

## Addendum #1 : TuneLab Models for Small Molecules

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The models listed below are representative examples and will evolve over time. Each model is documented by Lilly, including experimental protocols (assays), calculation protocols (how experimental readouts have been processed) and model algorithm.

Model Class	Endpoint Description	Type
Absorption	Kinetic solubility (pH 2, 0.1 mg/mL)	Classification
Absorption	Kinetic solubility (pH 2, 0.01 mg/mL)	Classification
Absorption	Kinetic solubility (pH 6, 0.1 mg/mL)	Classification
Absorption	Kinetic solubility (pH 6, 0.01 mg/mL)	Classification
Absorption	Kinetic solubility (pH 7.4, 0.1 mg/mL)	Classification
Absorption	Kinetic solubility (pH 7.4, 0.01 mg/mL)	Classification
Absorption	Apparent Permeability (MDCK)	Regression
Absorption	Apparent Permeability (MDCK)	Classification
Absorption	Thermodynamic Aqueous Solubility	Regression
Absorption	Human Passive Intestinal Permeability	Regression
Absorption (CNS)	P-gp Substrate Recognition	Classification
Distribution	Fraction Unbound Microsomal (human)	Regression
Distribution	Fraction Unbound Plasma (monkey)	Regression
Distribution	Fraction Unbound Plasma (rat)	Regression
Distribution	Fraction Unbound Plasma (human)	Regression
Distribution	Fraction Unbound Brain (human)	Regression
Distribution	Total Brain Concentration (human)	Regression
Distribution (CNS)	Kp Brain	Regression
Metabolism	Microsomal Apparent Intrinsic Clearance (mouse)	Regression
Metabolism	Microsomal Apparent Intrinsic Clearance (rat)	Regression
Metabolism	Microsomal Apparent Intrinsic Clearance (human)	Regression
Metabolism	Microsomal Metabolic Stability (mouse)	Regression
Metabolism	Microsomal Metabolic Stability (rat)	Regression

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Metabolism	Microsomal Metabolic Stability (human)	Regression
Metabolism	Microsomal Metabolic Stability (mouse)	Classification
Metabolism	Microsomal Metabolic Stability (rat)	Classification
Metabolism	Microsomal Metabolic Stability (human)	Classification
Metabolism	Microsomal Metabolic Stability (dog)	Classification
Metabolism	Microsomal Metabolic Stability (monkey)	Classification
Metabolism	Hepatocyte Apparent Intrinsic Clearance (mouse)	Regression
Metabolism	Hepatocyte Apparent Intrinsic Clearance (rat)	Regression
Metabolism	Hepatocyte Apparent Intrinsic Clearance (human)	Regression
Metabolism	Hepatocyte Apparent Intrinsic Clearance (dog)	Regression
Metabolism	IV Clearance (rat)	Regression
Metabolism	IV Vd Area (rat)	Classification
Metabolism	IV Clearance (rat)	Classification
Metabolism (DDI)	CYP % Inhibition (2C9)	Classification
Metabolism (DDI)	CYP % Inhibition (2D6)	Classification
Metabolism (DDI)	CYP % Inhibition (3A4)	Classification
Metabolism (DDI)	CYP % Inhibition (3A4) Time Dependent	Classification
Toxicity	Primary Hepatocyte Cytolethality (rat)	Classification
Toxicity	hERG Binding	Classification
Toxicity	Phospholipidosis (HepG2)	Classification
Toxicity	HepG2 Lysosomatropic	Classification
Toxicity	Mutagenicity (mini Ames)	Classification
Toxicity	Rat Primary Hepatocyte (RPH) Phospholipidosis	Classification