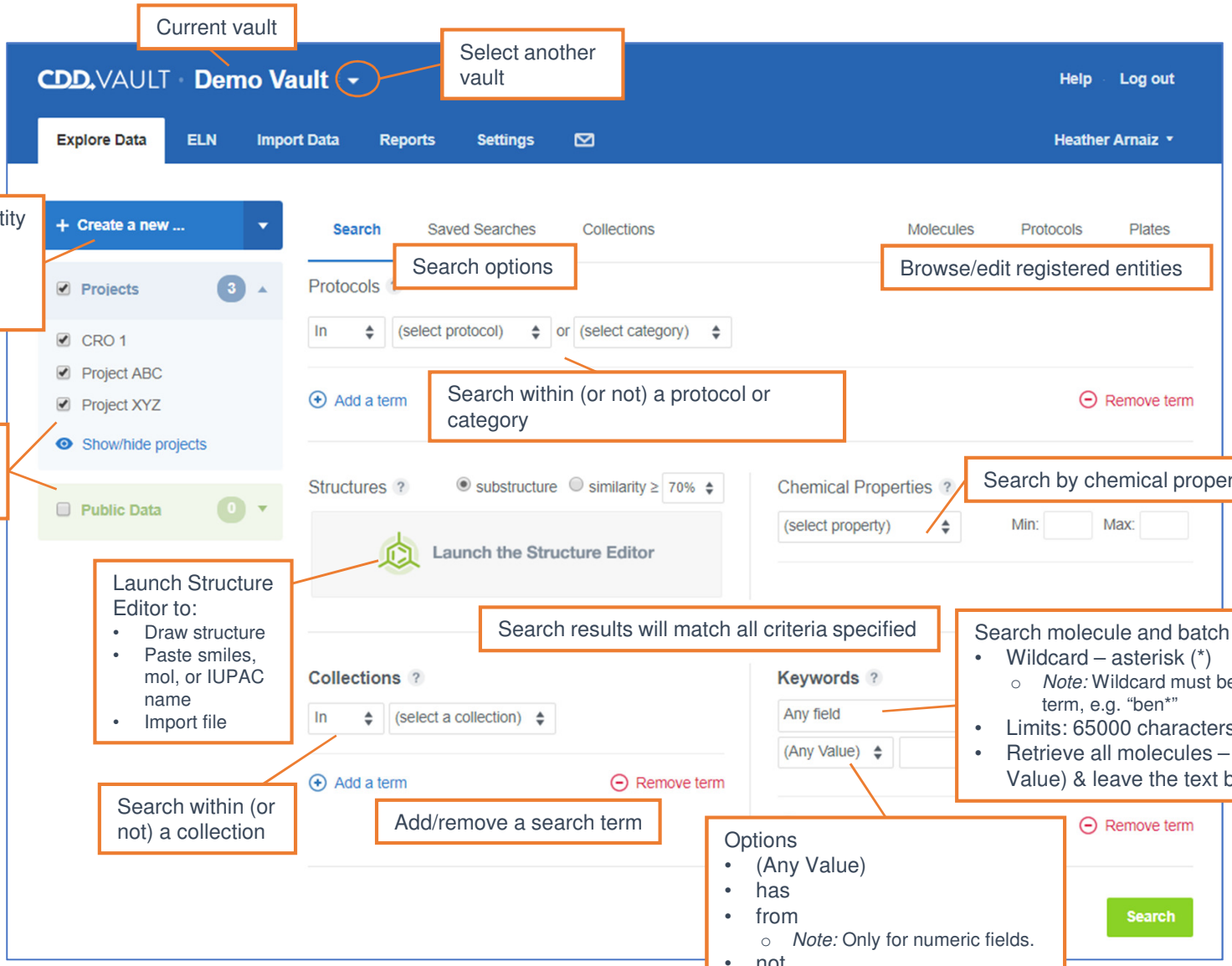
Explore Data

Search your data (or browse)



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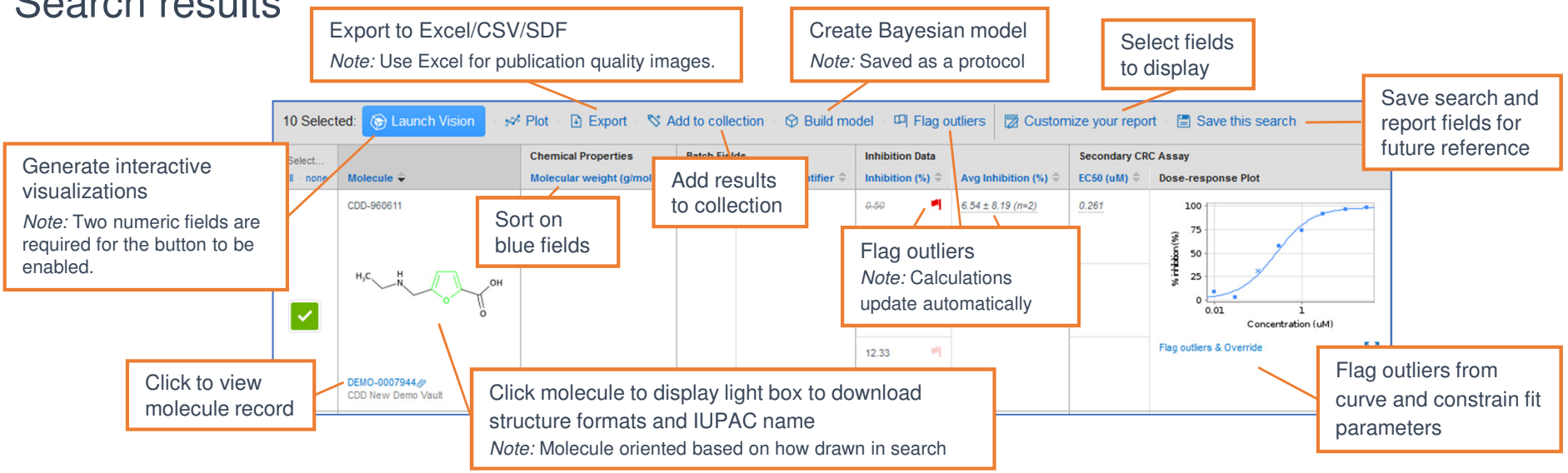
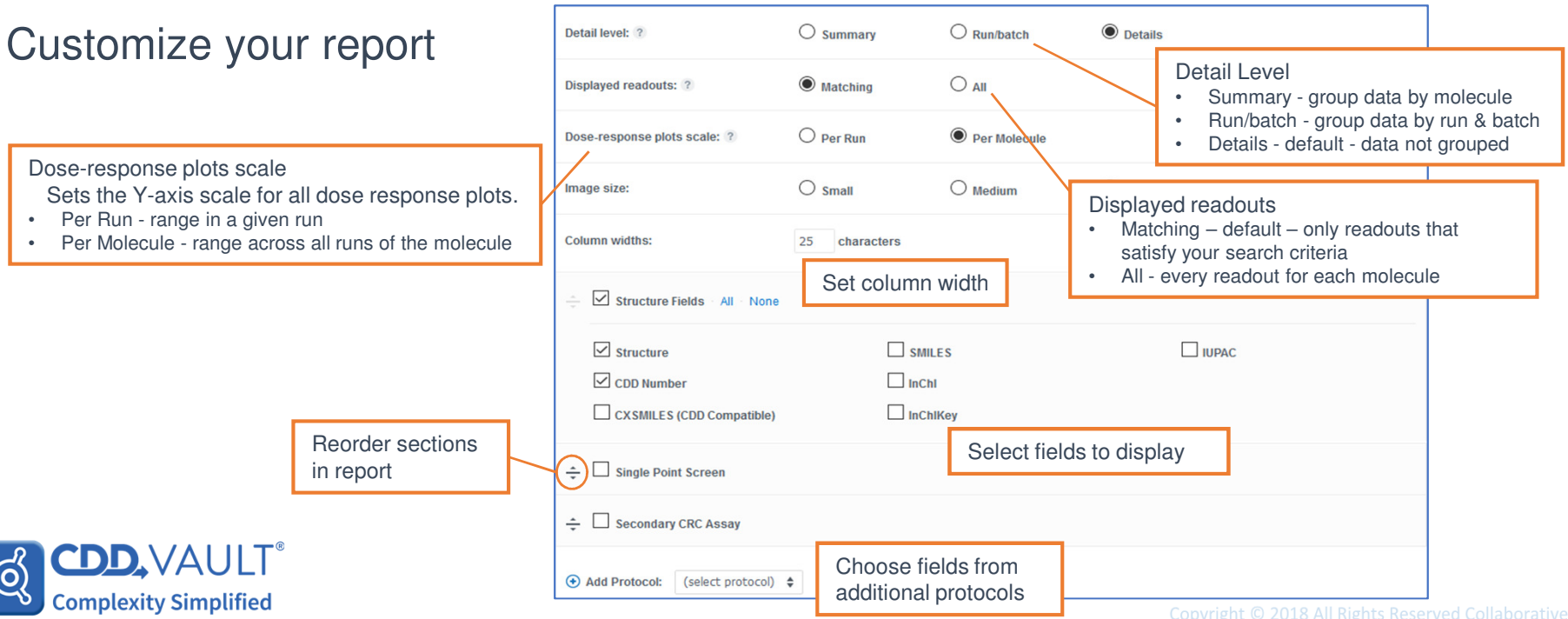
Explore Data

