:

Prepend each identifier with an optional prefix

Please address the following:

- If you map Molecule Name or Synonym you must also map Batch Name and vice versa.
- You must not map Image when adding readouts only.

Issues to be fixed before importing can occur

Save mapping as template for future use

Type of information to be registered

Note: To register records without structures, select "without structure" option

Use a saved mapping template, if available

Add data to existing molecules

Map fields

Note: System will map columns with similar names to fields

Issues to be fixed before importing can occur

Save mapping as template for future use

File format

Molecules

File types



CSV format

Unique batch field

Note: this can be used for uploading data

	A	B	C	D	E	F	G	H
1	Canonical_Smiles	CAS #	Purity	Vendor	Synonym	Catalog #	Amt	External ID
2	<chem>CC(NC(C)(C)C(=O)c1cccc(Cl)c1</chem>	34911-55-2	95	NIH	SAM001246723	CPD000058423	5	Sample-10-2
3	<chem>CNCC[C@H](Oc1cccc2ccccc12)c3cccs3</chem>		95	NIH	SAM001247059	CPD000449282	5	Sample-10-3
)cc3	128196-01-0	95	NIH	SAM001246668	CPD000469191	5	Sample-10-4

Use SMILES or mol file for structures

Note: Salts and solvents will be stripped by default

File type



Single point data

First row – column headers

Each type of data entered into a separate column

	A	B	C
1	SampleID	Inhibition	SEM
2	Sample-10-001	-10.336685	4.596999925
3	Sample-10-001	4.142833609	6.56848643
4	Sample-10-001	0.047860794	0.137099726
5	Sample-10-002	-4.29821	4.29821
6	Sample-10-002	8.835689174	0.158027477
7	Sample-10-002	3.668918207	4.560620974

A batch of a molecule may be uniquely identified by:

- Molecule name and Batch name
- Synonym and Batch name
- Batch field that is unique
- Plate and Well location – plate preregistered
- A combination of one of the first 3 options and Plate and Well location

e.g. Molecule name, Batch name, Plate and Well location

Dose response

Controls – if applicable

Note: do not need to be associated with a batch

	A	B	C	D	E	F
1	Molecule ID	Batch	Plate	Well	Conc	RLU
2			Plate 20180418	A01		2.82E+03
3			Plate 20180418	A02		30
4	DV-0000054	1	Plate 20180418	A04	0.01	3.37E+03
5	DV-0000048	1	Plate 20180418	A10	0.01	2.67E+03
6	DV-0000052	1	Plate 20180418	A12	0.01	3.34E+03
7	DV-0000053	1	Plate 2018041			

Samples

- 1 row per measurement
- Location of samples specified in file

Importing attachments

File format

File type ZIP

Name	Type
MicroscopyImage1.jpg	JPG File
MicroscopyImage2.jpg	JPG File
MicroscopyImage3.jpg	JPG File
MicroscopyImage4.jpg	JPG File
Secondary CRC Assay.csv	Microsoft Excel C

Create zip file containing attachments and CSV or SDF file.

Create SDF or CSV file as usual. Add a column for the attachment filename

	A	B	C	D	E	F
1	SampleID	Plate	Well	Conc (uM)	Raw (RLU)	Microscopy
2	Sample-10-001	Sample Plate 20151108	A10	0.01	2.67E+03	MicroscopyImage3.jpg
3	Sample-10-001	Sample Plate 20151108	B10	0.03	2.84E+03	
4	Sample-10-001	Sample Plate 20151108	C10	0.1	2.04E+03	
5	Sample-10-001	Sample Plate 20151108	D10	0.3	1.25E+03	
6	Sample-10-001	Sample Plate 20151108	E10	1	775	
7	Sample-10-001	Sample Plate 20151108	F10	3	255	
8	Sample-10-001	Sample Plate 20151108	G10	10	1	
9	Sample-10-001	Sample Plate 20151108	H10	30	63	
10	Sample-10-001	Sample Plate 20151108	I10	0.01	2.44E+	
11	Sample-10-001	Sample Plate 20151108	J10	0.03	3.22E+03	
			08 K10	0.1	2.53E+03	
			08 L10	0.3	1.68E+03	
			08 M10	1	628	
			08 N10	3	267	
			08 O10	10	109	
			08 P10	30	84	
18	Sample-10-002	Sample Plate 20151108	A20	0.01	2.73E+03	MicroscopyImage2.jpg
19	Sample-10-002	Sample Plate 20151108	B20	0.03	3.00E+03	

