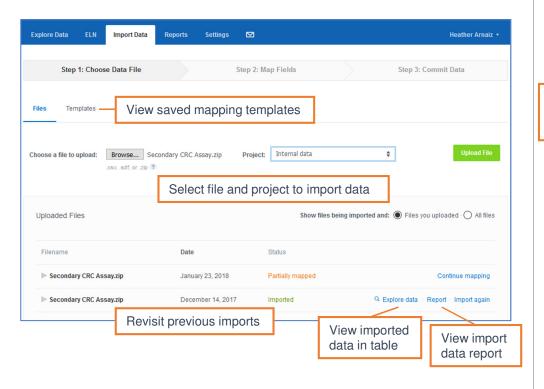# Import Data

Choose file

Map fields

Type of information to be registered

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

Add data to existing molecules

Use a saved mapping template, if available

View saved mapping templates

Select file and project to import data

Map fields

Note: System will map columns with similar names to fields

Revisit previous imports

View imported data in table

View import data report

Issues to be fixed before importing can occur

Save mapping as template for future use

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File format

Molecules

File types — SDF, CSV

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	CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1	34911-55-2	95	NIH	SAM001246723	CPD000058423	5	Sample-10-2
3	CNCC[C@H](Oc1cccc2ccccc12)c3cccs3		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 — CSV

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 20180418			

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

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Importing attachments

File format

File type

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

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

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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

View mapping
- Create template from mapping

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 b...   [ACCEPT] [REJECT]

▶ 7 New Batches (2 indirectly rejected)

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

⚠ Suspicious Events · Usually unexpected. Associated records will not be imported except if you choose otherwise.   [ACCEPT] [REJECT]

▼ 2 Existing Molecules Associated with New Project

The molecule will be associated with the target project. Learn more...

Suspicious events
- Problems in registration
- Decide to Accept or Reject

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

Click down arrow to see details of noteworthy or suspicious events

Export problematic data to fix and reimport, as desired

[Commit Data Import] [Reject Data Import]

Commit or Reject Import

Report

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

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

[+ Create a new ... ▼]   Search   Saved Searches   Col...

Import status

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

View mapping
- Create template from mapping

This data import was committed   🔍 Explore imported data

⊕ 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

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]

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