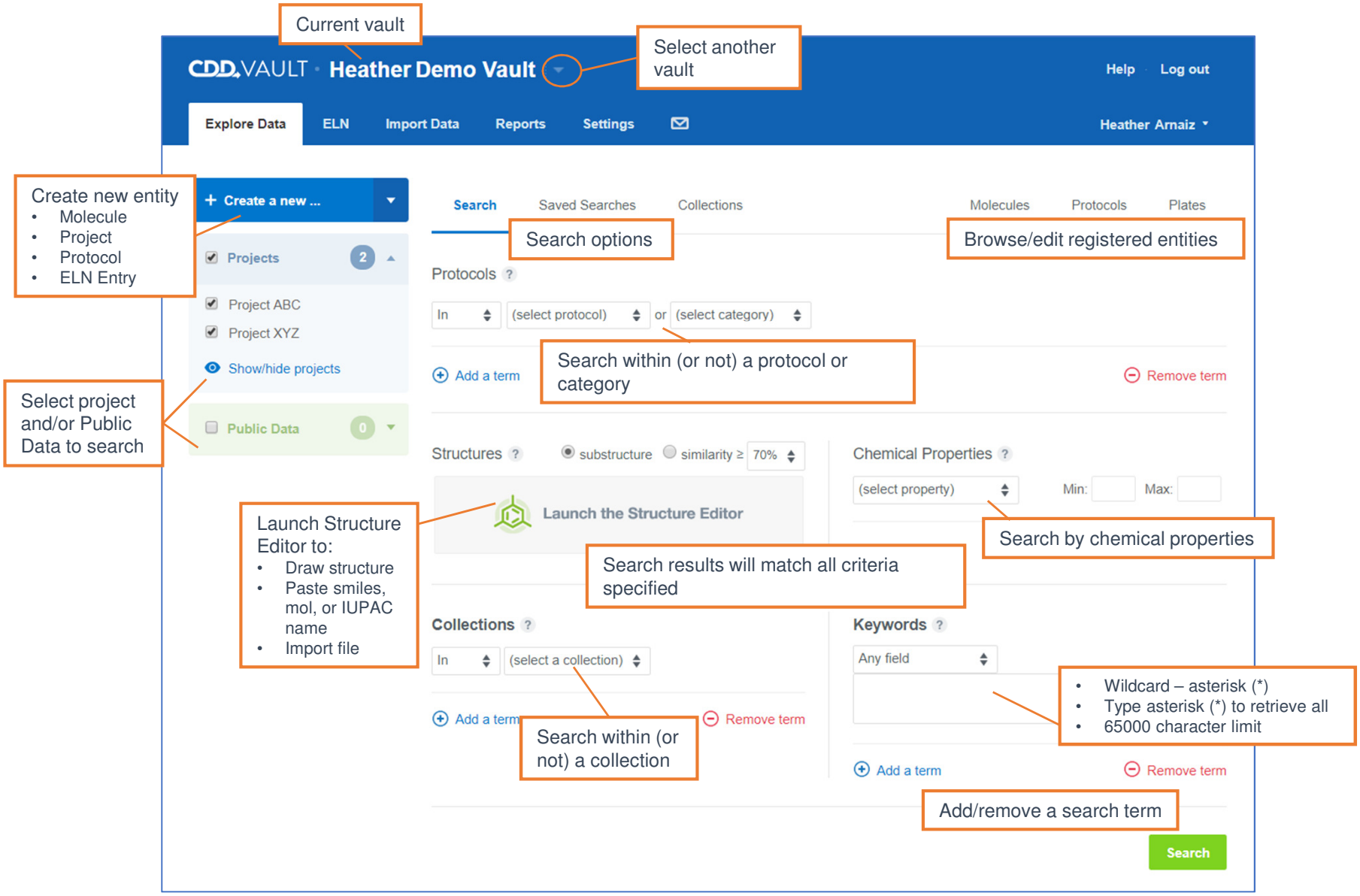
Explore Data

Search your data (or browse)



