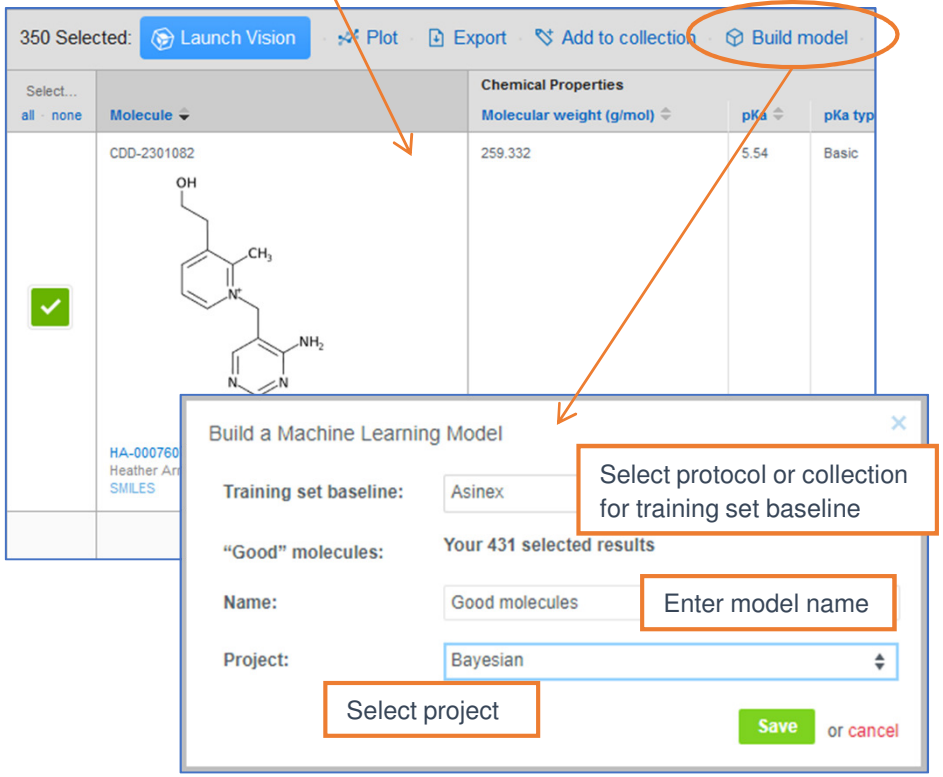
Data Modeling

Create a model

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

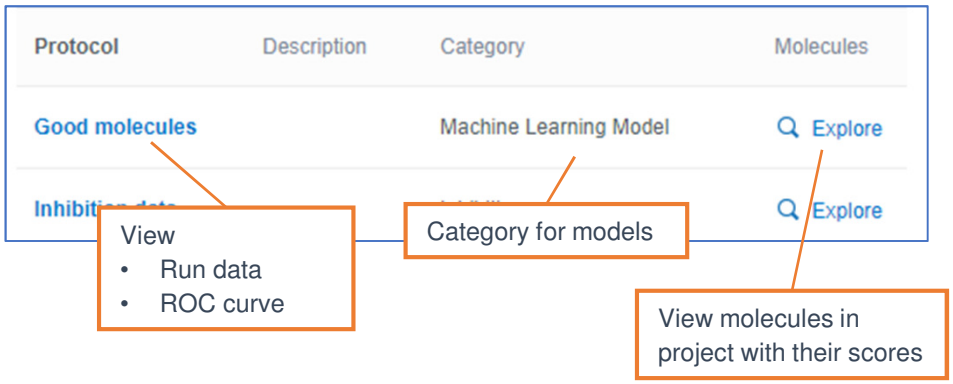


Select protocol or collection for training set baseline

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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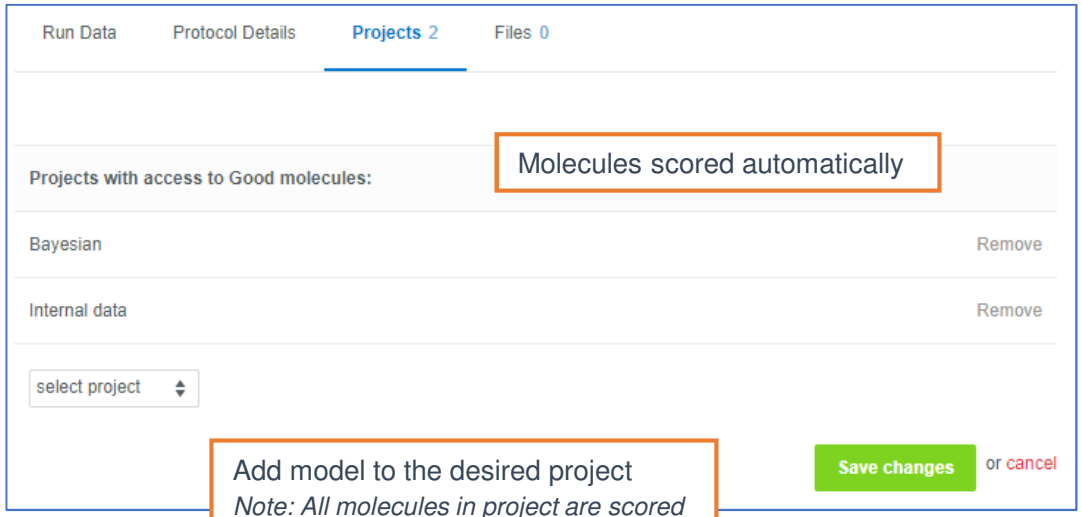
Data Modeling

Quality of model

On Protocol Details tab

Use a model



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