Enter filename of attachment
Note: Attachment only needed once per batch

A batch of a molecule may be uniquely identified by:

- Molecule name and Batch name
- Synonym and Batch name
- Batch field that is unique
- Plate and Well location – plate preregistered
- A combination of one of the first 3 options and Plate and Well location
e.g. Molecule name, Batch name, Plate and Well location

Import Data

Commit Data

Step 1: Choose Data File | Step 2: Map Fields | **Step 3: Commit Data**

File: Benzodiazepines.sdf (Review mapping) | Project: Bayesian | Owner: Heather Arnaiz

This data import is ready for review

- 7 records will be imported - Only records that are not associated with any rejected event will be imported.
- 2 records will be rejected - You will be able to download these records and their specific issues once you commit.

Noteworthy Events - Usually fine. Associated records will be imported unless you choose otherwise.

- 7 New Batches (2 indirectly rejected)

Suspicious Events - Usually unexpected. Associated records will not be imported except if you choose otherwise.

- 2 Existing Molecules Associated with New Project

Line #	Record #	Molfile	Event Description
1	1	BENZOEXAM...M.END	REJECTED: Molecule HA-0000962 associated with project Bayesian
58	2	BENZOEXAM...M.END	REJECTED: Molecule HA-0000156 associated with project Bayesian

Export

Commit Data Import | Reject Data Import

View mapping

- Create template from mapping

Noteworthy events

- Things to be aware of
- Decide to Accept or Reject

Suspicious events

- Problems in registration
- Decide to Accept or Reject

Click down arrow to see details of noteworthy or suspicious events

Export problematic data to fix and reimport, as desired

Commit or Reject Import

Report

Explore Data | ELN | Import Data | Reports | Settings | [Email]

Your Current Import: Benzodiazepines.sdf Processed (2 Suspicious Events) Email me updates

+ Create a new ... | Search | Saved Searches | [Cancel]

Step 1: Choose Data File | Step 2: Map Fields | **Step 3: Commit Data**

File: Benzodiazepines.sdf (Review mapping) | Project: Bayesian | Owner: Heather Arnaiz

Import details for Benzodiazepines.sdf: Queued (#1) Email me updates

Cancel Import

Explore Data | ELN | **Import Data** | Reports | Settings | [Email] | Heather Arnaiz

File: Benzodiazepines.sdf (Review mapping) | Project: Bayesian | Owner: Heather Arnaiz

This data import was committed

- 7 records imported - View or export registered molecules
- 2 records rejected - Export rejected records to fix and re-import the problematic data

Explore imported data

View imported records

View or export records

Noteworthy Events - Usually fine. Associated records will be imported unless you choose otherwise.

- 7 New Batches (2 indirectly rejected)

Suspicious Events - Usually unexpected. Associated records will not be imported except if you choose otherwise.

- 2 Existing Molecules Associated with New Project

Import status

I changed my mind – Cancel the import

View mapping

- Create template from mapping

View imported records

View or export records

Protocols

Create a new protocol

Explore Data ELN Impo

+ Create a new ...

