

Configuration

Settings > Vault

Terminology [Edit terminology](#)

Vault Settings

Entry:	experiment
Protocol:	assay
Readout_definition:	readout
Run:	run
Molecule:	compound
Batch:	lot

Use your terminology in your Vault

General Vault setting

Multiple compounds with the same structure are NOT allowed.
To enable this feature (e.g. to archive structures with different but unique identifiers) please contact support@collaborativedrug.com.

Email alerts: summary only

Project association via data import: 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

3 Projects [Create a new project](#)

CRO 1	View data	Delete
Project ABC	View data	Delete

Create new projects

Edit project or assign members

Read-Add or higher role needed to create a project

Members

5 Members [Add a member](#)

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

Create new members

Manage Vault members

Vault Admin privileges needed for all pages except Projects

General

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		is optional
Notebook	Text		or Vendor is required
Vendor	Text		or Notebook is required
Sample ID	Text	✓	is optional
Initial Amount	Number		

Create batch fields

Specify batch field is:

- Unique value across Vault
- Required or optional

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

Configuration

Projects

Delete project
Note: All data must be removed from project first

Rename project

Delete

Add/Edit

Edit settings

Members ?

Name	Edit Data	Manage
Heather Arnaiz	✓	✓
Maria Edwards	<input type="checkbox"/>	<input type="checkbox"/> Remove

Control permissions

- Edit Data
 - Checked – user has vault role
 - Unchecked – read only or read export depending on vault role
- Manage
 - Checked – Manage users

Select user from drop down
Note: Only members of a vault can be added to a project

- Select a user -
- Select a user -
Sylvia Ernst

Members

Your role

- Click to view table of permissions for all roles

Add a member

- First name
- Last name
- Email
- Role

Edit or delete member

Heather Arnaiz Vault Administrator

Add a member

Name	Access	Date Added	Projects	Email	API Keys	Actions
Heather Arnaiz	vault admin					<input type="checkbox"/> <input type="checkbox"/>

First name: John
Last name: Doe
Email: john.doe@company.com
Access role: Readonly

Configuration

Batch fields

Settings > Vault > Batch fields

Create batch fields at any time

Add/Edit Batch Fields

Name	Data Type	Must be Unique	This Field
Date	Date		is optional
External ID	Text	✓	is optional

CAS #

Name	Data Type	Must be Unique	This Field
Purity		<input type="checkbox"/>	is optional
Type		<input checked="" type="checkbox"/>	is optional
Image		<input type="checkbox"/>	is optional

Value is unique for across the vault

- Uniqueness checked at registration.
- Can be used to identify a batch when importing data.

Reorder batch fields

+ Add a batch field

+ Add a batch field

Supported data types:

- Text
- Number
- Date
- Pick list
- File

Enforce business rules:

- Must be unique
- Is required
- Is optional

Update batch fields or cancel

Explore Data

Search your data (or browse)

The screenshot shows the CDD Vault interface for 'Heather Demo Vault'. The interface includes a top navigation bar with 'Explore Data', 'ELN', 'Import Data', 'Reports', and 'Settings'. A user profile 'Heather Arnaiz' is visible in the top right. The main content area is divided into several sections:

- Left Panel:** A 'Create a new ...' dropdown menu lists 'Molecule', 'Project', 'Protocol', and 'ELN Entry'. Below it, a 'Projects' section shows 'Project ABC' and 'Project XYZ' with checkboxes, and a 'Public Data' section with a '0' count.
- Search Options:** A 'Search' section with tabs for 'Search', 'Saved Searches', and 'Collections'. It includes a 'Search options' box and a 'Browse/edit registered entities' box.
- Protocols:** A section for filtering by protocol, with options to search 'In' a specific protocol or category.
- Structures:** A section for filtering by structure type (substructure or similarity) and a 'Launch the Structure Editor' button.
- Chemical Properties:** A section for filtering by chemical properties, with a dropdown for '(select property)' and input fields for 'Min' and 'Max'.
- Collections:** A section for filtering by collection, with a dropdown for '(select a collection)'.
- Keywords:** A section for filtering by keywords, with a dropdown for 'Any field' and a text input field.

