

# 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
- from
  - Note: Only for numeric fields.
- 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

Structure: CCNC(C)Cc1oc(C(=O)O)c1

DEMO-0007944  
CDD New Demo Vault

0-50 6.54 ± 8.19 (n=2) 0.261

12.33

% Inhibition (%) vs Concentration (uM)

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)

Dose-response plots scale

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