Search results



Customize your report



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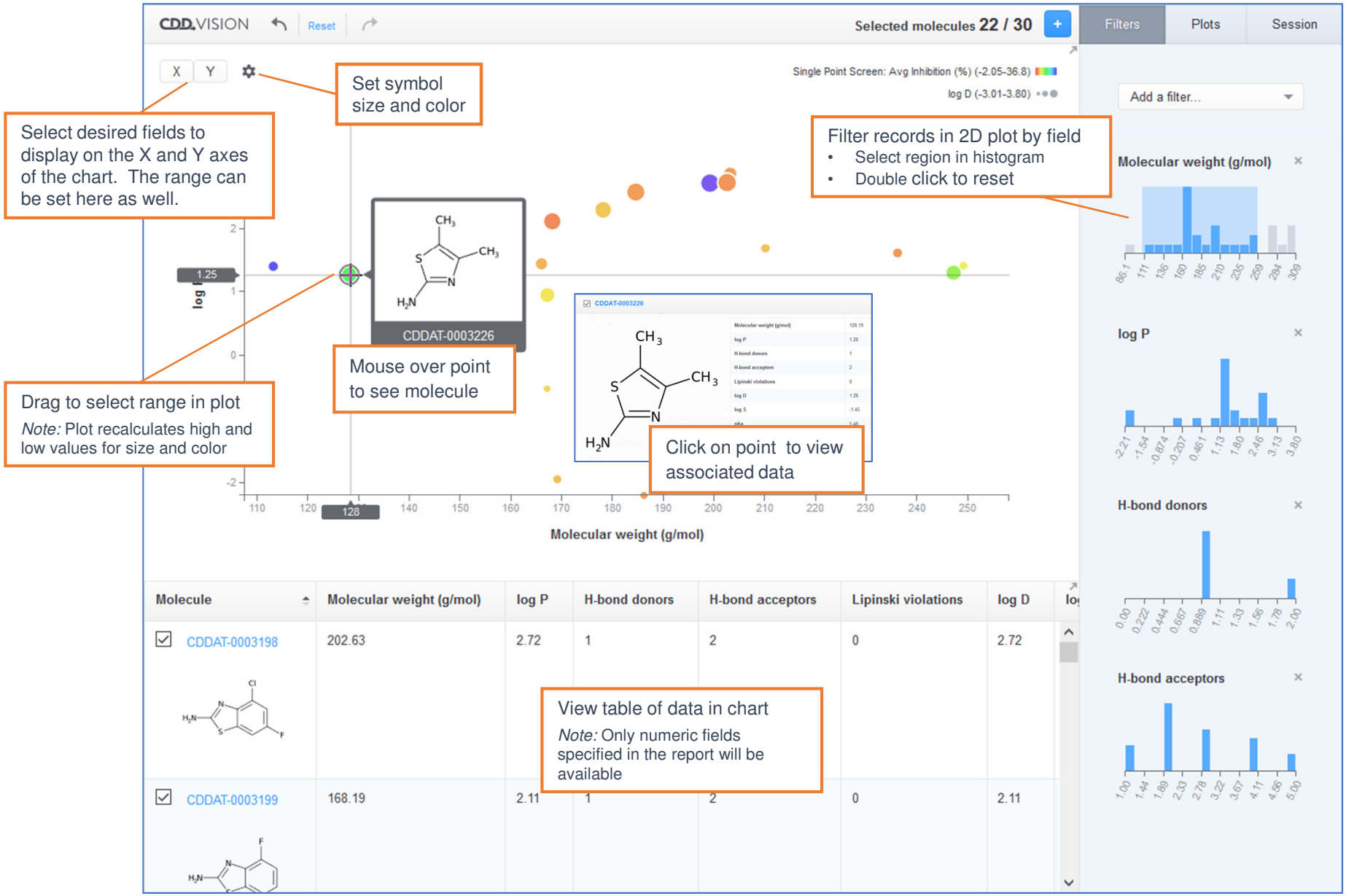
Vision

Filters



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Vision

Plots

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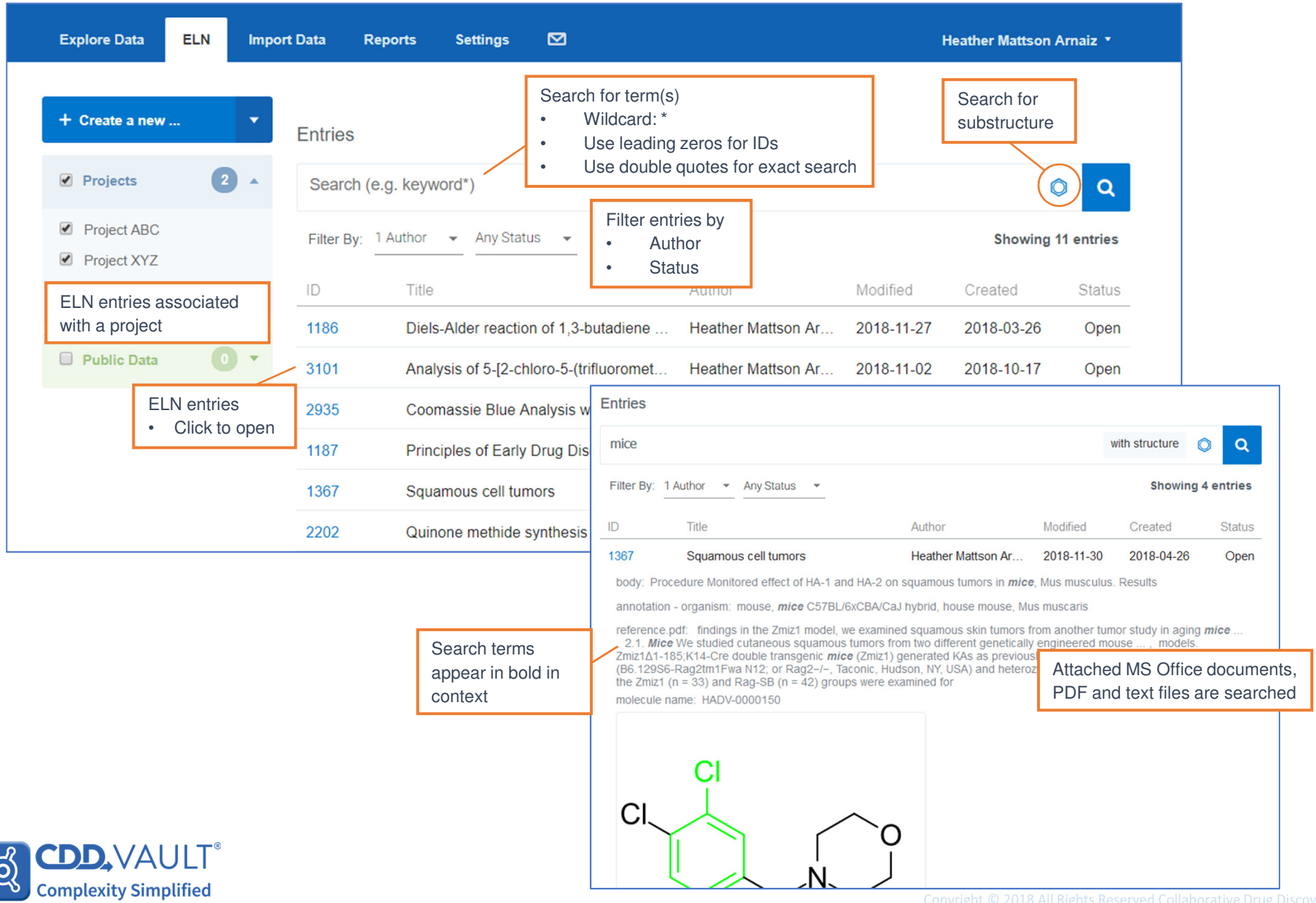
ELN

Search entries



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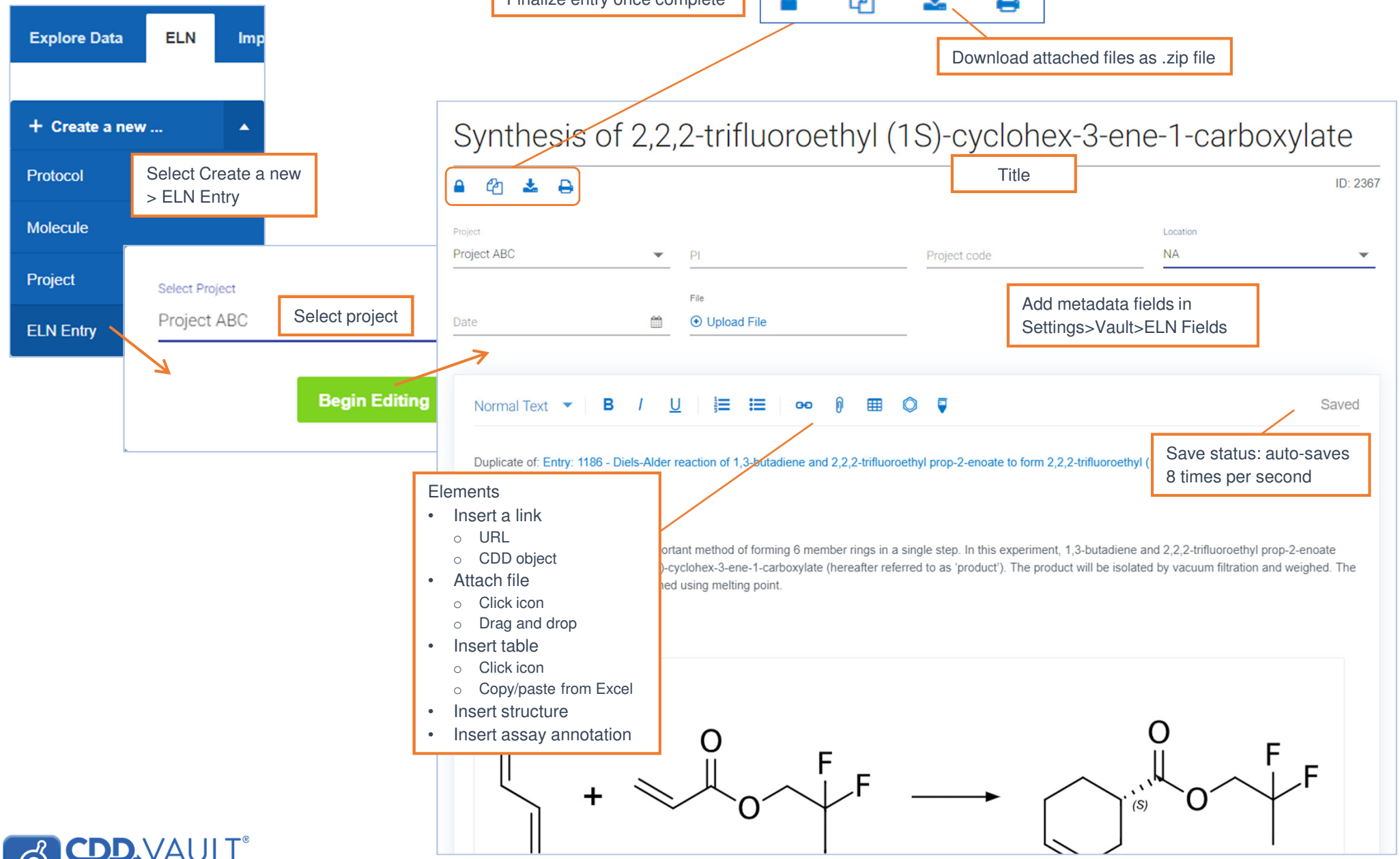
ELN