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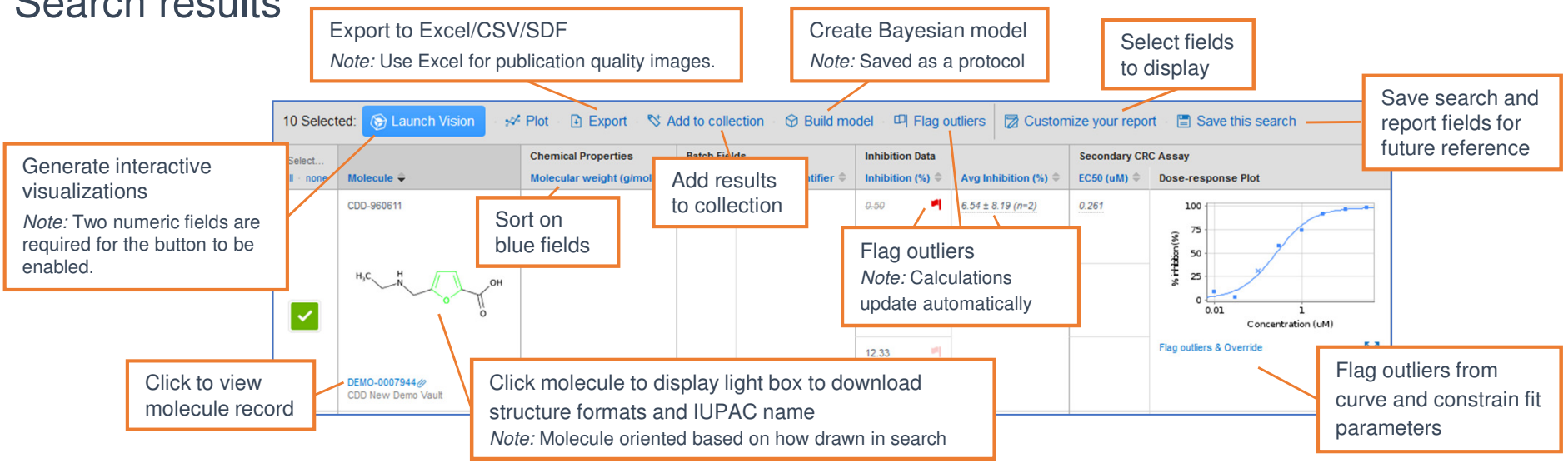
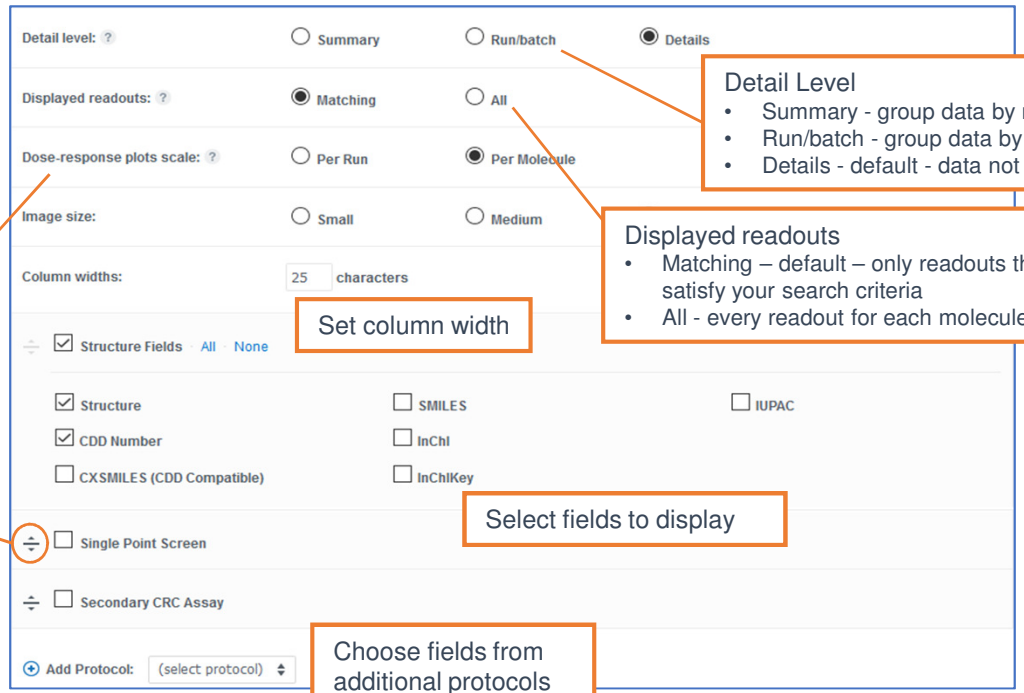
Explore Data

Search results



Customize your report



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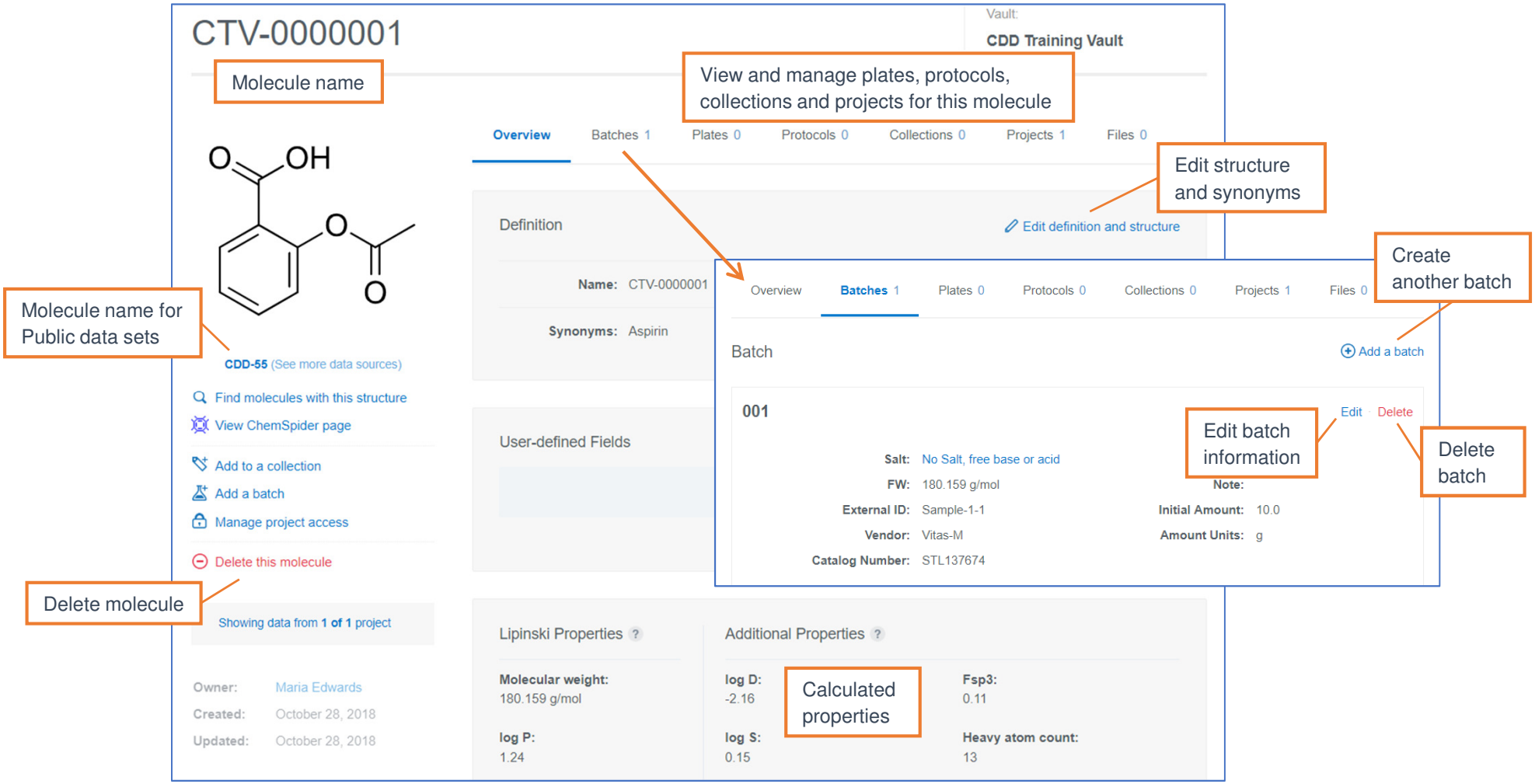
Molecules

