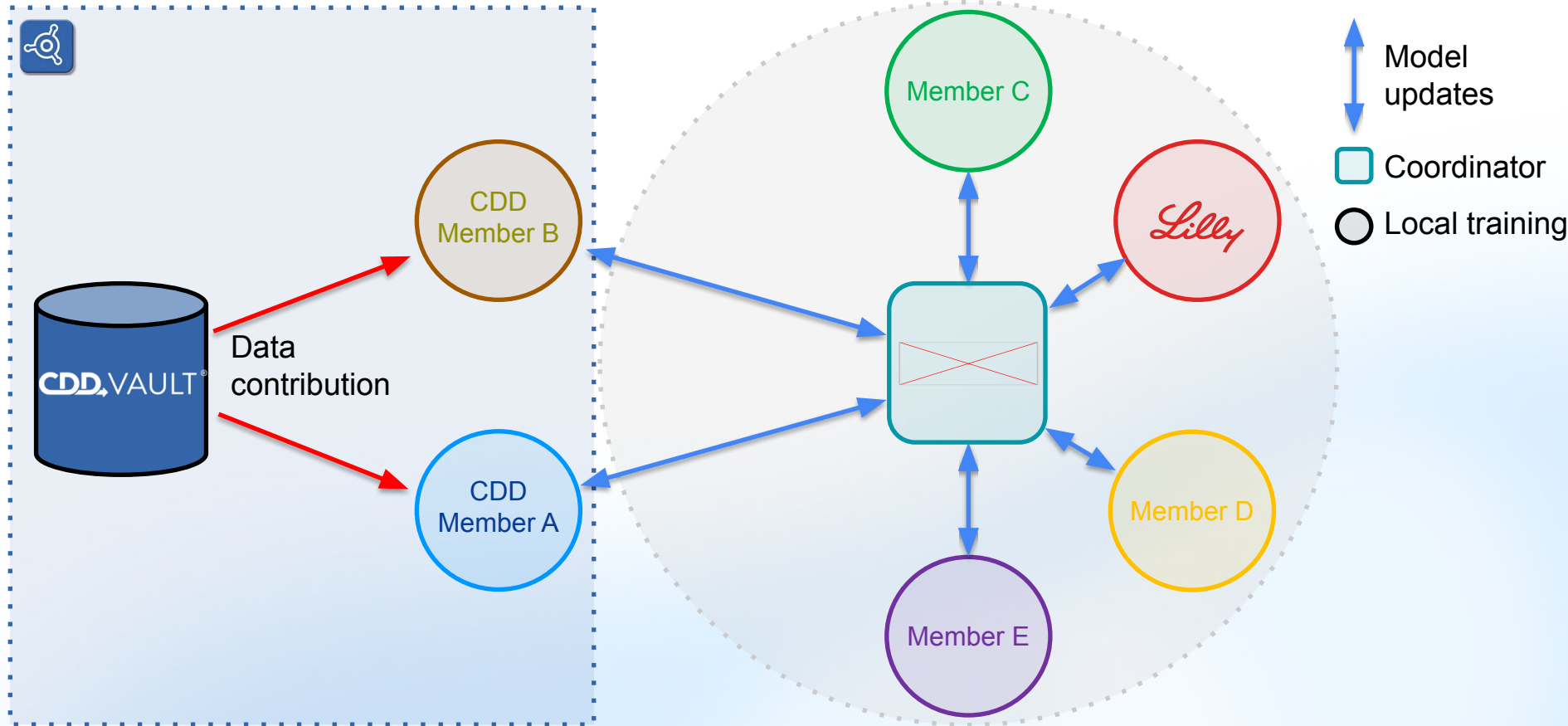
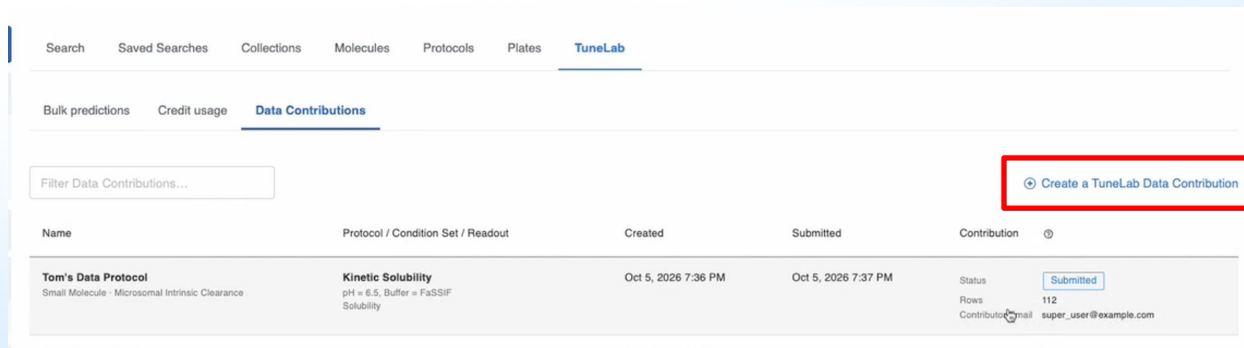