Create new entry



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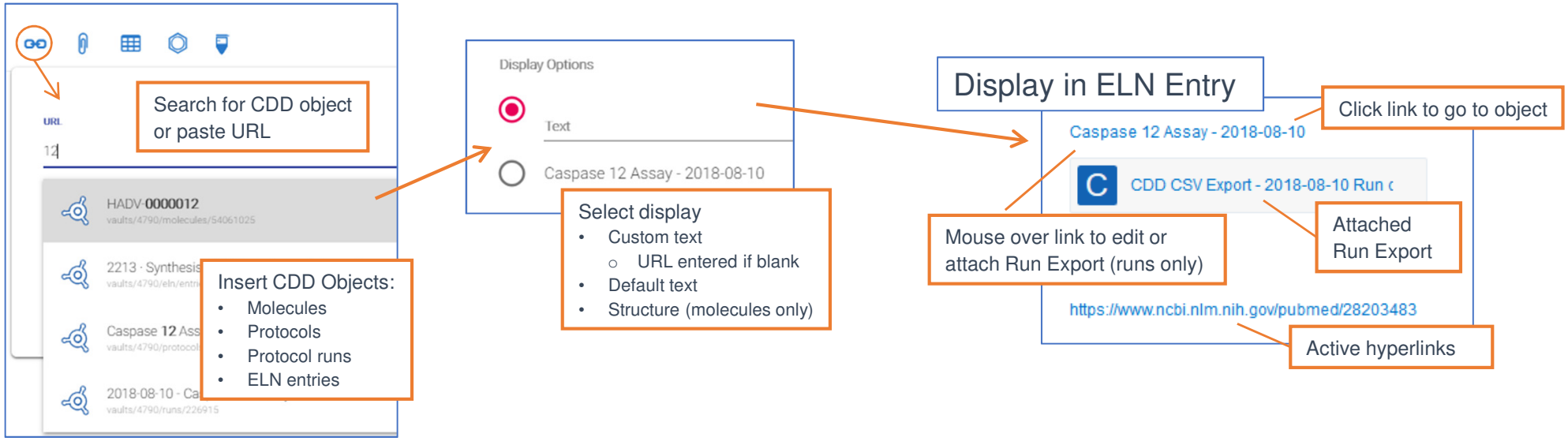
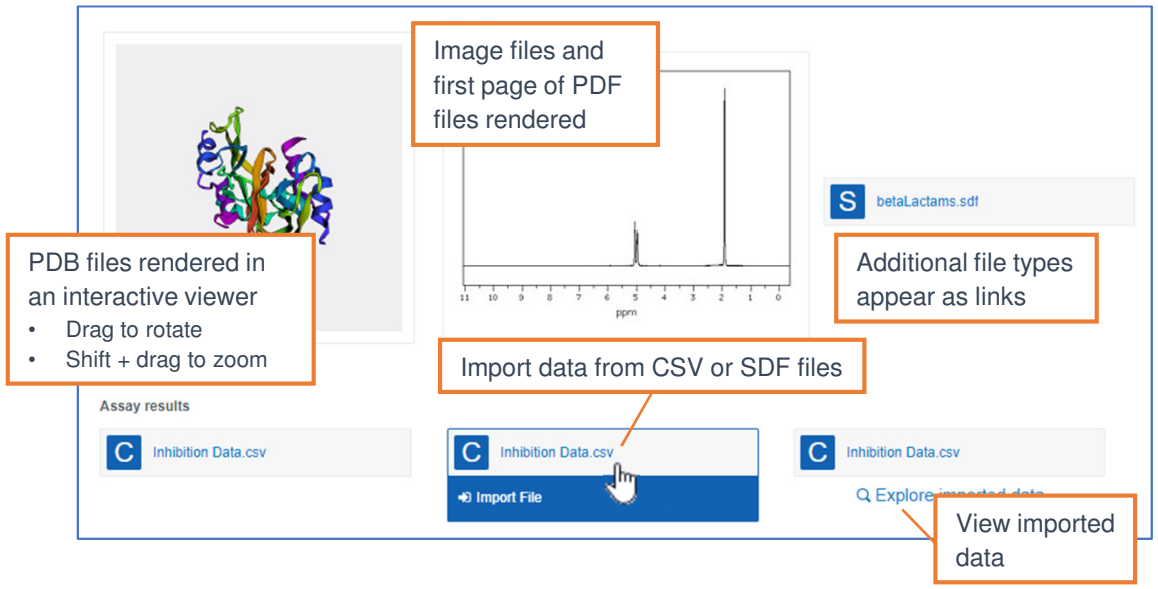
ELN Elements

Links



File Attachments



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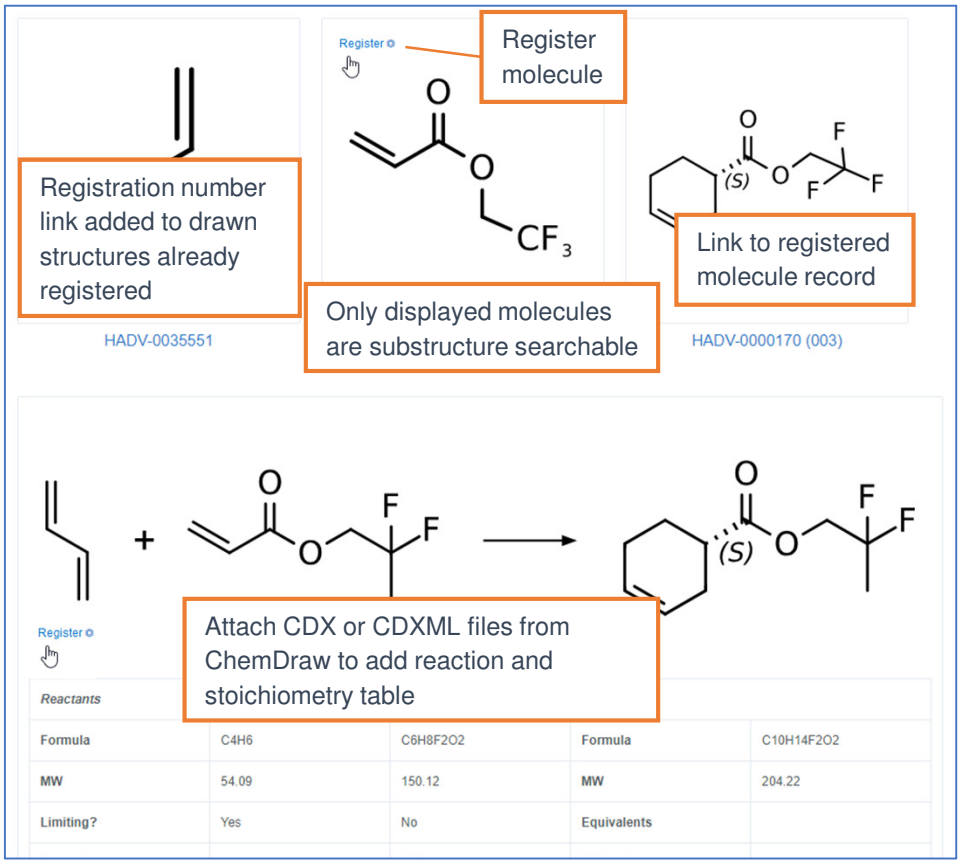
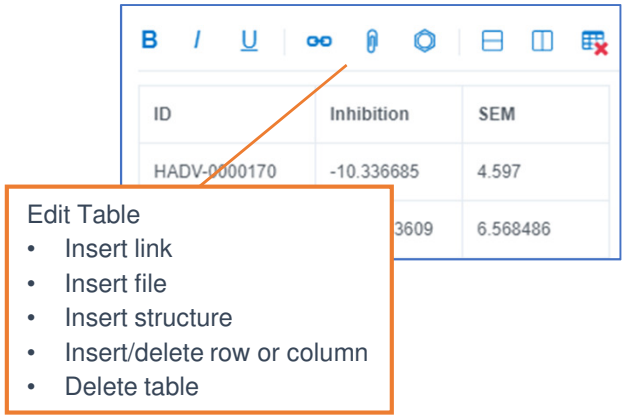
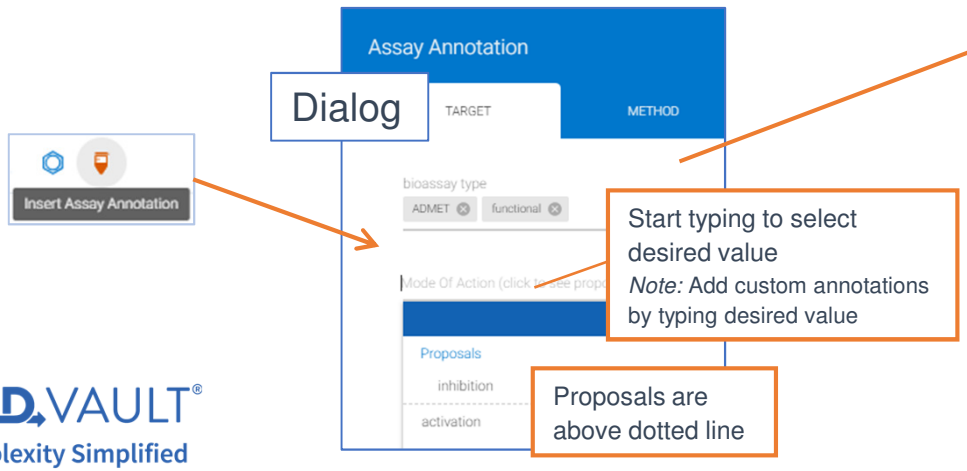
Molecules and Reactions