Explore data > Molecules



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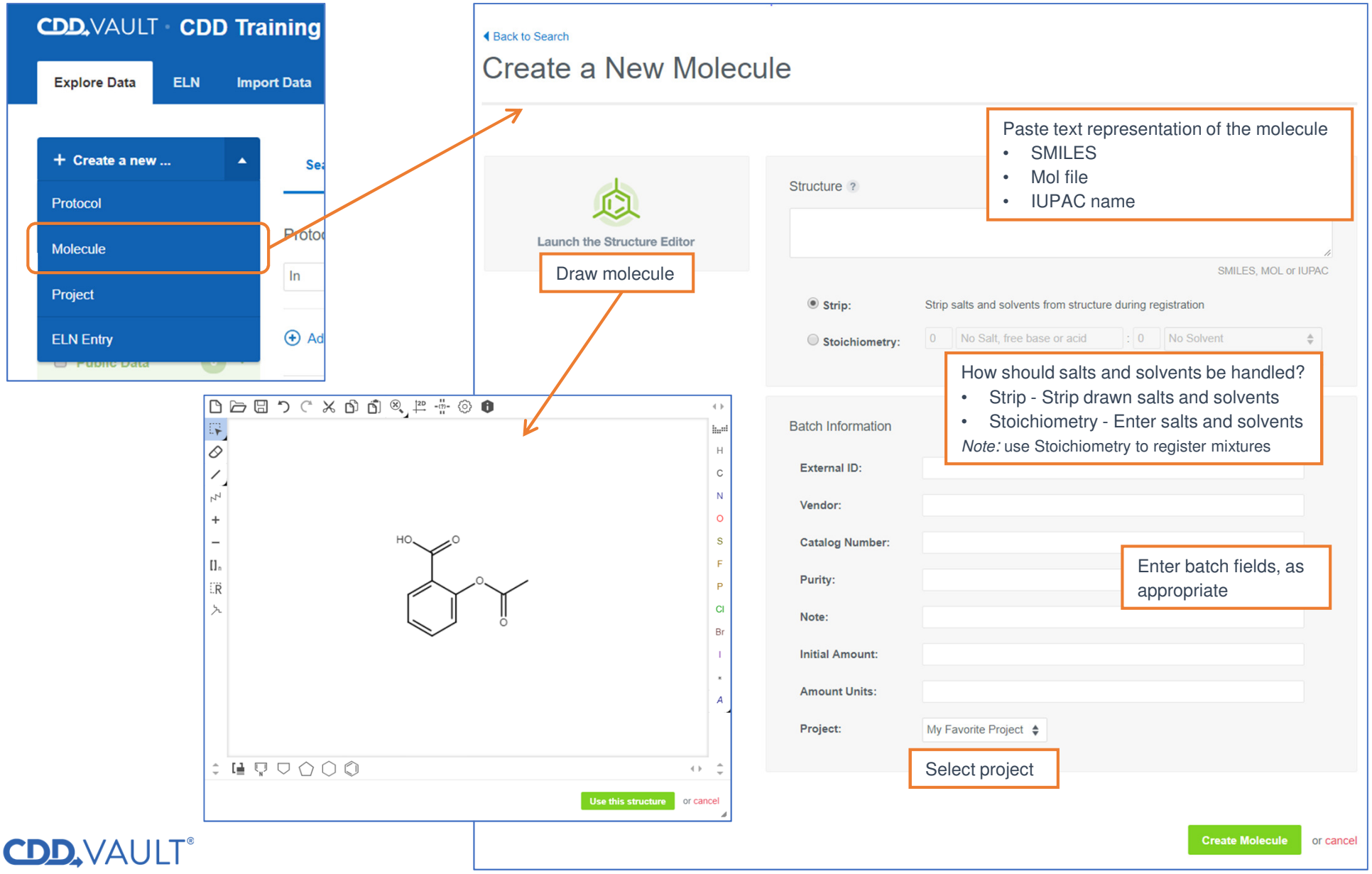
Molecules

