

Explore Data

Search your data (or browse)

The screenshot shows the CDD Vault interface for the 'Heather Demo Vault'. The interface includes a top navigation bar with 'Explore Data', 'ELN', 'Import Data', 'Reports', and 'Settings'. A dropdown menu for 'Current vault' is shown, with a callout 'Select another vault'. The main content area is divided into sections for 'Search', 'Saved Searches', and 'Collections'. The 'Search' section includes filters for 'Molecules', 'Protocols', and 'Plates'. A callout 'Search options' points to the search filters. A callout 'Browse/edit registered entities' points to the 'Molecules', 'Protocols', and 'Plates' tabs. The 'Search' section also includes a 'Protocols' filter with a callout 'Search within (or not) a protocol or category'. The 'Structures' section includes a 'Launch the Structure Editor' button with a callout 'Launch Structure Editor to: Draw structure, Paste smiles, mol, or IUPAC name, Import file'. The 'Chemical Properties' section includes a callout 'Search by chemical properties'. The 'Collections' section includes a callout 'Search within (or not) a collection'. The 'Keywords' section includes a callout 'Add/remove a search term' and a list of search tips: 'Wildcard – asterisk (*)', 'Type asterisk (*) to retrieve all', and '65000 character limit'. A 'Search' button is located at the bottom right.

Current vault

Select another vault

Help · Log out

Heather Arnaiz

Explore Data ELN Import Data Reports Settings

Create new entity

- Molecule
- Project
- Protocol
- ELN Entry

Projects 2

- Project ABC
- Project XYZ

Show/hide projects

Public Data 0

Search Saved Searches Collections

Molecules Protocols Plates

Search options

Browse/edit registered entities

Protocols ?

In (select protocol) or (select category)

Add a term Search within (or not) a protocol or category Remove term

Structures ? substructure similarity \geq 70%

Launch the Structure Editor

Search results will match all criteria specified

Chemical Properties ?

(select property) Min: Max:

Search by chemical properties

Collections ?

In (select a collection)

Add a term Search within (or not) a collection Remove term

Keywords ?

Any field

- Wildcard – asterisk (*)
- Type asterisk (*) to retrieve all
- 65000 character limit

Add/remove a search term

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

Structure: CCNCc1oc(C(=O)O)c1

Graph: % Inhibition (%) vs Concentration (uM)

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

Structure Fields: All None

Structure SMILES IUPAC

CDD Number InChI

CXSMILES (CDD Compatible) InChIKey

Single Point Screen

Secondary CRC Assay

Add Protocol: (select protocol)

Dose-response plots scale
Sets the Y-axis scale for all dose response plots.

- Per Run - range in a given run
- Per Molecule - range across all runs of the molecule

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

Set column width

Select fields to display

Reorder sections in report

Choose fields from additional protocols

Molecules

Explore data > Molecules

CTV-0000001 Vault: CDD Training Vault

Molecule name

CC(=O)Oc1ccc(cc1)C(=O)O

Molecule name for Public data sets

CDD-55 (See more data sources)

- Find molecules with this structure
- View ChemSpider page
- Add to a collection
- Add a batch
- Manage project access
- Delete this molecule

Delete molecule

Showing data from 1 of 1 project

Owner: Maria Edwards
Created: October 28, 2018
Updated: October 28, 2018

View and manage plates, protocols, collections and projects for this molecule

Overview **Batches 1** Plates 0 Protocols 0 Collections 0 Projects 1 Files 0

Edit structure and synonyms

Definition [Edit definition and structure](#)

Name: CTV-0000001

Synonyms: Aspirin

User-defined Fields

Create another batch

Batch [Add a batch](#)

001

Edit batch information

Delete batch

Salt: No Salt, free base or acid
FW: 180.159 g/mol
External ID: Sample-1-1
Vendor: Vitas-M
Catalog Number: STL137674

Note:
Initial Amount: 10.0
Amount Units: g

Calculated properties

Lipinski Properties ?		Additional Properties ?	
Molecular weight:	180.159 g/mol	log D:	-2.16
log P:	1.24	log S:	0.15
		Fsp3:	0.11
		Heavy atom count:	13

Molecules

Single registration

Explore Data | **ELN** | **Import Data**

+ Create a new ...

- Protocol
- Molecule**
- Project
- ELN Entry

Back to Search

Create a New Molecule

Launch the Structure Editor

Draw molecule

Paste text representation of the molecule

- SMILES
- Mol file
- IUPAC name

Structure ?

SMILES, MOL or IUPAC

Strip: Strip salts and solvents from structure during registration

Stoichiometry: 0 No Salt, free base or acid : 0 No Solvent

How should salts and solvents be handled?

 - Strip - Strip drawn salts and solvents
 - Stoichiometry - Enter salts and solvents

Note: use Stoichiometry to register mixtures

Batch Information

External ID:

Vendor:

Catalog Number:

Purity:

Note:

Initial Amount:

Amount Units:

Project: My Favorite Project

Select project

Enter batch fields, as appropriate

Use this structure or **cancel**

Create Molecule or **cancel**

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 page > Protocol Name > 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

Formula =

`average([Inhibition data -> Inhibition (%)])`

Aggregation: Aggregate by batch 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

X: Concentration Unit: uM
Example: Concentration, Molar...

Y: Raw Unit: RLU
Example: % Inhibition, RFU, raw data...

Options

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

Fit Parameters:

Normalization:

Type: % inhibition or activation

Name: % inhibition

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

Specify Fit Parameters

Min, Max, and Hill Slope:

- Do not constrain values (use best fit)
- Constrain values

At least one point must be outside of this range
Otherwise, result will be reported as "> maximum concentration tested"

Inactive Range:

- 3 Standard Deviations from the negative control mean
- Custom

Set activity range that defines inactive compounds

IC50

Data Calculations: Display Format: 3 significant figures

Select desired calculation from list or choose Custom for another option

Add another calculation, e. g. IC90

[Add a data calculation](#)

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: **Browse...** Secondary CRC Assay.zip Project: Internal data **Upload File**

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 previously imports

Map fields

Type of information to be registered
Note: To register records without structures, select "without structure" option

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

File: Secondary CRC Assay.zip **Apply a mapping template...**

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

Use a saved mapping template, if available

	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

Next

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

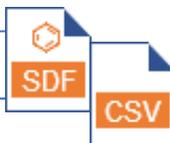
Save this mapping as a template... **Process File**

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
	<chem>c3ccc(F)cc3</chem>	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

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
- 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

Import Data

Commit Data

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

File: Benzodiazepines.sdf (Review mapping) **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 or Reject Import

- Commit Data Import
- Reject Data Import

Click down arrow to see details of noteworthy or suspicious events

Export problematic data to fix and reimport, as desired

- Noteworthy events**
 - Things to be aware of
 - Decide to Accept or Reject
- Suspicious events**
 - Possible problems in registration
 - Decide to Accept or Reject

Report

Explore Data | ELN | Import Data | Reports | Settings | **Import status**

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

+ Create a new ... Search Saved Searches

Heather Arnaiz

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

I changed my mind – Cancel the import

Cancel Import

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

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

This data import was committed **View imported records**

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

View or export records

Noteworthy Events · Usually fine. Associated records will be imported except if you choose otherwise.

- 7 New Batches (2 indirectly rejected) **ACCEPTED**

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

- 2 Existing Molecules Associated with New Project **REJECTED**