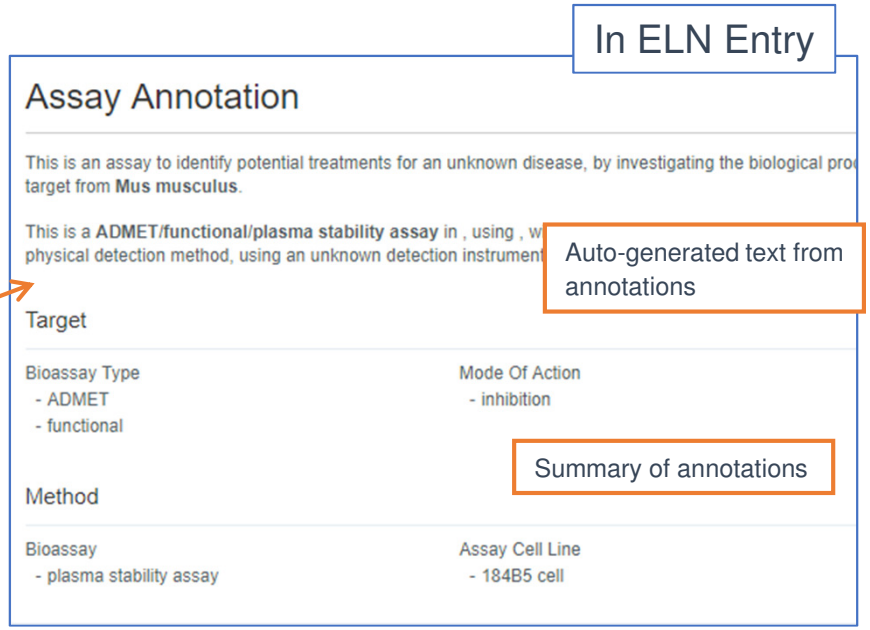


Tables



Assay Annotation





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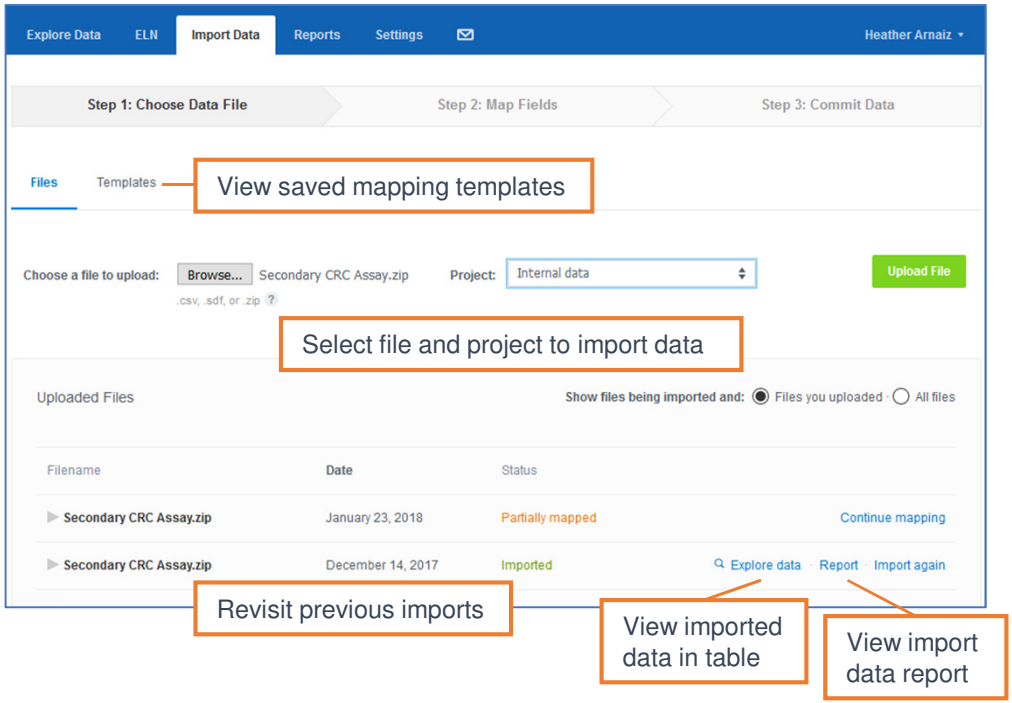
Import Data

Choose file



View saved mapping templates

Select file and project to import data

Revisit previous imports

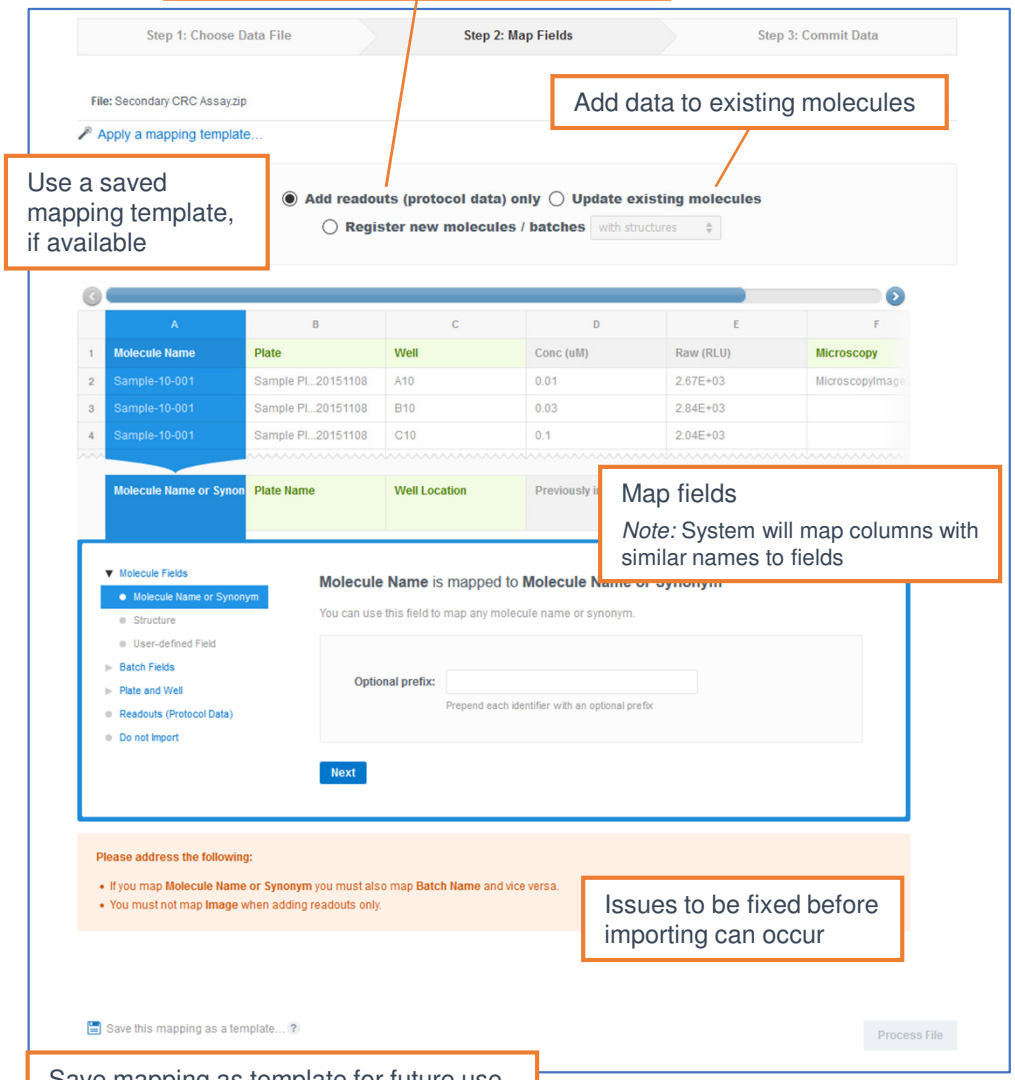
View imported data in table

View import data report

Map fields

Type of information to be registered

Note: To register records without structures, select “without structure” option



Use a saved mapping template, if available

Add data to existing molecules

Map fields

Note: System will map columns with similar names to fields

Issues to be fixed before importing can occur

Save mapping as template for future use

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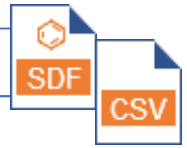
File format

Molecules

File types



CSV format

	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
4	)cc3	128196-01-0	95	NIH	SAM001246668	CPD000469191	5	Sample-10-4

Unique batch field

Note: this can be used for uploading data

Use SMILES or mol file for structures

Note: Salts and solvents will be stripped by default

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
- A combination of one of the first 3 options and Plate and Well location

e.g. 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	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

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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 C

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

View mapping
- Create template from mapping

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

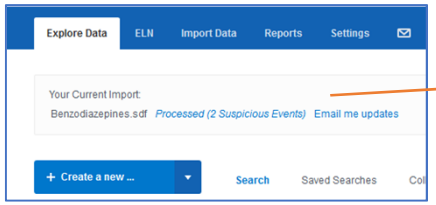
Suspicious events
- Problems in registration
- Decide to Accept or Reject

Click down arrow to see details of noteworthy or suspicious events

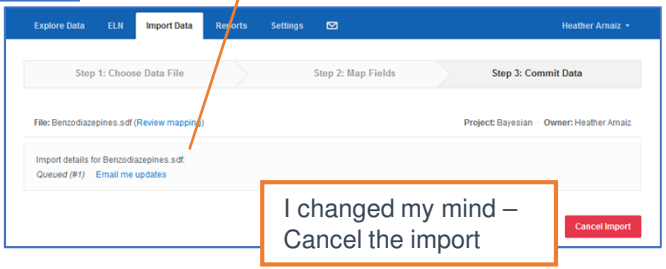
Export problematic data to fix and reimport, as desired