Single registration



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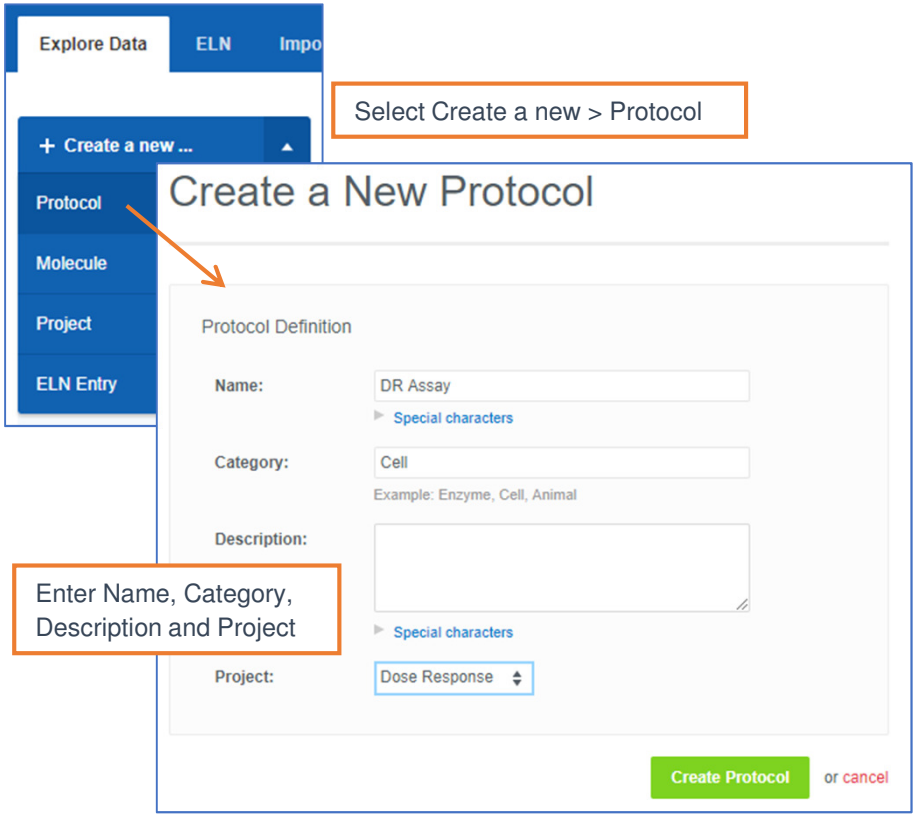
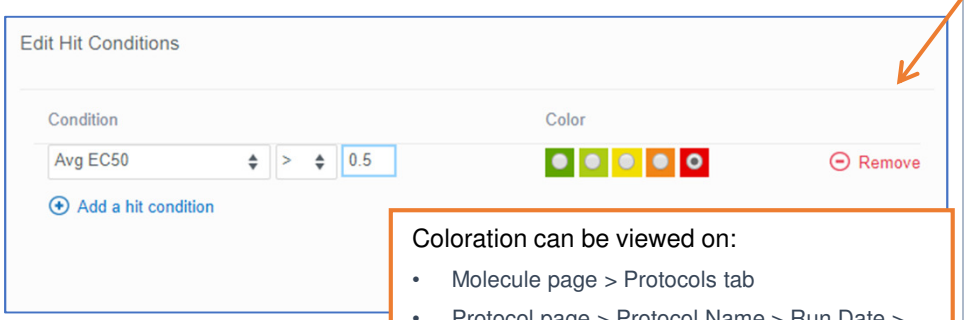
Protocols