Protocol
Molecule
Project
ELN Entry

Create a New Protocol

Protocol Definition

Name: DR Assay
Special characters

Category: Cell
Example: Enzyme, Cell, Animal

Description:

Project: Dose Response

Create Protocol or cancel

Select Create a new > Protocol

Enter Name, Category, Description and Project

Run Data Protocol Details Projects 1 Files 0

Protocol Definition

Edit protocol definition

Name: DR Assay

Category: Cell

Description:

Edit Readout Definitions

Add a readout definition

Add a dose-response calculation

Add a calculated readout definition

Hit Conditions

Add stop light color coding to readout definitions based on readout value

Control Layouts

Positive control (hit) Negative control Reference molecule

Protocol Default 96-well Control Layout

Protocol Default 384-well Control Layout

Protocol Default 1536-well Control Layout

Add a plate-specific control layout

Click to Edit

	01	02	03	04	05	06	07	08	09	10	11	12
A												
B												
C												
D												
E												
F												
G												
H												

Location of samples specified in the import file

Full plate not required

Define control layout for a specific plate after upload

Toggle between Positive, Negative, Reference molecule & not specified

Searching across protocols with the same value for category
Note: Recommend using a limited vocabulary

Add a readout definition to hold a value, e.g. Raw Data

Add a dose response calculation

Add a custom calculation on data in readout definitions – can be across multiple protocols

Edit Hit Conditions

Condition: Avg EC50 > 0.5

Color: [Green] [Yellow] [Red]

Remove

Add a hit condition

Coloration can be viewed on:

- Molecule page > Protocols tab > Protocol name
- Protocols page > Protocol Name > desired run date > All Data tab

Readout Definitions

Add a Readout Definition

Name to use for the readout in CDD Vault

Store biological data

Options

- Text
- Numeric
- Date
- Pick list
- File

Description:

Adds aggregation for calculations and searching. Calculations aggregate on protocol condition, e. g. If species is protocol condition, average inhibition is calculated over batch/run/species.

Add a calculated readout definition

Only number data type supported

Perform calculations on readout definitions

Precision to be displayed

Type function name to select from list Syntax

- [readout definition name]
- <protocol condition name>
- {chemical property name}

Perform calculations over

- Batch and run
- Batch and protocol
- Molecule and protocol

Add calculated readout definition or cancel

Add a dose response readout definition

Calculate relative dose response

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

Field names in CDD Vault for raw dose response data

Options

- Normalize within each plate
- Normalize within each run
- Already normalized
- No controls (do not normalize)

Specify Fit Parameters

Options

- % inhibition or activation
- Requires positive and negative controls to be specified
- % negative control

Set activity range that defines inactive compounds

Select desired calculation from list or choose Custom for another option

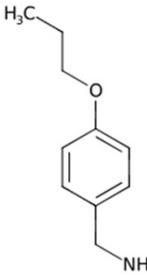
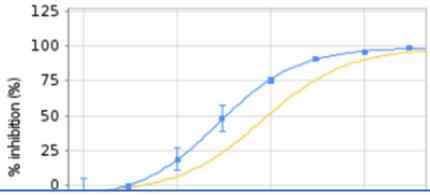
Add another calculation, e. g. IC90

Quality Control

Protocols > Protocol name > Run date

Select... all · none Molecule \downarrow IC50 (uM) \downarrow Dose-response Plot

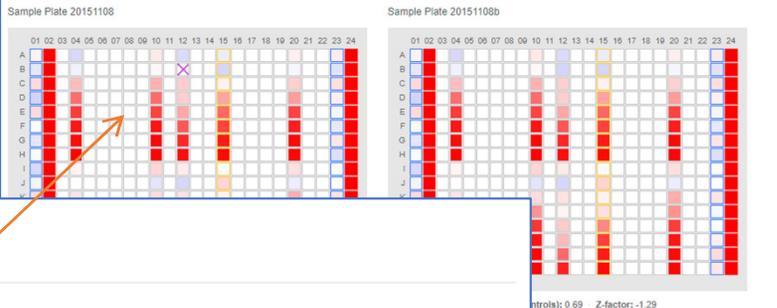
CDD-960699 0.274

Heat Map Viewer

Protocol: Secondary CRC Assay Run: 2018-02-12 Conditions: Raw (RLU) Readout definition: Raw (RLU)