Federated Learning



- Prepare and submit data contributions within CDD Vault
 - Lilly uses provided information to decide whether or not to include data in existing models
 - If not use right away, data may be incorporated in new models
 - Account administrators can prepare and submit data contributions



Search Saved Searches Collections Molecules Protocols Plates **TuneLab**

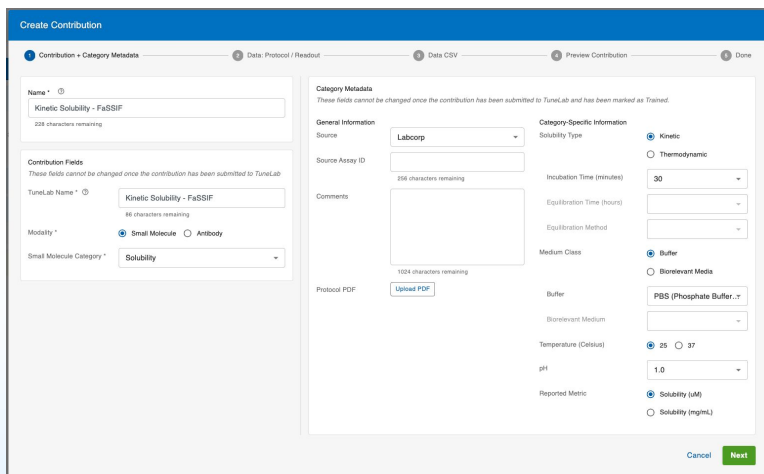
Bulk predictions Credit usage **Data Contributions**

Filter Data Contributions...

[Create a TuneLab Data Contribution](#)

Name	Protocol / Condition Set / Readout	Created	Submitted	Contribution	
Tom's Data Protocol Small Molecule - Microsomal Intrinsic Clearance	Kinetic Solubility pH = 6.5, Buffer = FaSSiF Solubility	Oct 5, 2026 7:36 PM	Oct 5, 2026 7:37 PM	Status Rows Contributor	Submitted 112 super_user@example.com

- Data contribution is a four-step process
 1. Characterize your data using contribution dependent forms
 2. Associate protocol data (readouts and conditions) with your contribution



Create Contribution

1 Contribution + Category Metadata 2 Data: Protocol / Readout 3 Data CSV 4 Preview Contribution 5 Done

Name *
Kinetic Solubility - FaSSiF
228 characters remaining

Contribution Fields
These fields cannot be changed once the contribution has been submitted to TuneLab.
TuneLab Name *
Kinetic Solubility - FaSSiF
86 characters remaining

Modality *
☒ Small Molecule ☐ Antibody

Small Molecule Category *
Solubility

Category Metadata
These fields cannot be changed once the contribution has been submitted to TuneLab and has been marked as Trained.