Create a new protocol



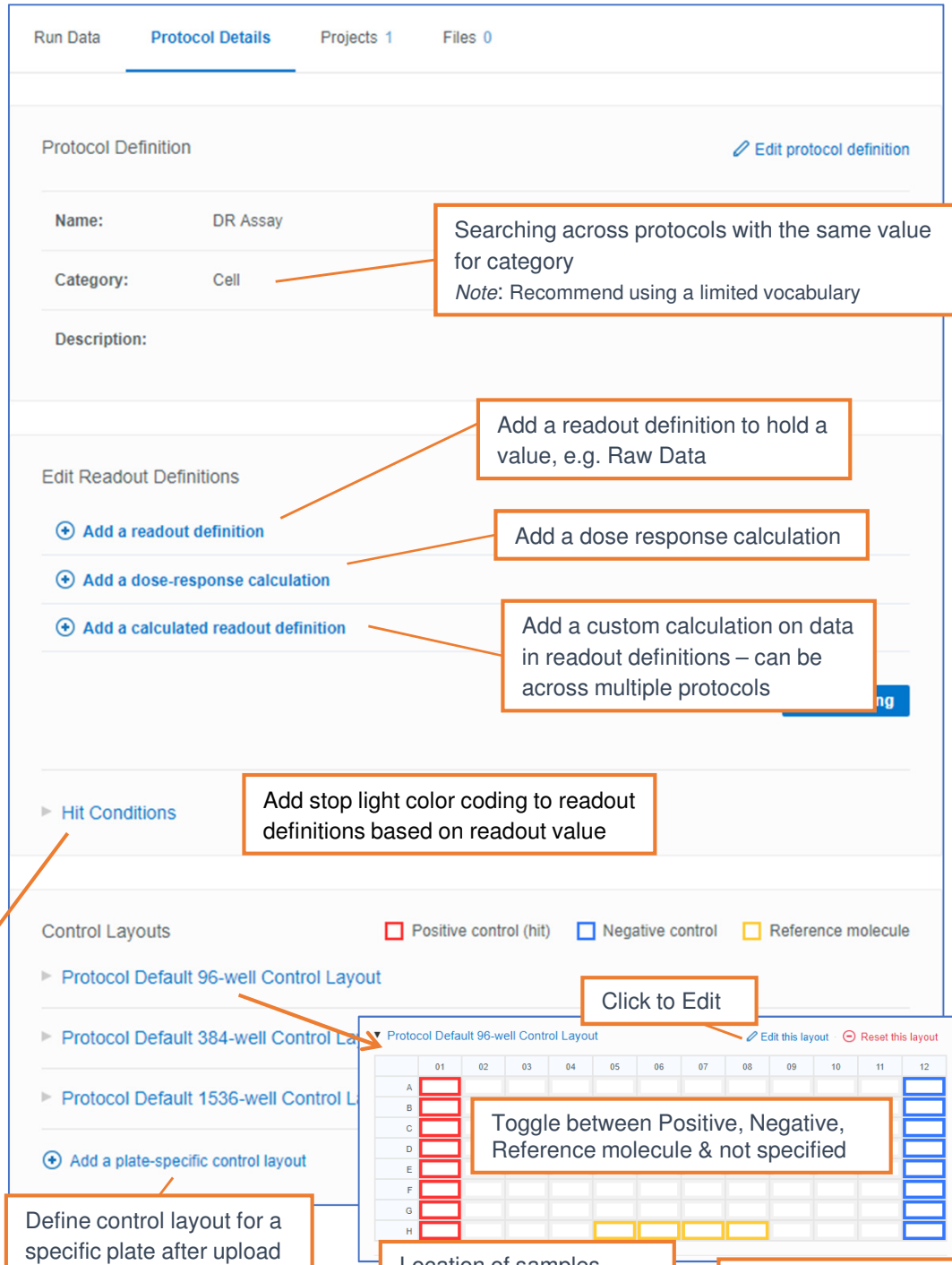
Select Create a new > Protocol

Enter Name, Category, Description and Project



Coloration can be viewed on:

- Molecule page > Protocols tab
- Protocol page > Protocol Name > Run Date > All Data tab



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

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

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

Click to Edit

Toggle between Positive, Negative, Reference molecule & not specified

Define control layout for a specific plate after upload

Location of samples specified in the import file

Full plate not required

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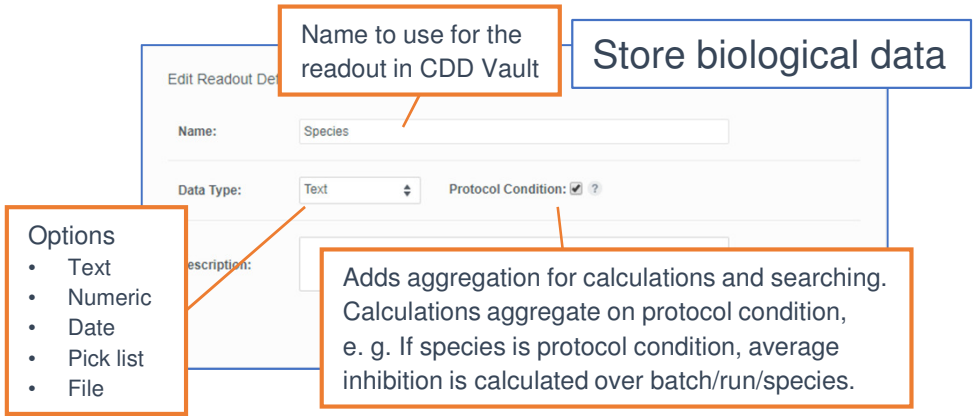
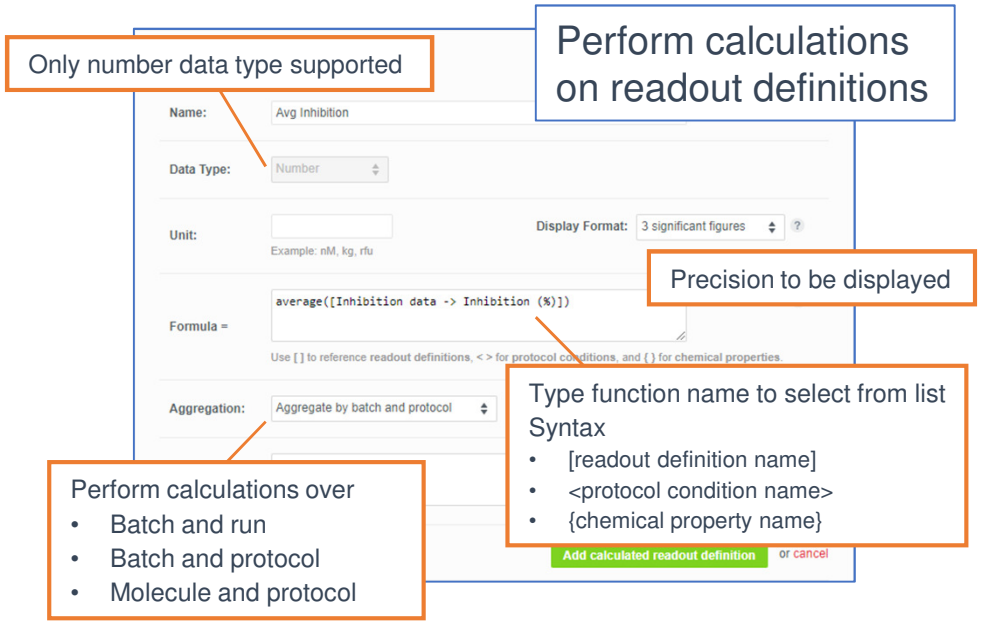
Readout Definitions