View scatter plot for all data



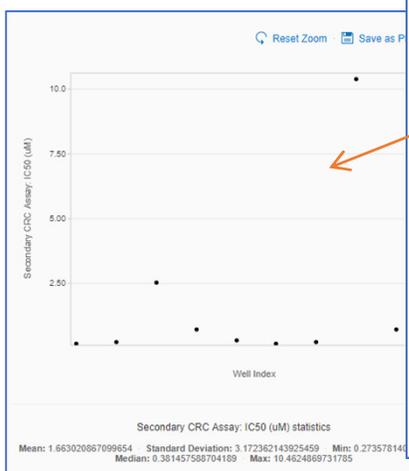
Data Summary All Data Run Details Files 1

View readouts View scatter plot View all heat maps Export readouts Create ELN experiment

Export csv file of readouts Create ELN entry with link to run results

	2 Plates	Raw (RLU) Z'-factor (controls)	IC50 (uM) Reference molecule intercept	Raw (RLU) Positive control mean	Raw (RLU) Negative control mean
Protocol Averages:		0.69 \pm 0.00 (n = 4 plates)	0.797 \pm 0.00 (n = 4 plates)	30.5 \pm 11.6 (n = 4 plates)	2.94E+03 \pm 287 (n = 4 plates)
Sample Plate 20151108	Delete	0.69	0.797 (n = 1)	30.5 \pm 11.6 (n = 32)	2.94E+03 \pm 287 (n = 32)
Sample Plate 20151108b	Delete	0.69	0.797 (n = 1)	30.5 \pm 11.6 (n = 32)	2.94E+03 \pm 287 (n = 32)

Z'-factor, RM intercept, control means per plate and per protocol



Delete plate

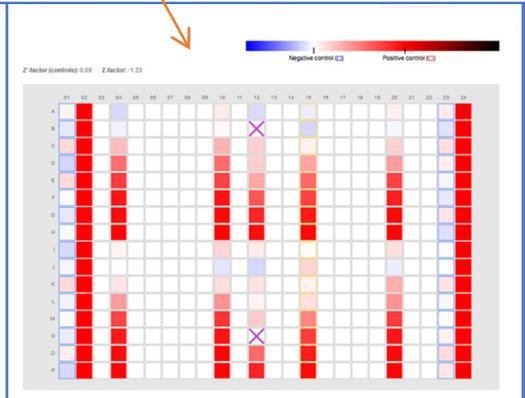


Plate Details Projects 1 Plate Map

	01	02	03	04	05	06	07	08	09	10	11	12	13
A				HA-0000077						HA-0000001		HA-0000003	
B				HA-0000077						HA-0000001		HA-0000003	
C				HA-0000077						HA-0000001		HA-0000003	
D				HA-0000077						HA-0000001		HA-0000003	
E				HA-						HA-		HA-	

View sample layout

Quality Control

From Protocol page

- Breadcrumbs
- Click Protocol name to Protocol Run Data page
 - Click Run date to go to Data Summary page

Heat Map Viewer

Protocol: Secondary CRC Assay Run: 2018-02-12

Readout definition: Raw (RLU) (selected)

Select readout definition to display

View scatter plot for all data

Sample Plate 20151108 Sample Plate 20151108b

Z'-factor (controls): 0.69 Z-factor: -1.29

DATA SOURCE

Protocol: Secondary CRC Assay
Run: 2018-02-12

CONFIGURE AXES

Select which data you want to use for each axis of the scatter plot.

X: Well Index (selected) Y: Secondary CRC Assay: IC50 (uM) (selected)

Select Axes

DATA POINTS

Show: All points (selected)

Point Size: Large (selected)