General Information
Source
Labcorp
Source Assay ID

256 characters remaining
Comments

1024 characters remaining
Protocol PDF
[Upload PDF](#)

Category-Specific Information
Solubility Type
☒ Kinetic ☐ Thermodynamic
Incubation Time (minutes)
30
Equilibration Time (hours)

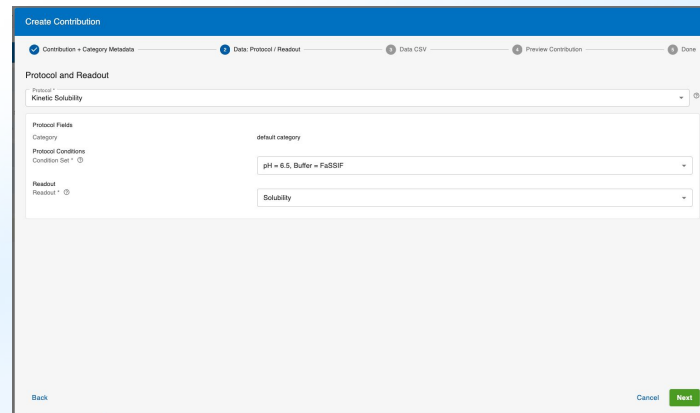
Equilibration Method

Medium Class

Buffer
PBS (Phosphate Buffer, ...
Bio-relevant Medium

Temperature (Celsius)
☒ 25 ☐ 37
pH
1.0
Reported Metric
☒ Solubility (uM) ☐ Solubility (mg/mL)

[Cancel](#) [Next](#)



Create Contribution

1 Contribution + Category Metadata 2 Data: Protocol / Readout 3 Data CSV 4 Preview Contribution 5 Done

Protocol and Readout
Private *
Kinetic Solubility

Protocol Fields
Category
default category
Protocol Conditions
Condition Set *
pH = 6.5, Buffer = FaSSiF
Readout
Readout *
Solubility

[Back](#) [Cancel](#) [Next](#)

- Data contribution is a four-step process
 3. Decide which data will be released for training
 4. Review and submit the data
- Submitted data will be included in the next training cycle

Create Contribution

1 Contribution - Category Metadata 2 Data Protocol / Readout 3 Data CSV 4 Preview Contribution 5 Done

112 of 112 rows included in submission

Filter rows by molecule or ID All Rows

Include Row in Submission	Molecule ID	ID	SMILES	Operator	Value	Date
☒	<chem>CCO</chem> KSF-001	1070782024	CCCC	=	12.4	2019-03-05
☐	<chem>CCCO</chem> KSF-002	1070782025	CCCCC	=	13.7	2019-11-18
☒	<chem>CCCCO</chem> KSF-003	1070782026	CCCCC	=	15	
☒	<chem>CCCCCO</chem> KSF-004	1070782027	CCCCCCC	=	16.3	2019-03-05
☒	<chem>CCCCCO</chem> KSF-005	1070782028	CCCCCCCC	=	17.6	2019-11-18

Back Cancel Next

Create Contribution

1 Contribution - Category Metadata 2 Data Protocol / Readout 3 Data CSV 4 Preview Contribution 5 Done

TuneLab Name: Kinetic Solubility - FullSDF
Molecule: Small Molecule
Category: Solubility
Contributor: super_user@example.com

Category Metadata

Property	Value
Source	Library
Source Assay ID	-
Solubility Type	Kinetic
Medium Class	Buffer
Buffer	PBS (Phosphate Buffered Saline)
Temperature (Celsius)	25
pH	7.5
Incubation Time (minutes)	30
Reported Metric	Solubility (uM)
Comments	-