Commit or Reject Import

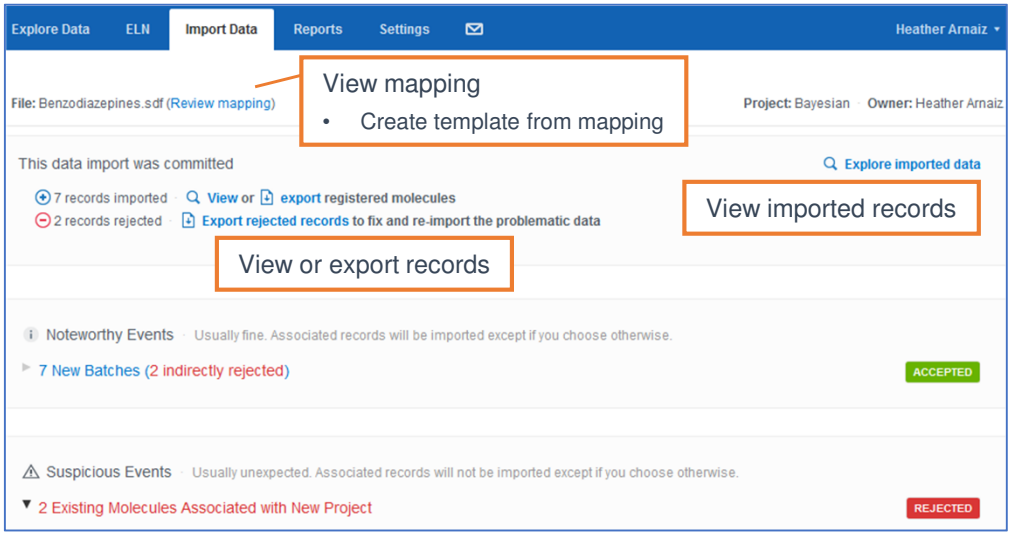
Report



Import status



I changed my mind – Cancel the import



View mapping
- Create template from mapping

View imported records

View or export records

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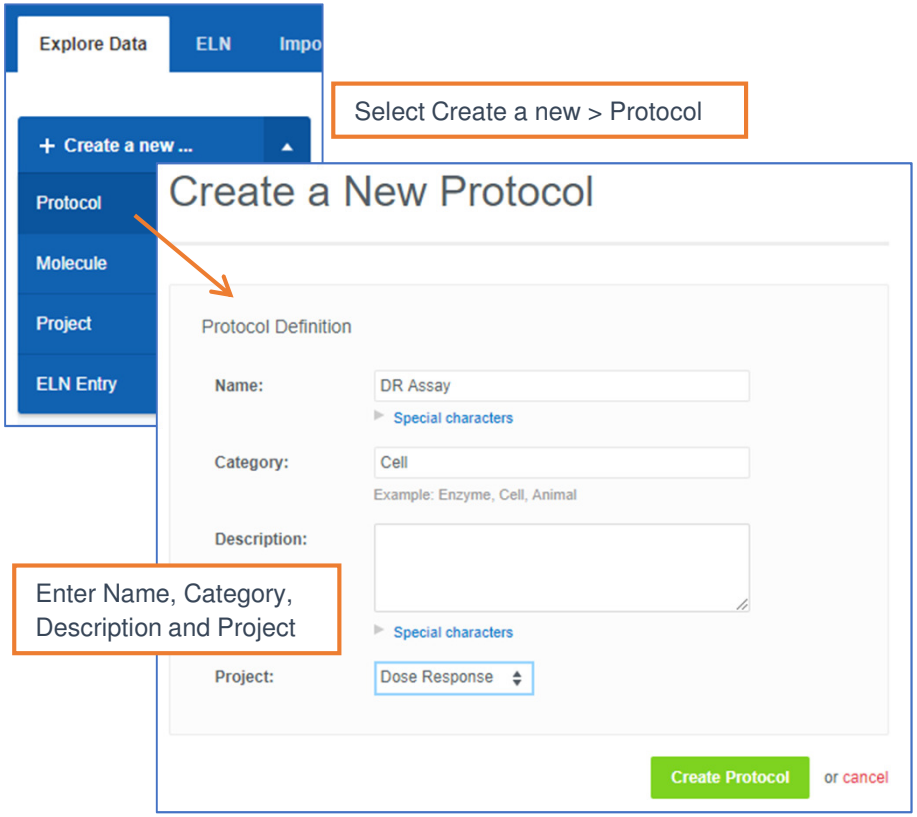
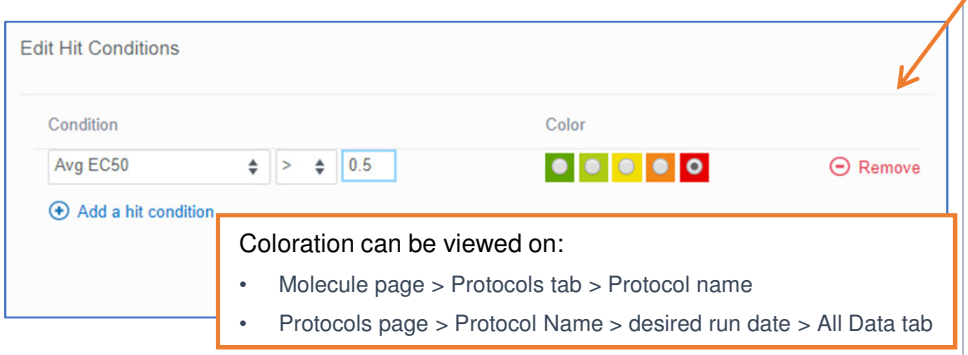
Protocols

Create a new protocol





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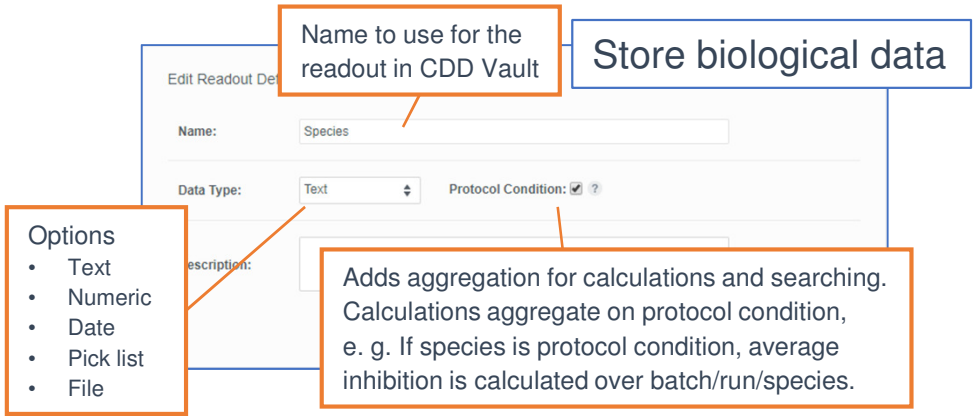
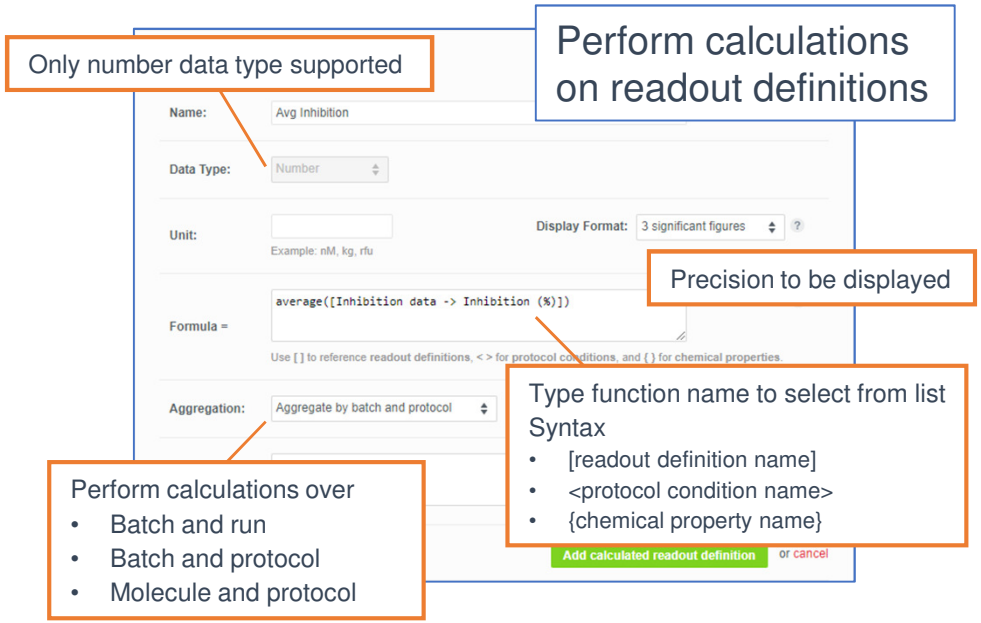
Readout Definitions