Callout boxes provide additional information:

- 'Current vault' points to the vault name in the top bar.
- 'Select another vault' points to the vault selection dropdown.
- 'Create new entity' points to the 'Create a new ...' dropdown.
- 'Select project and/or Public Data to search' points to the 'Projects' and 'Public Data' sections.
- 'Launch Structure Editor to:' points to the 'Launch the Structure Editor' button, with sub-points: 'Draw structure', 'Paste smiles, mol, or IUPAC name', and 'Import file'.
- 'Search results will match all criteria specified' points to the search criteria section.
- 'Search within (or not) a protocol or category' points to the 'Protocols' section.
- 'Search by chemical properties' points to the 'Chemical Properties' section.
- 'Search within (or not) a collection' points to the 'Collections' section.
- 'Add/remove a search term' points to the 'Add a term' and 'Remove term' buttons.
- 'Wildcard – asterisk (*)' points to the 'Keywords' section, with sub-points: 'Type asterisk (*) to retrieve all' and '65000 character limit'.

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: CCNC1=CC=C(O)O1

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

CDD.VAULT · CDD Training

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

Add a dose-response calculation

Add a calculated readout definition

Hit Conditions

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

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

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

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

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

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

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

Import Data

Choose file

The screenshot shows the 'Import Data' interface with the 'Choose Data File' step active. The navigation bar includes 'Explore Data', 'ELN', 'Import Data', 'Reports', 'Settings', and a user profile 'Heather Arnaiz'. The main area has three steps: 'Step 1: Choose Data File', 'Step 2: Map Fields', and 'Step 3: Commit Data'. Under 'Files', there is a link to 'View saved mapping templates'. The 'Choose a file to upload' section has a 'Browse...' button, the filename 'Secondary CRC Assay.zip', a 'Project' dropdown set to 'Internal data', and an 'Upload File' button. Below this, the 'Uploaded Files' section shows a table with columns for 'Filename', 'Date', and 'Status'. Two entries for 'Secondary CRC Assay.zip' are listed: one from January 23, 2018, with a 'Partially mapped' status, and another from December 14, 2017, with an 'Imported' status. A 'Revisit previously imports' callout points to the 'Imported' entry.

View saved mapping templates

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

Uploaded 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

The screenshot shows the 'Map Fields' step of the import process. The navigation bar is the same as in the previous screenshot. The main area has three steps: 'Step 1: Choose Data File', 'Step 2: Map Fields', and 'Step 3: Commit Data'. The 'File' is 'Secondary CRC Assay.zip' and there is an 'Apply a mapping template...' button. Below this, there are radio buttons for 'Add readouts (protocol data) only', 'Update existing molecules', and 'Register new molecules / batches with structures'. A callout 'Add data to existing molecules' points to the 'Update existing molecules' option. Below the radio buttons is a table with columns A-F and rows 1-4. Row 1 has headers: 'Molecule Name', 'Plate', 'Well', 'Conc (uM)', 'Raw (RLU)', and 'Microscopy'. Row 2 has values: 'Sample-10-001', 'Sample Pl._20151108', 'A10', '0.01', '2.67E+03', and 'Microscopy/mag...'. Below the table, there is a 'Map fields' section with a dropdown for 'Molecule Name or Synonym' and a 'Next' button. A callout 'Map fields' points to this section, with a note: 'System will map columns with similar names to fields'. Below the mapping section, there is a 'Please address the following:' section with two bullet points: 'If you map Molecule Name or Synonym you must also map Batch Name and vice versa.' and 'You must not map Image when adding readouts only.' A callout 'Issues to be fixed before importing can occur' points to this section. At the bottom, there is a 'Save this mapping as a template...' button and a 'Process File' button. A callout 'Save mapping as template for future use' points to the 'Save this mapping as a template...' button.

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

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.



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

Single point data

File type 

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

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

Dose response

Controls – if applicable

Note: do not need to be associated with a batch

	A	B	C	D	E	
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

Noteworthy events

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

Suspicious events

- Possible 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

Report

Explore Data | ELN | Import Data | Reports | Settings | ✉

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

Import status

+ Create a new ... Search Saved Searches Col

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

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

View imported records

Explore imported 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)

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

- 2 Existing Molecules Associated with New Project

REJECTED