

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 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

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

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 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

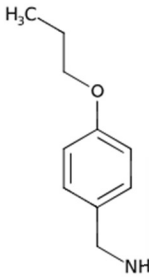
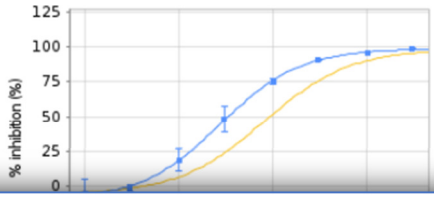
Add another calculation, e. g. IC90

Quality Control

Protocols > Protocol name > Run date

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

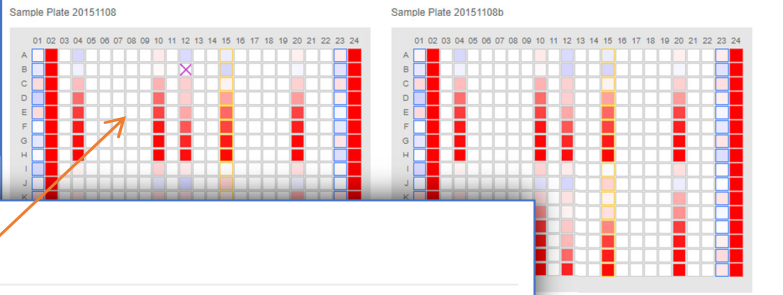
CDD-960699 0.274

Heat Map Viewer

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

View scatter plot for all data



Sample Plate 20151108 Sample Plate 20151108b

Controls: 0.69 Z-factor: -1.29

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

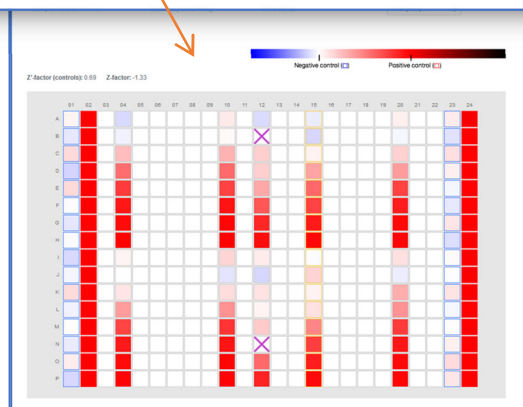
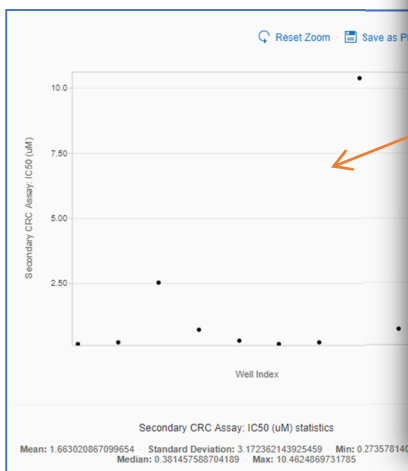


Plate Details Projects 1 Plate Map

	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