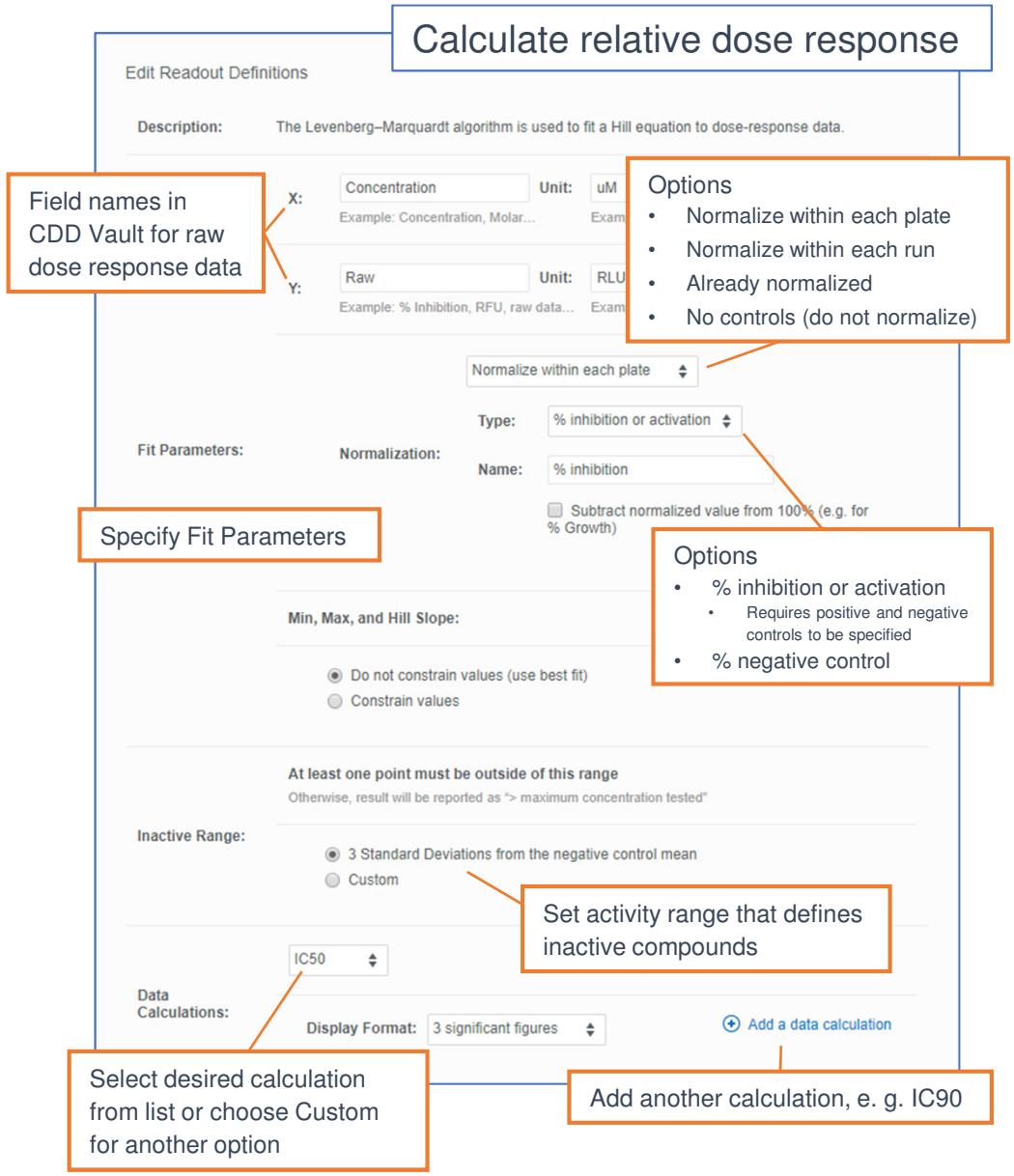
Add a Readout Definition



Add a calculated readout definition



Add a dose response readout definition



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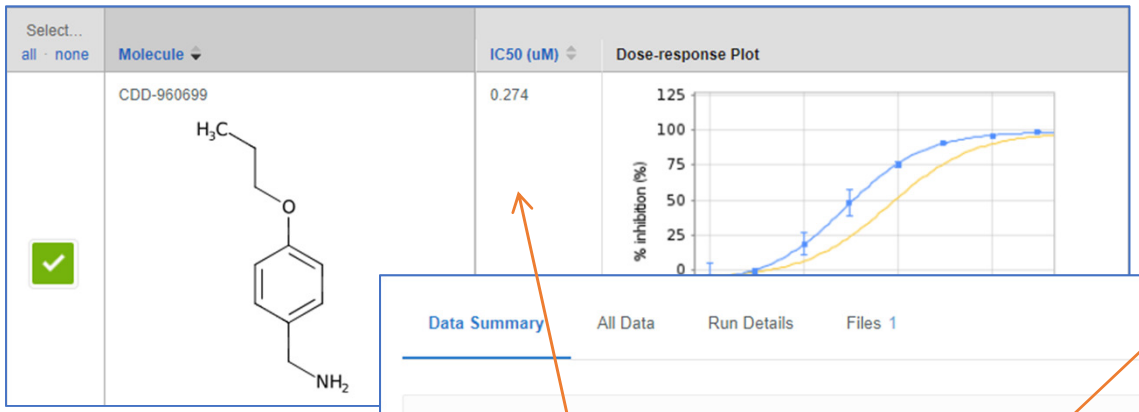
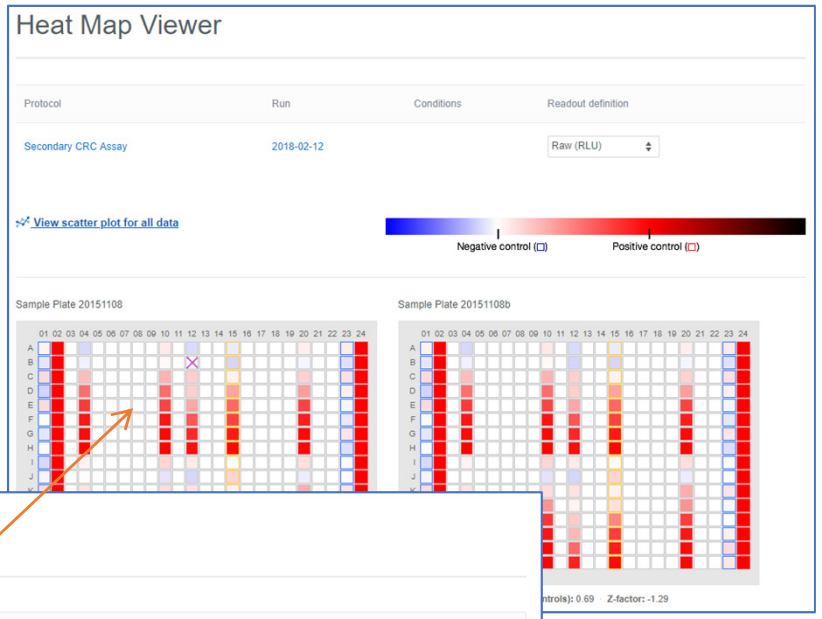
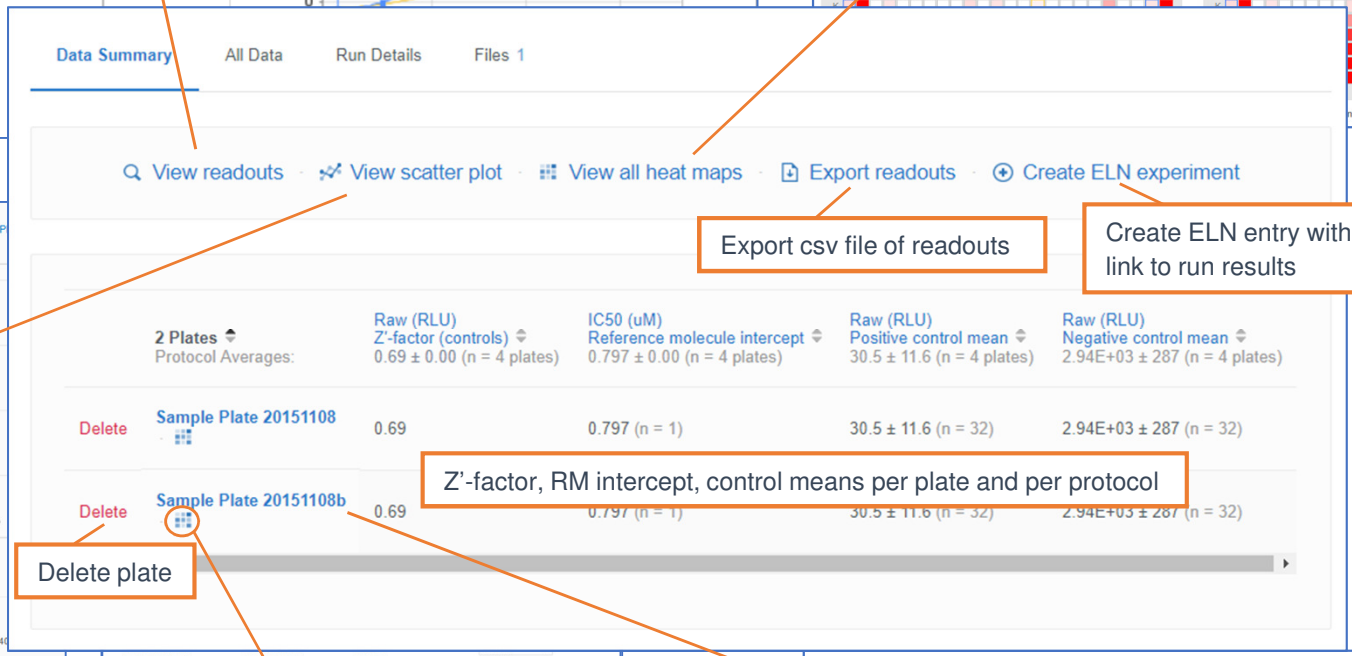
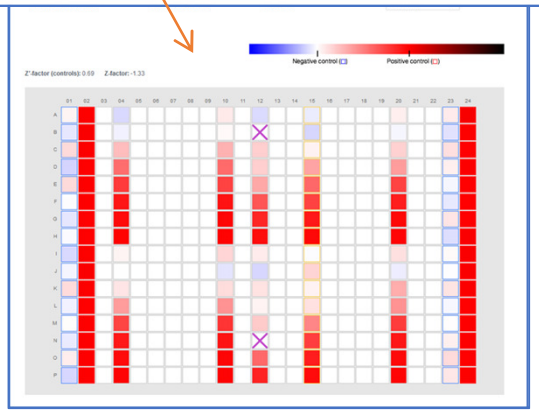
Quality Control