Data

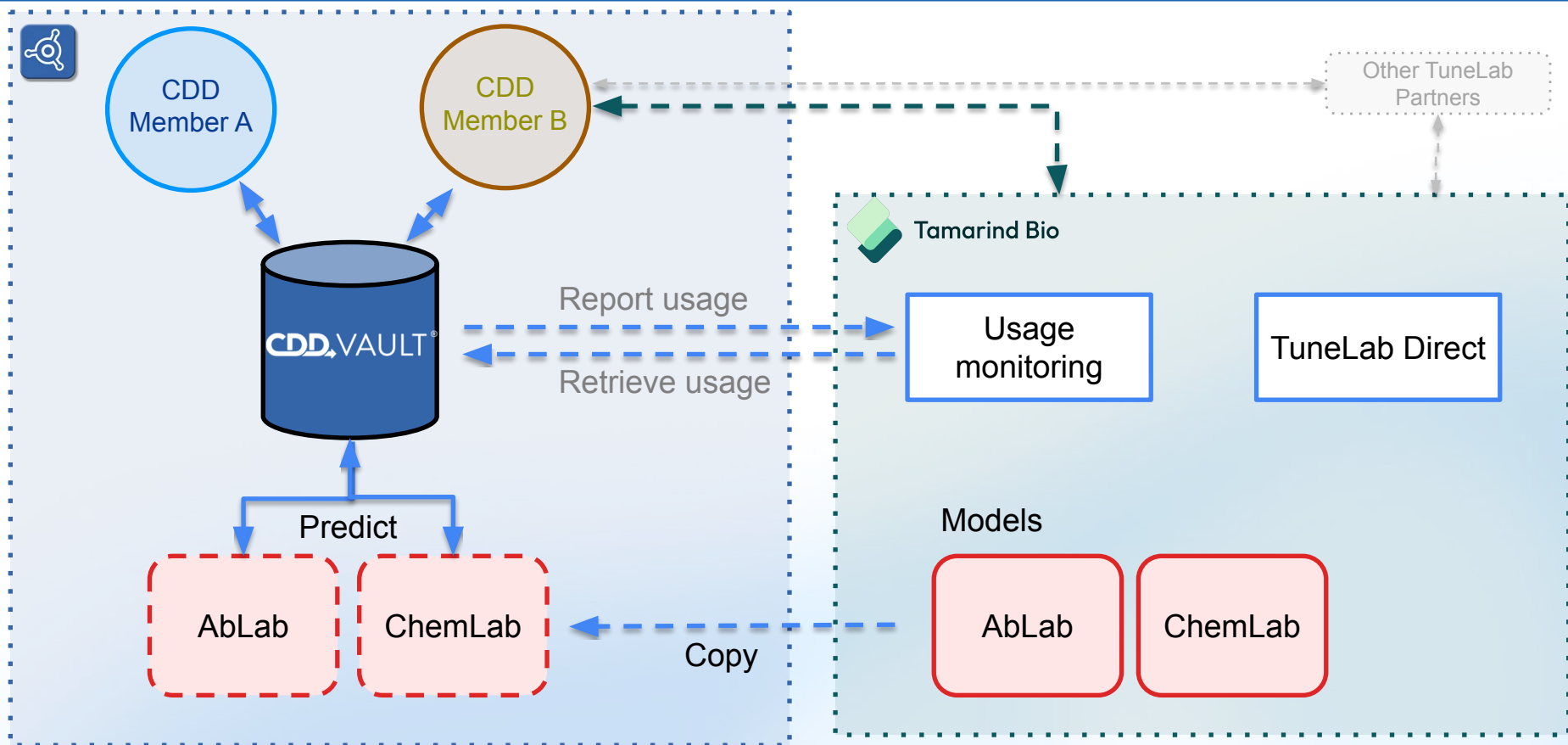
Protocol: Kinetic Solubility
Condition Set: pH = 7.5, Buffer = FullSDF
Readout: Solubility
Name: 112

Download CSV Help Data

ID	SMILES	Operator	Value	Date
1070782024	CCCC	=	12.4	2019-03-05
1070782026	CCCCC	=	15	
1070782027	CCCCCCC	=	16.3	2019-03-05
1070782028	CCCCCCCC	=	17.6	2019-11-18
1070782029	CCCCCCCCC	=	18.9	

Back Cancel Submit to TuneLab

Inference



Inference – Model Selection

1. Select existing models
2. Quickly filter models
3. Lists the selected models
4. For quick access, use sets of models
5. Check your current prediction quota