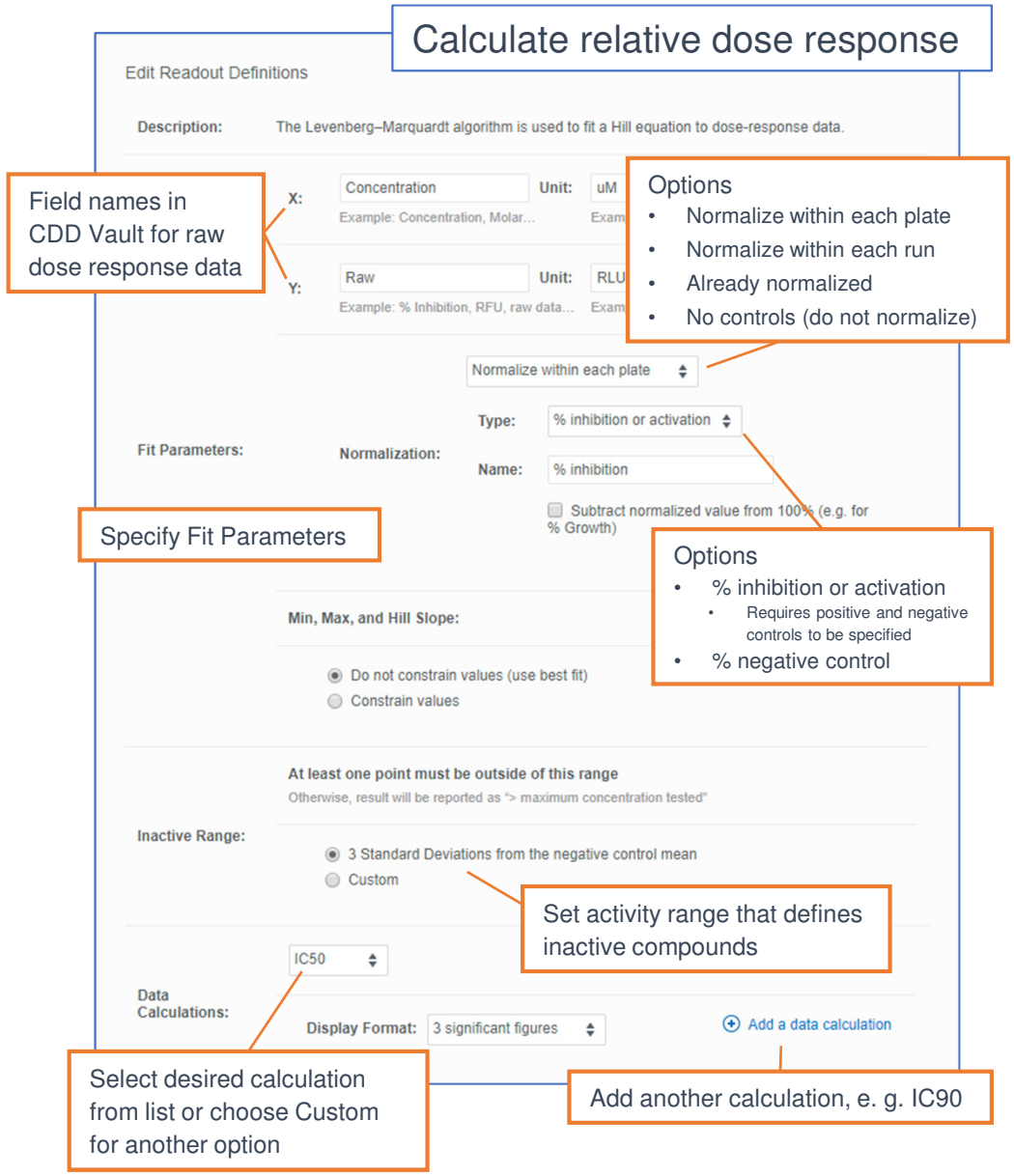
Add a Readout Definition



Add a calculated readout definition



Add a dose response readout definition



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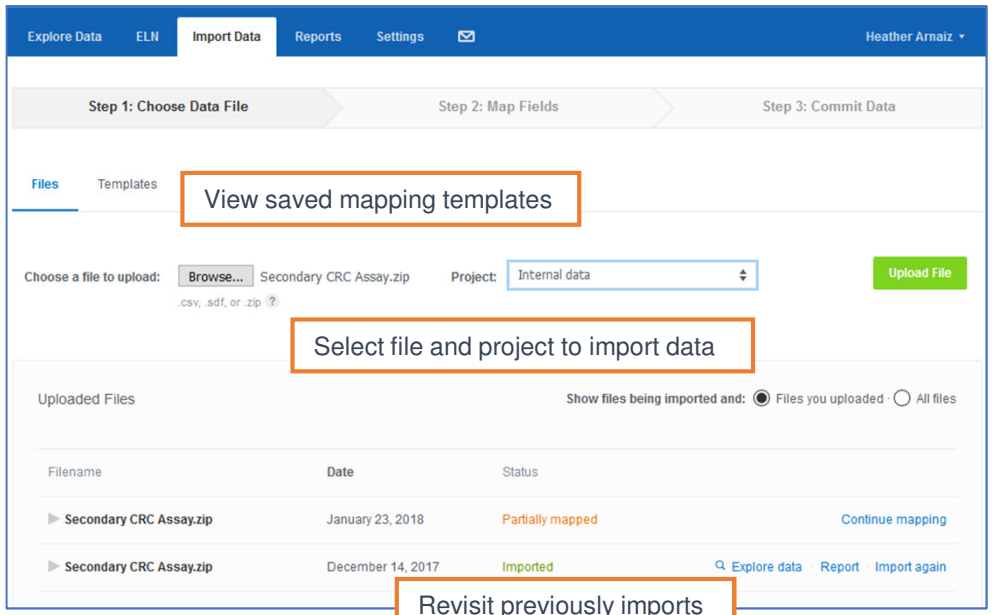
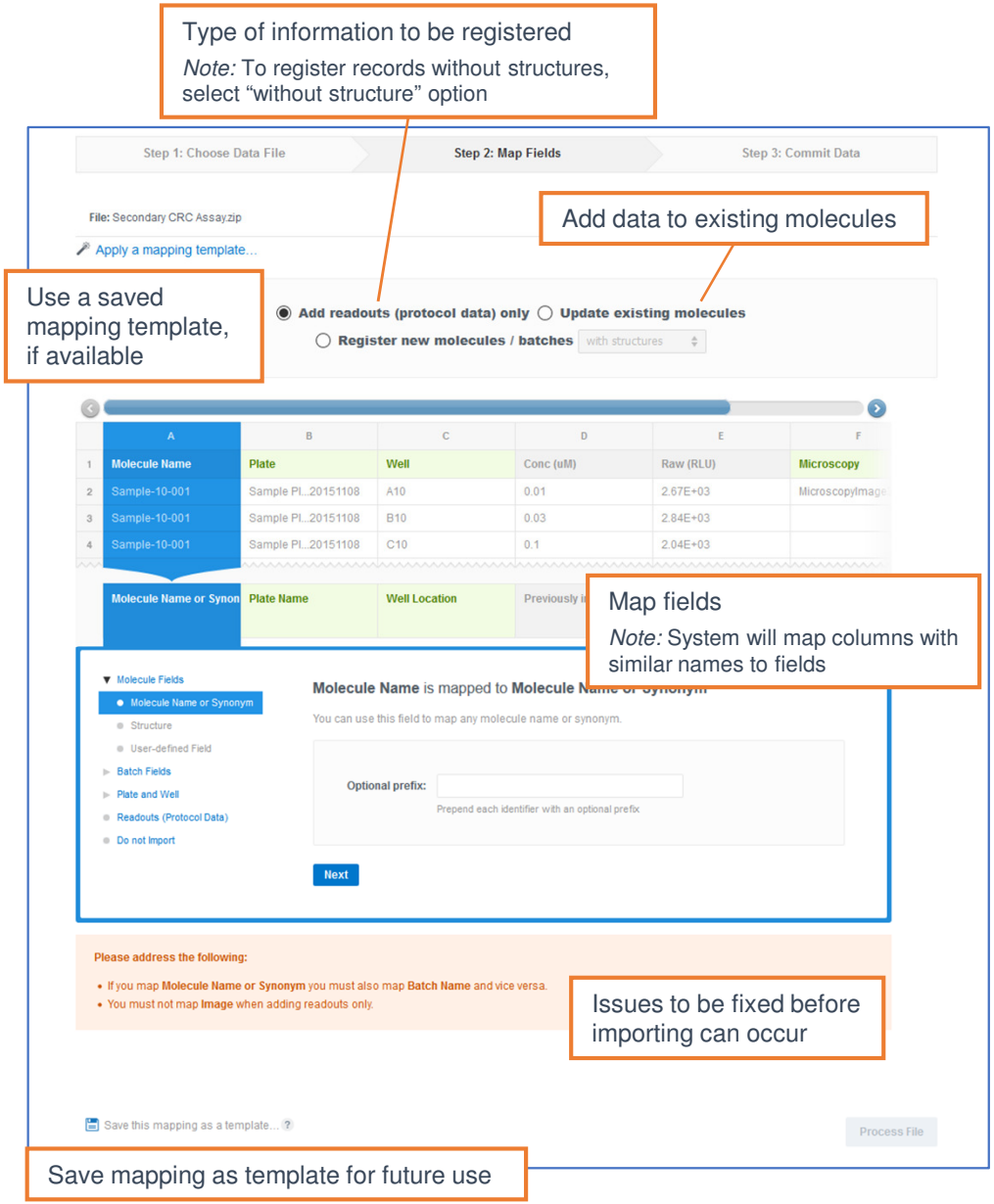
Import Data

Choose file



Map fields



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File format

Molecules

File types: SDF, CSV

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
	)c3ccc(F)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