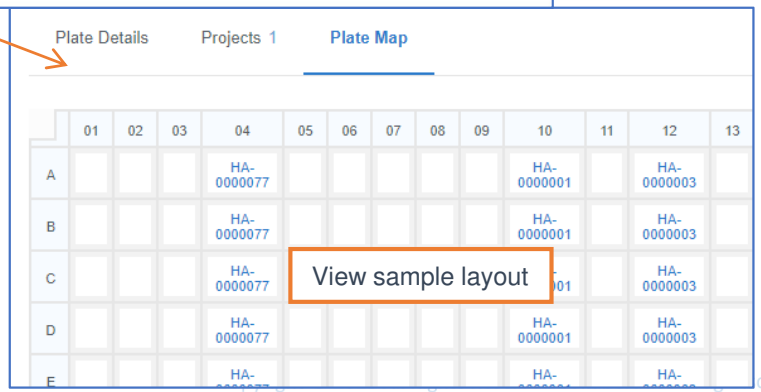
Protocols > Protocol name > Run date











Export csv file of readouts

Create ELN entry with link to run results

Z'-factor, RM intercept, control means per plate and per protocol

Delete plate

View sample layout

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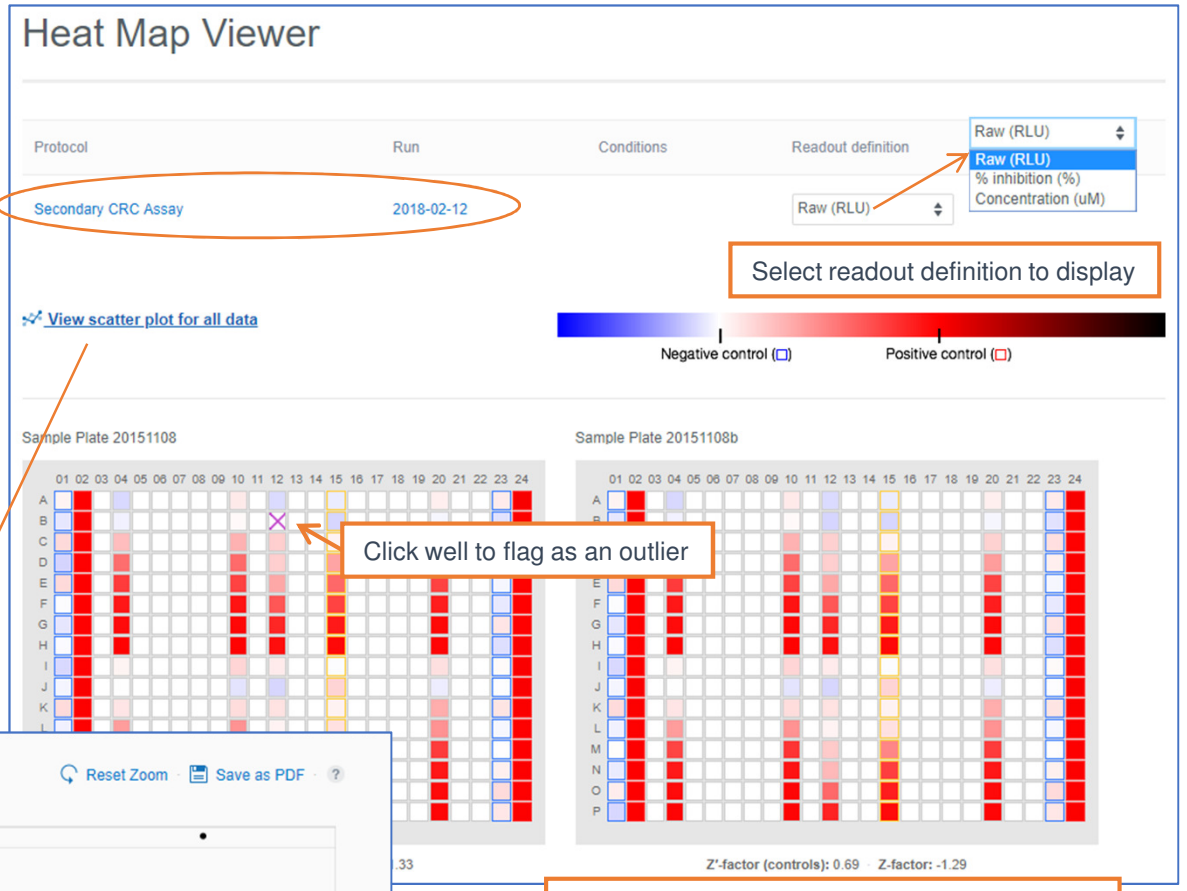
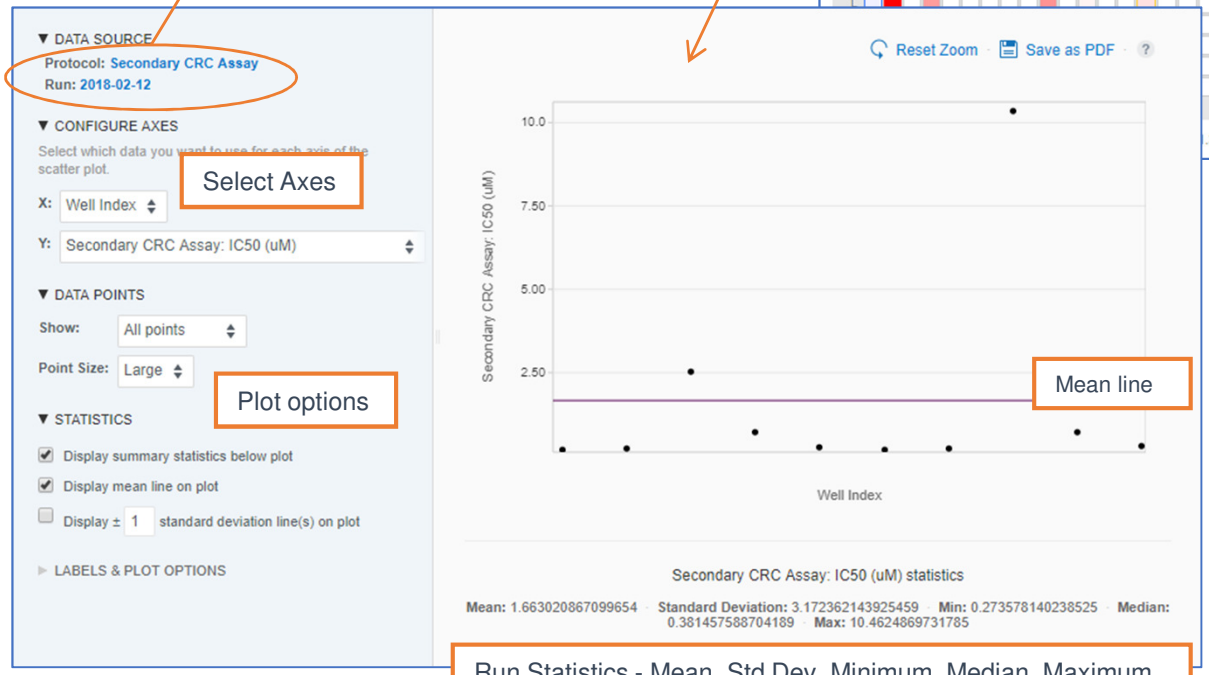
Quality Control

From Protocol page



Breadcrumbs
- Click Protocol name to Protocol Run Data page
- Click Run date to go to Data Summary page



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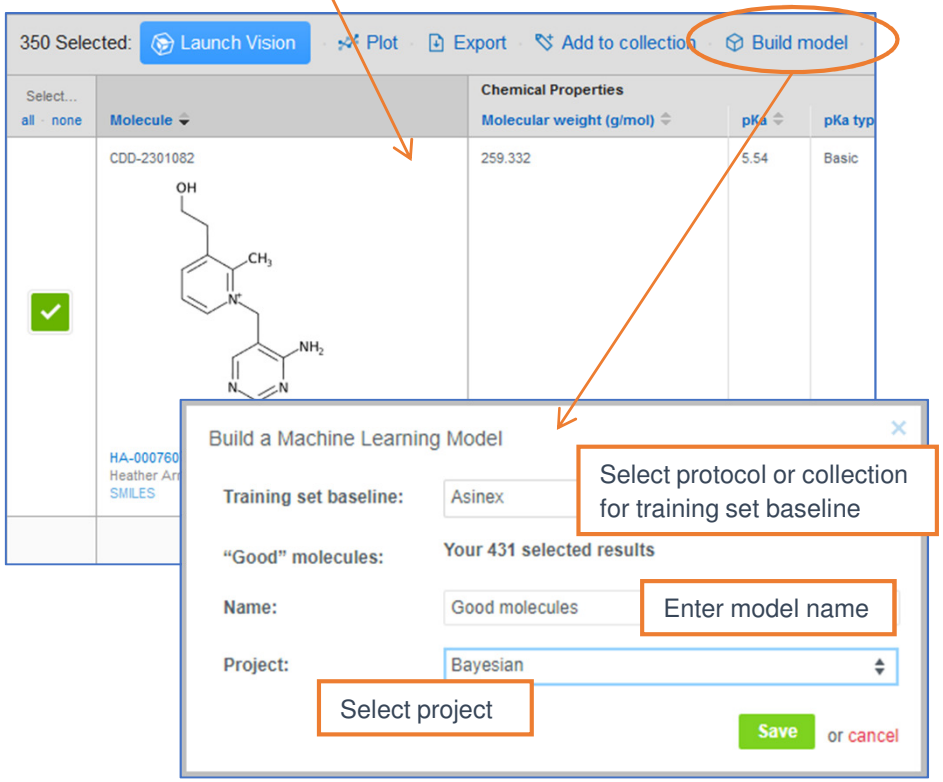
Data Modeling

Create a model

Retrieve a list of “Good” molecules from a:
- Search
- Saved search
- Collection

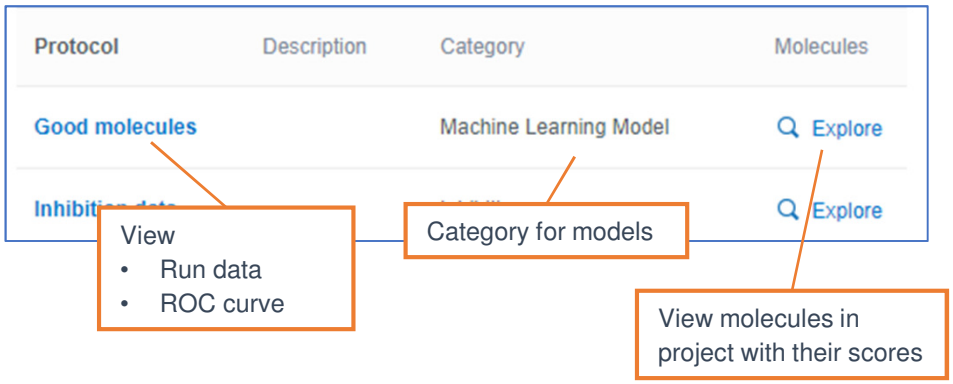


Select protocol or collection for training set baseline

Enter model name

Select project

Model are treated as Protocols



View
- Run data
- ROC curve

Category for models

View molecules in project with their scores

Readout definitions calculated

Name	Description
Score	Relative score (higher is better)
Applicability	Fraction of structural features shared with the training set
Maximum similarity	Maximum Tanimoto/Jaccard similarity to any “good” molecules

Algorithm

Modified Bayesian model with FCFP6 descriptors

Model:	CDD's open source modified Bayesian model described in Xia et al. 2004.
Descriptors:	CDD's open source FCFP6 fingerprints described in Rogers and Hahn 2010.