Select TuneLab models

4

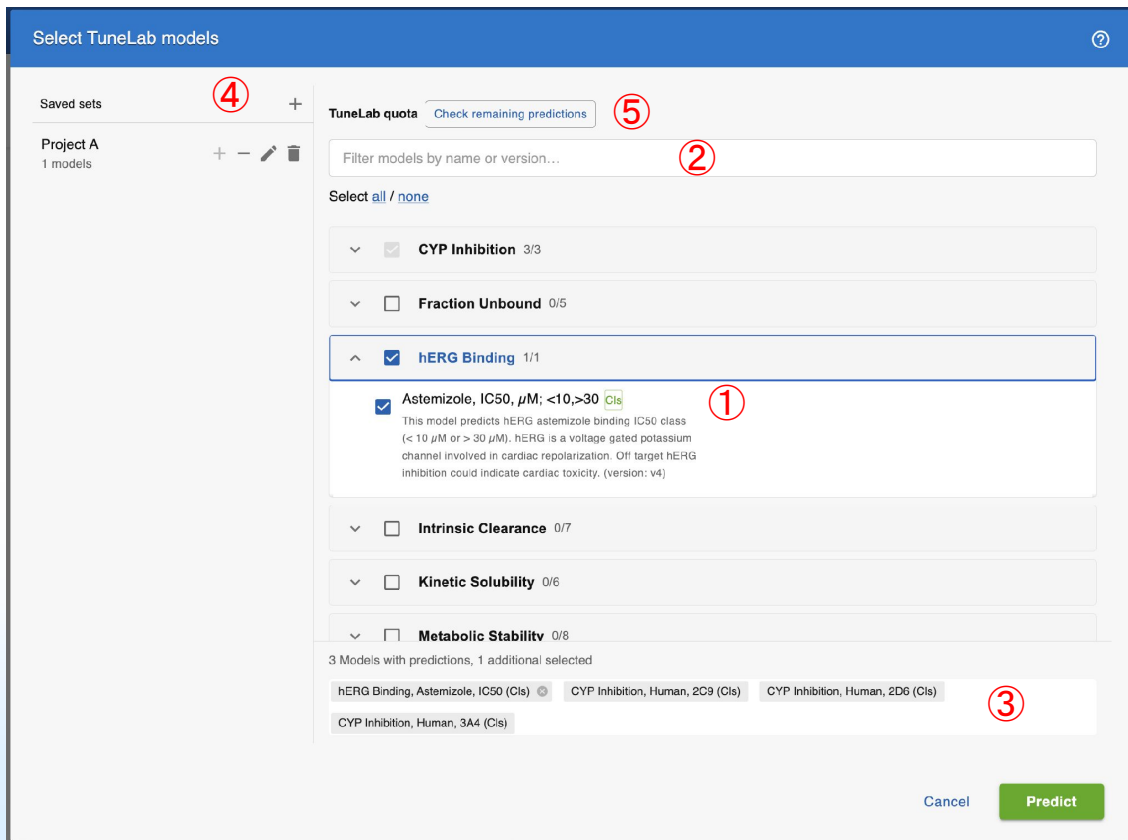
5

2

1

3

Cancel Predict



Project A
1 models

TuneLab quota [Check remaining predictions](#)

Filter models by name or version...

Select all / none

☒ CYP Inhibition 3/3

☐ Fraction Unbound 0/5

☒ hERG Binding 1/1

☒ Astemizole, IC50, μM ; <10,>30 CIs
This model predicts hERG astemizole binding IC50 class (< 10 μM or > 30 μM). hERG is a voltage gated potassium channel involved in cardiac repolarization. Off target hERG inhibition could indicate cardiac toxicity. (version: v4)

☐ Intrinsic Clearance 0/7

☐ Kinetic Solubility 0/6

☐ Metabolic Stability 0/8

3 Models with predictions, 1 additional selected

hERG Binding, Astemizole, IC50 (CIs) CYP Inhibition, Human, 2C9 (CIs) CYP Inhibition, Human, 2D6 (CIs)

CYP Inhibition, Human, 3A4 (CIs)