Plot options

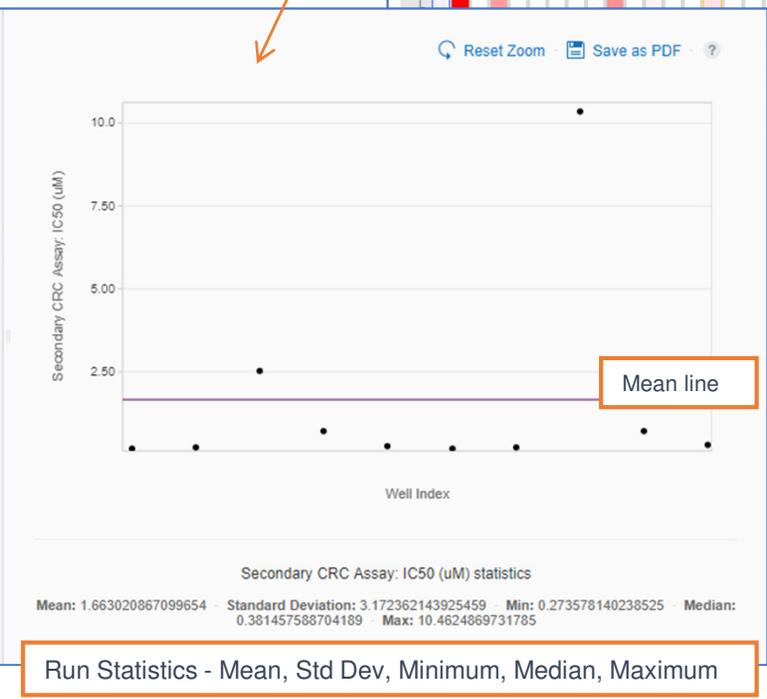
STATISTICS

Display summary statistics below plot

Display mean line on plot

Display ± 1 standard deviation line(s) on plot

LABELS & PLOT OPTIONS



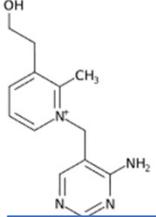
Data Modeling

Create a model

Retrieve a list of "Good" molecules from a:

- Search
- Saved search
- Collection

350 Selected: [Launch Vision](#) [Plot](#) [Export](#) [Add to collection](#) [Build model](#)

Select...	Molecule	Chemical Properties
all none		Molecular weight (g/mol) pKa pKa typ
<input checked="" type="checkbox"/>	CDD-2301082 	259.332 5.54 Basic

Build a Machine Learning Model

Training set baseline: Asinex

"Good" molecules: Your 431 selected results

Name: Good molecules

Project: Bayesian

Save or cancel

Model are treated as Protocols

Protocol	Description	Category	Molecules
Good molecules		Machine Learning Model	Explore
Inhibitors data		Machine Learning Model	Explore

Readout definitions calculated

Name	Description
Score	Relative score (higher is better)
Applicability	Fraction of structural features shared with the training set
Maximum similarity	Maximum Tanimoto/Jaccard similarity to any "good" molecules

Algorithm

Modified Bayesian model with FCFP6 descriptors

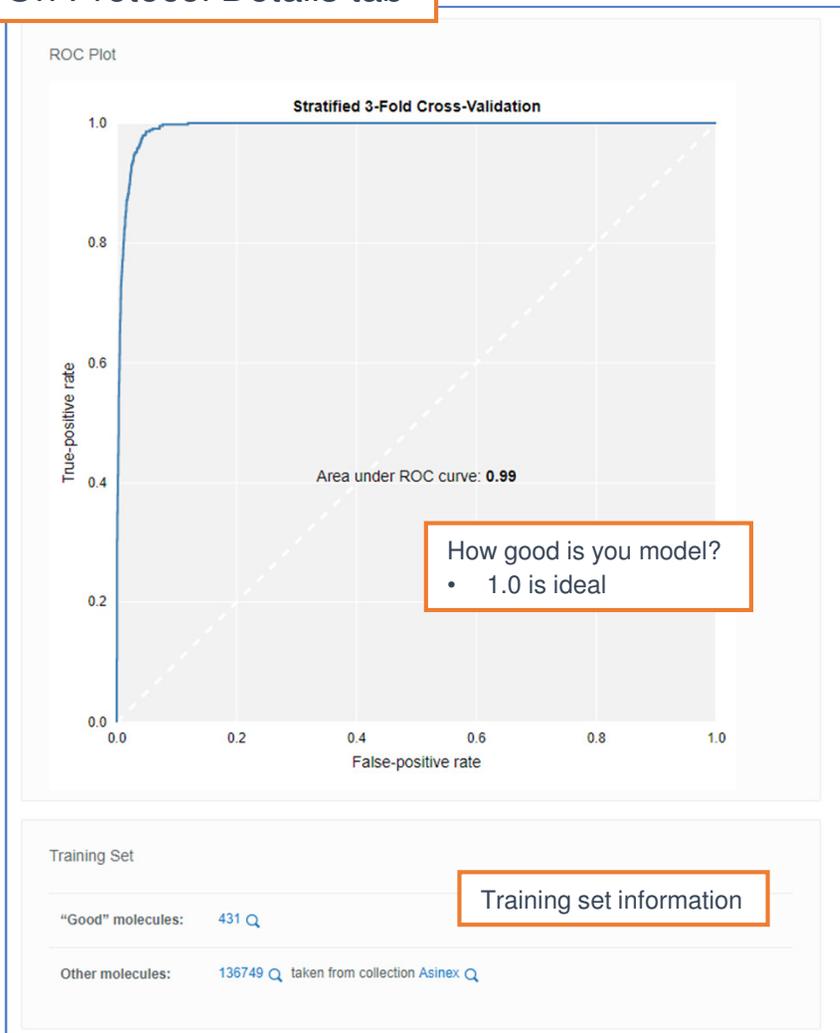
Model: CDD's open source modified Bayesian model described in Xia et al. 2004.