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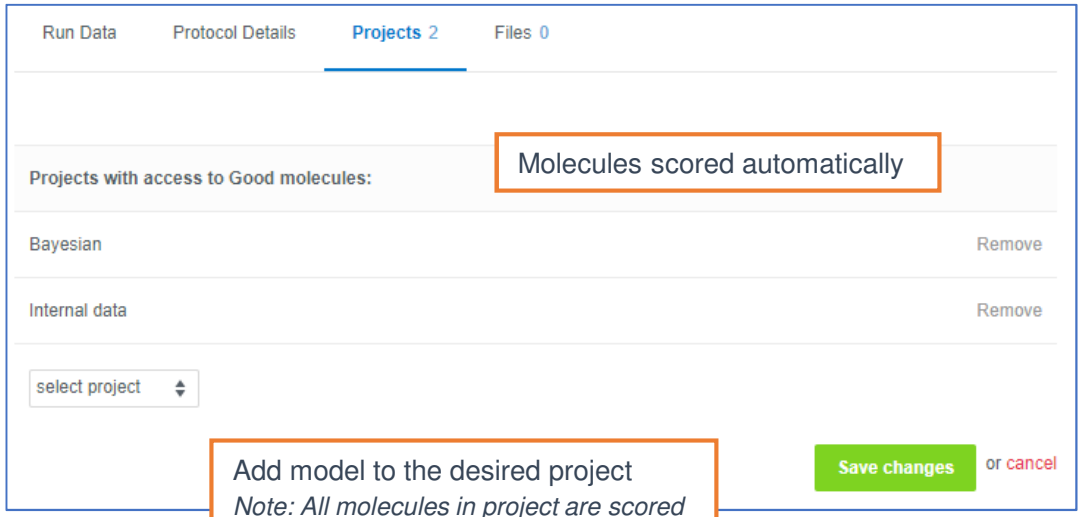
Data Modeling

Quality of model

On Protocol Details tab

Use a model



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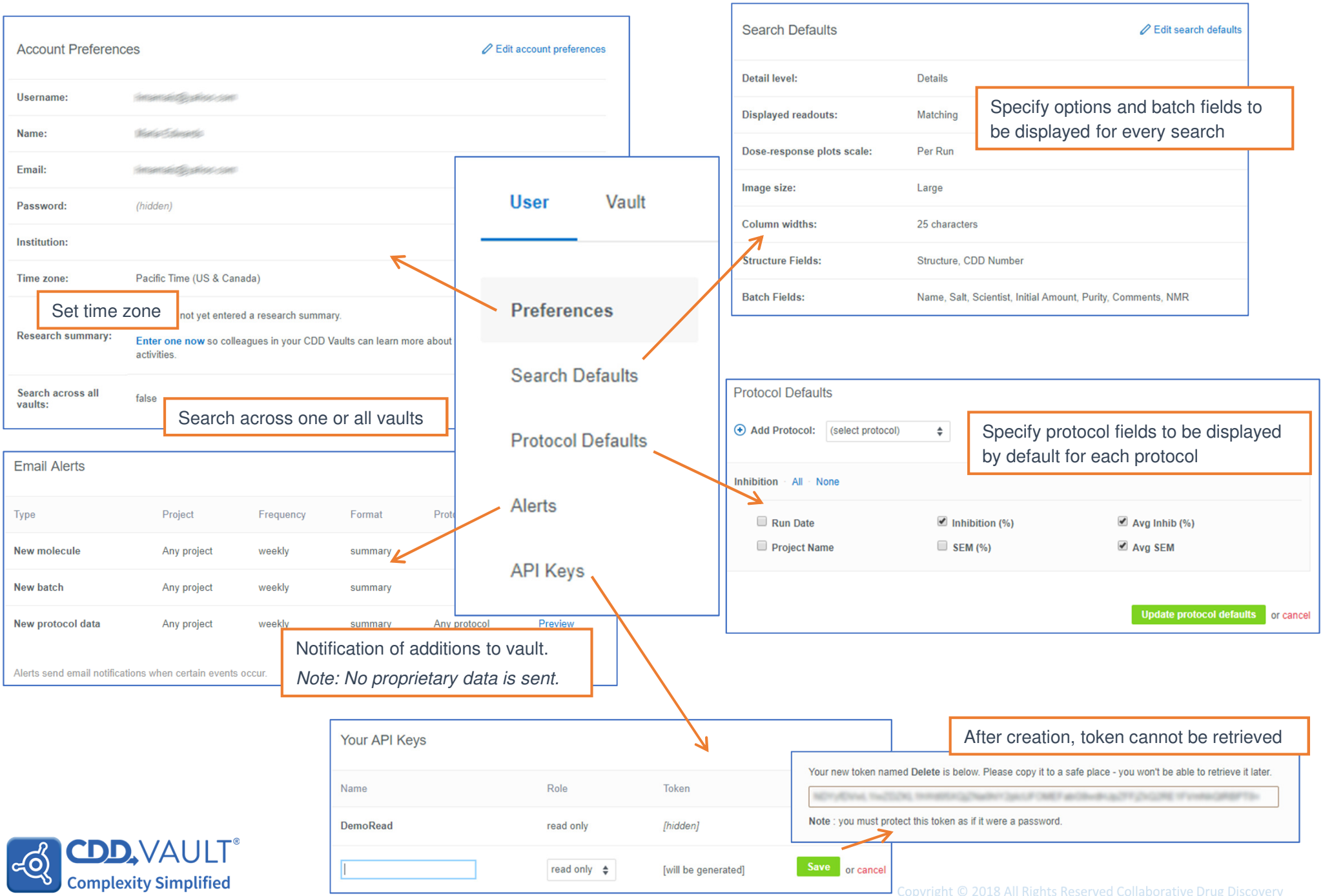
Settings > User



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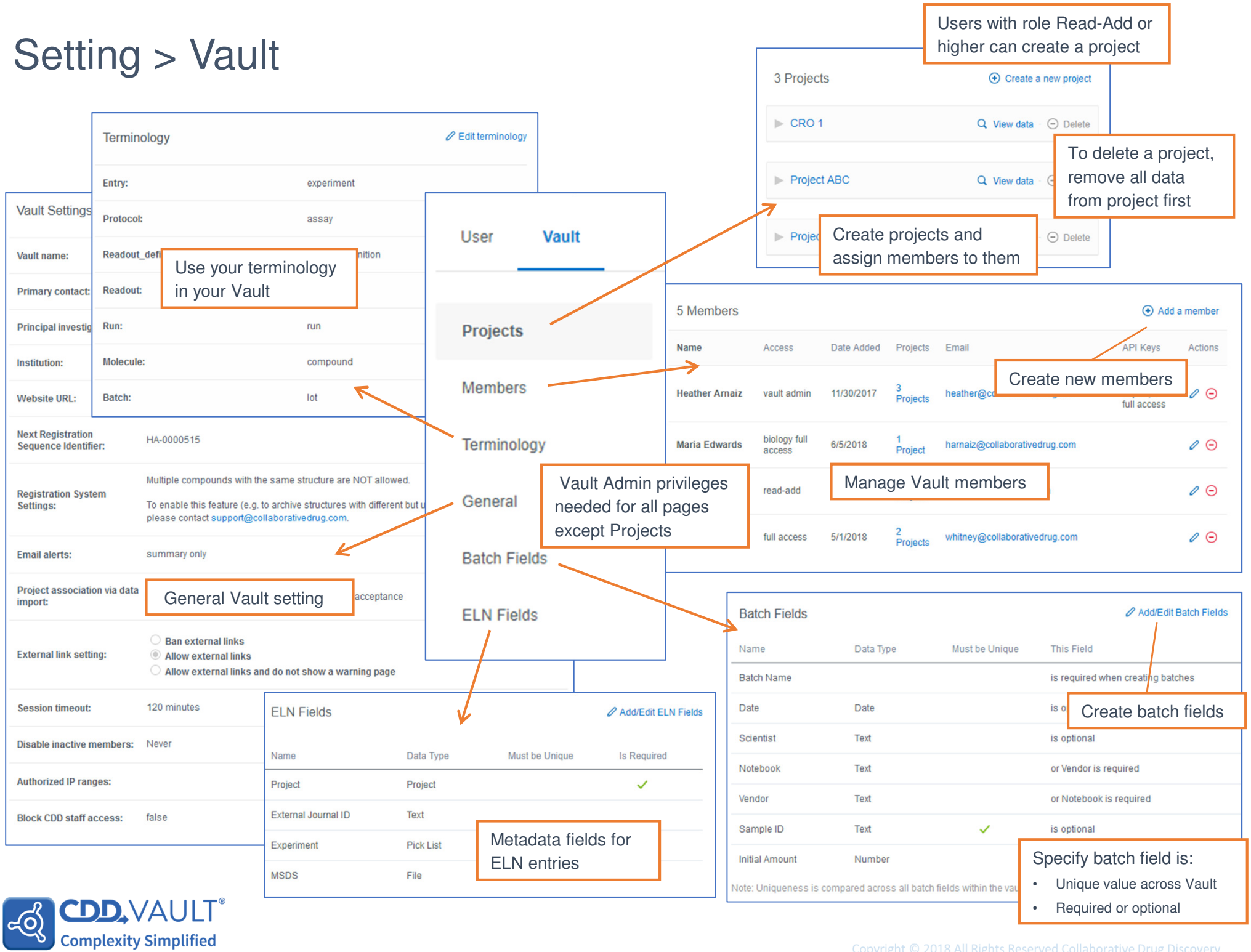
Setting > Vault



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