Cancel Predict

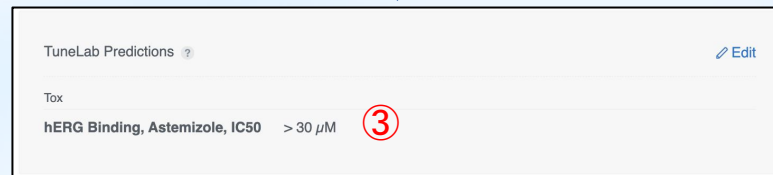
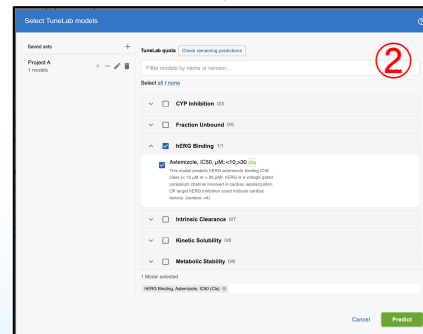
- Predictions reflect uncertainty, e.g.
 - Regression: 46.5 (14.9-145) 10^{-6} cm/sec
 - Classification: extensive (uncertain)
- Conformal prediction with 90% coverage

TuneLab Predictions 			
Absorption			
Permeability Papp, MDCK, AB		3.90 (0.400–38.0) 10 ⁴ cm/sec	
Distribution			
Fraction Unbound			
Species	Brain	Liver Microsomes	Plasma
Human	0.417 (0.179–0.968)	0.874 (0.598–1.00)	1.00 (0.549–1.00)
Monkey			1.00 (0.565–1.00)
Rat			1.00 (0.546–1.00)
Metabolism			
Intrinsic Clearance			
Species	Hepatocytes (μL/min/million cells)	Liver Microsomes (μL/min/mg)	
Dog	5.51 (1.71–17.7)		
Human	1.69 (0.753–3.81)	3.28 (0.747–14.4)	
Mouse	1.05 (0.205–5.43)	7.98 (2.12–30.0)	
Rat	1.35 (0.387–4.71)	8.05 (1.96–33.1)	
Metabolic Stability			
Species	% parent loss	> 60% turnover	
Dog		not extensive	
Human	6.24 (0.00–22.8)	not extensive	
Monkey		not extensive	
Mouse	14.1 (0.00–37.3)	not extensive	
Rat	12.4 (0.00–34.8)	not extensive	
Metabolism (DDI)			
CYP Inhibition			
2C9	< 50%		
2D6	< 50%		
3A4	< 50%		
Physchem			
Kinetic Solubility			
pH 2.0	> 0.01 mg/mL	> 0.1 mg/mL	
pH 6.0	> 0.01 mg/mL	> 0.1 mg/mL	
pH 7.4	> 0.01 mg/mL	> 0.1 mg/mL	
Tox			
hERG Binding, Astemizole, IC50			> 30 μM
Phospholipidosis, HepG2			> 40 μM
Primary Hepatocyte Cytolethality, Rat, LC50			non-lethal