Descriptors: CDD's open source FCFP6 fingerprints described in Rogers and Hahn 2010.

Data Modeling

Quality of model

On Protocol Details tab



Use a model

Run Data Protocol Details **Projects 2** Files 0

Projects with access to Good molecules: **Molecules scored automatically**

Bayesian Remove

Internal data Remove

select project [v](#)

Save changes or **cancel**

Add model to the desired project
Note: All molecules in project are scored

Recalculating statistics and calculations for the following protocols:

- Good molecules

Banner is displayed while molecules are being scored

Setting > Vault

Terminology [Edit terminology](#)

Entry: experiment

Protocol: assay

Vault name: Readout_definition

Primary contact: Readout: **Use your terminology in your Vault**

Principal investigator: Run: run

Institution: Molecule: compound

Website URL: Batch: lot

Next Registration Sequence Identifier: HA-0000515

Registration System Settings: Multiple compounds with the same structure are NOT allowed. To enable this feature (e.g. to archive structures with different but up to you please contact support@collaboratedrug.com.

Email alerts: summary only

Project association via data import: **General Vault setting** acceptance

External link setting:

- Ban external links
- Allow external links
- Allow external links and do not show a warning page

Session timeout: 120 minutes

Disable inactive members: Never

Authorized IP ranges:

Block CDD staff access: false

User Vault

Projects

Members

Terminology

General

Batch Fields

ELN Fields

ELN Fields [Add/Edit ELN Fields](#)

Name	Data Type	Must be Unique	Is Required
Project	Project		✓
External Journal ID	Text		
Experiment	Pick List		
MSDS	File		

Metadata fields for ELN entries

3 Projects [Create a new project](#)

- CRO 1 [View data](#) [Delete](#)
- Project ABC [View data](#) [Delete](#)
- Project [View data](#) [Delete](#)

Users with role Read-Add or higher can create a project

To delete a project, remove all data from project first

Create projects and assign members to them

5 Members [Add a member](#)

Name	Access	Date Added	Projects	Email	API Keys	Actions
Heather Arnaiz	vault admin	11/30/2017	3 Projects	heather@collaboratedrug.com	full access	Edit Delete
Maria Edwards	biology full access	6/5/2018	1 Project	harnaiz@collaboratedrug.com		Edit Delete
	read-add					Edit Delete
	full access	5/1/2018	2 Projects	whitney@collaboratedrug.com		Edit Delete

Create new members

Manage Vault members

Batch Fields [Add/Edit Batch Fields](#)

Name	Data Type	Must be Unique	This Field
Batch Name			is required when creating batches
Date	Date		is optional
Scientist	Text		or Vendor is required
Vendor	Text		or Notebook is required
Sample ID	Text	✓	is optional
Initial Amount	Number		

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

Create batch fields

Specify batch field is:

- Unique value across Vault
- Required or optional