File type: CSV

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

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

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

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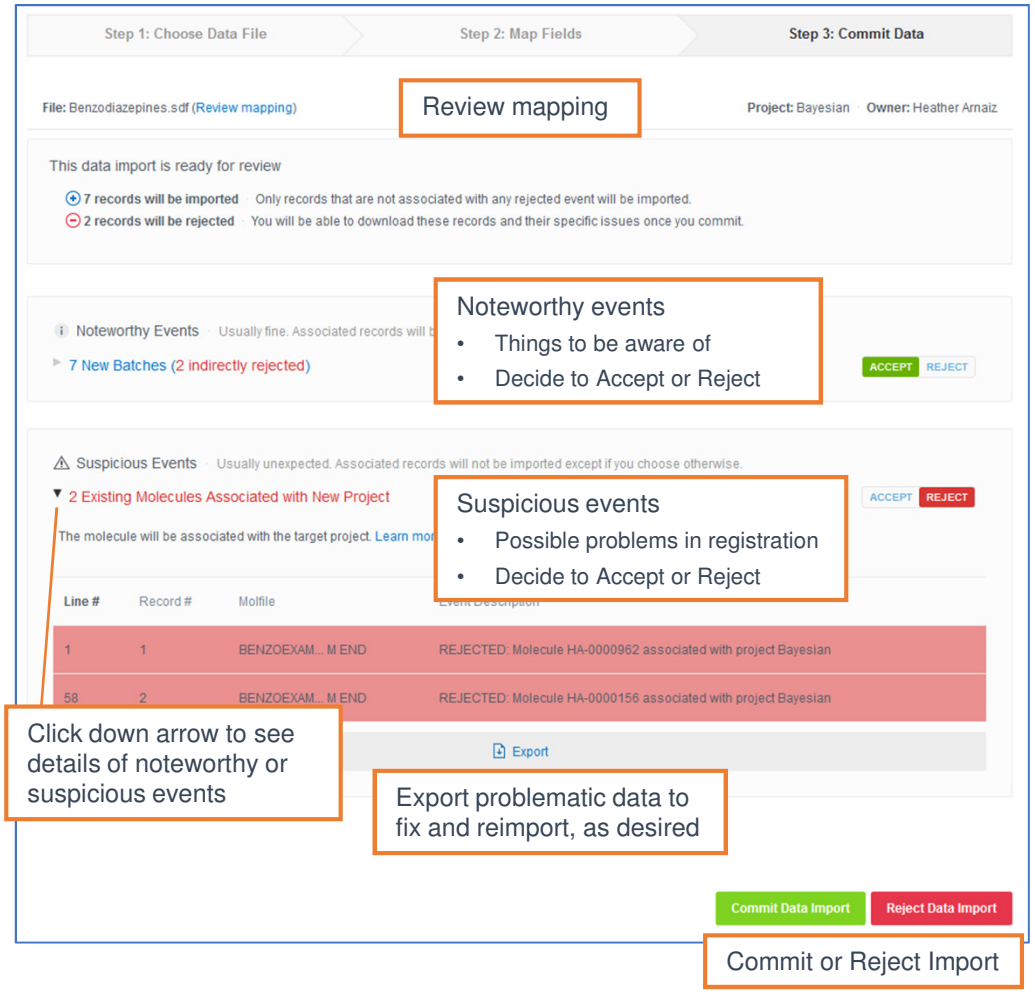
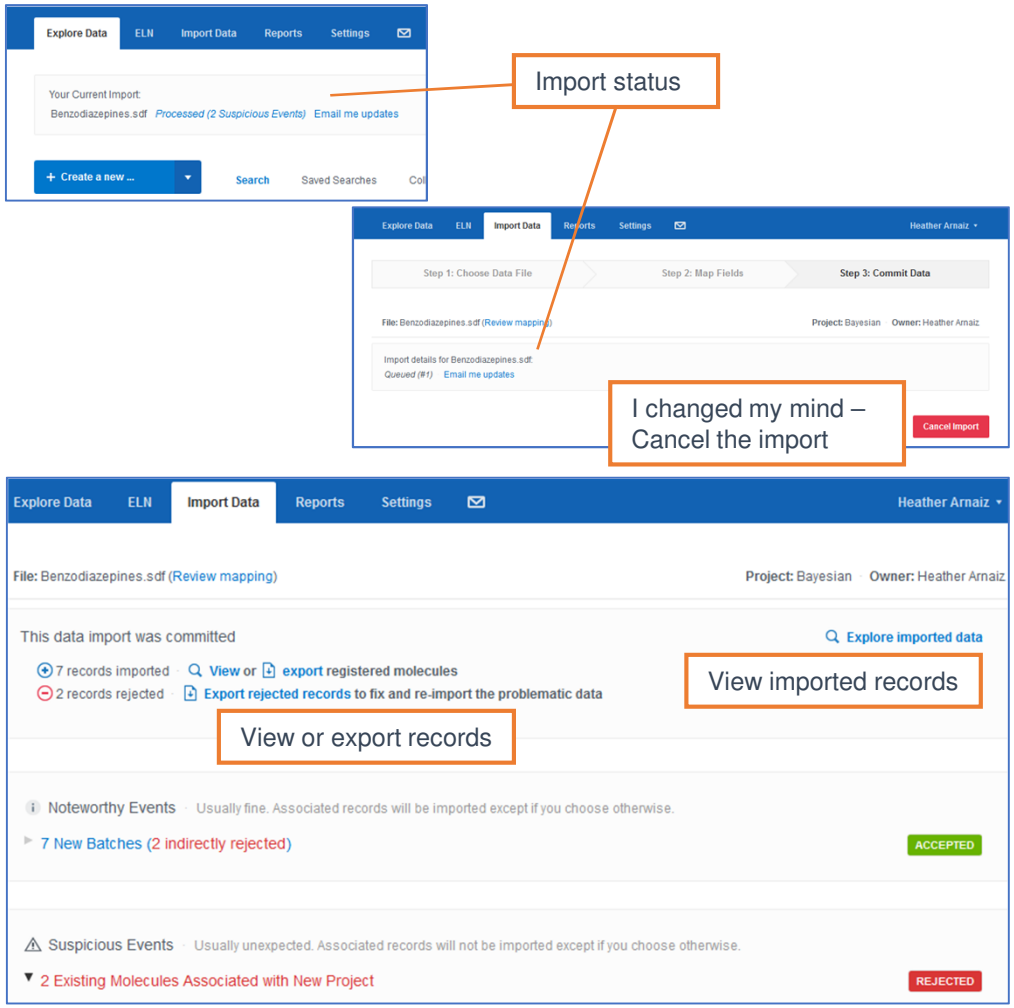
Import Data

Commit Data



Report



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