Inference – How to make predictions

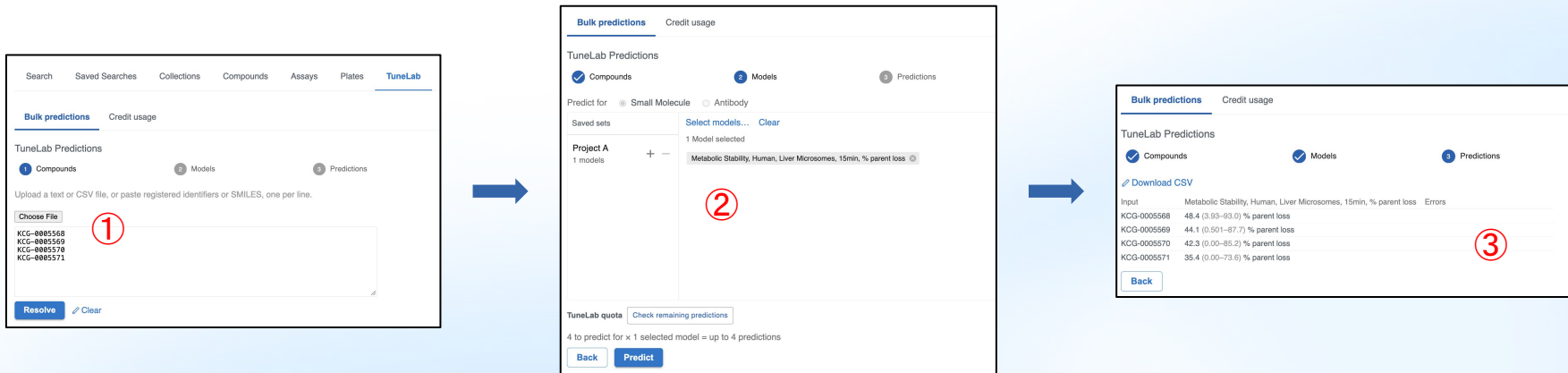
- New section on the molecule page

1. Select the *Edit* button
2. Select the property you want to predict
3. Results show up in the new section



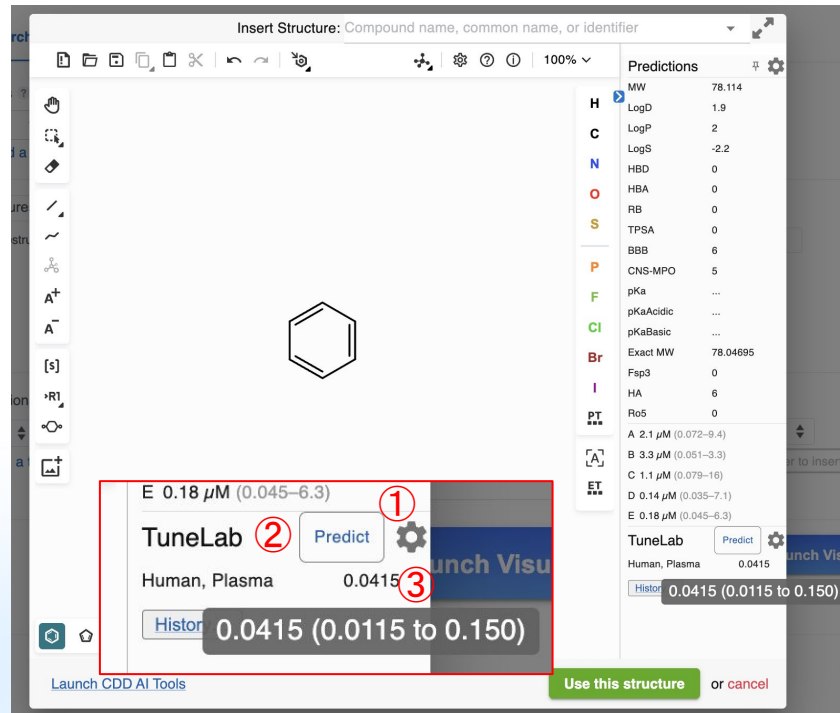
Inference – How to make predictions

- Bulk predictions available from the new TuneLab section
 1. Enter structures as SMILES or identifiers
 2. Select the property you want to predict
 3. Predictions are added to your Vault and can be downloaded



Inference – How to make predictions

- New TuneLab section in the monitor side panel
 1. Select models
 2. Draw the structure and click on [Predict]
 3. Prediction is shown. Mouse over to see Uncertainty is shown



The screenshot displays the CDD VAULT interface. At the top, a search bar is labeled "Insert Structure: Compound name, common name, or identifier". Below it, a benzene ring structure is drawn in the center. On the right, a "Predictions" panel lists various properties: MW (78.114), LogD (1.9), LogP (2), LogS (-2.2), HBD (0), HBA (0), RB (0), TPSA (0), BBB (6), CNS-MPO (5), pKa (---), pKaAcidic (---), pKaBasic (---), Exact MW (78.04695), Fsp3 (0), HA (6), Ro5 (0), and several ADMET predictions (A, B, C, D, E) with their respective ranges. At the bottom, a "TuneLab" section is highlighted with a red box. It shows a prediction for "Human, Plasma" with a value of 0.0415 and a range of (0.0115 to 0.150). The "Predict" button is circled in red with a '2', and the "Launch Visu" button is circled in red with a '3'. A "History" button is also visible. At the bottom right, there are buttons for "Use this structure" and "or cancel".