# ADMET Models

The following is a list of the different ADMET endpoints studied. For classification, conformal prediction is used to calculate a confidence (how certain the model is that the prediction is a singleton) and a credibility. In the case of regression, a 95% prediction interval (predictions at the 0.025 and 97.5 percentiles) is calculated and provides a range for the predictions on an individual observation. Narrow prediction intervals indicate a lower uncertainty associated with the prediction.

| Model | Type | Predicted Value |
|---|---|---|
| Anticommensal effect on the human gut microbiota | Binary Classification | Positive = anticommensal; Negative = commensal |
| Aqueous Solubility (in Phosphate Buffered Saline) | Binary Classification | Active: moderate/high solubility; Inactive: low solubility |
| Blood Brain Barrier Permeability | Binary Classification | Yes: BBB permeable; No: not BBB permeable |
| Breast Cancer Resistance Protein Inhibition | Binary Classification | Inhibitor/Non-inhibitor |
| Human Oral Bioavailability | Binary Classification | High: $F \geq 50\%$ ; Low: $F < 50\%$ |
| CYP450 inhibition (1A2/2C9/2C19/2D6/A4) | Binary Classification | Active = inhibitor; Inactive: Non-inhibitor |
| CYP450 inhibition (2C8) | Binary Classification | Inhibitor/Non-inhibitor |
| DMSO Solubility | Binary Classification | Soluble/Insoluble |
| $pK_a$ | Regression | $pK_a$ |
| Madin–Darby canine kidney Permeability | Regression | $\log P_{app}$ predicted |
| Human Intestinal Absorption | Binary Classification | Positive: $HIA \geq 30\%$ ; Negative: $HIA < 30\%$ |
| Human Liver Microsomal Stability | Binary Classification | Positive/Stable: $T_{\frac{1}{2}} > 30$ min; Negative/Unstable ($T_{\frac{1}{2}} \leq 30$ min) |
| Hepatocellular organic anion transporting polypeptide Inhibition | Binary Classification | Yes: inhibitor; No: Non-inhibitor |

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| Model | Type | Predicted Value |
|---|---|---|
| Distribution coefficient ($\log D$ at pH 7.4) | Regression | $\log D$ |
| $\log S$ | Regression | $\log S$ |
| Drug affinity to human serum albumin | Regression | $\log K_{HSA}$ |
| 50% hemolytic dose | Regression | $\log HD_{50}$ |
| Skin Penetration | Regression | $\log\ K_p$ |
| Organic Cation Transporter 2 inhibition | Binary Classification | Inhibitor/Non-inhibitor |
| Multidrug and Toxin Extrusion Transporter 1 Inhibition | Binary Classification | Inhibitor/Non-inhibitor |
| Substratesof P-glycoprotein | Binary Classification | P:Substrate; N: Non-substrate |
| Inhibitors of P-glycoprotein | Binary Classification | P:Inhibitor; N: Non-inhibitor |
| Human plasma protein binding | Multiclass | Low/Medium/High |
| Carcinogenecity | Binary Classification | Carcinogen/Non-Carcinogen |
| Rat acute oral toxicity | Multiclass | EPA1: highest toxicity; EPA2: moderately toxic; EPA3: slightly toxic; EPA4: Safe |
| AMES mutagenecity | Binary Classification | Active: Mutagen ; Inactive: Non-mutagen |
| Metabolic Intrinsic Clearance | Multiclass | Stable/Moderate/Unstable |
| Human Bile Salt Export Pump Inhibition | Binary Classification | Active: Inhibitor; Inactive: Non-inhibitor |
| Drug-Induced Choleostasis | Binary Classification | Positive/Negative |
| Drug-induced Ototoxicity | Binary Classification | Yes/No |
| Rhabdomyolysis | Binary Classification | Yes/No |

| Model | Type | Predicted Value |
|---|---|---|
| hERG Liability | Binary Classification | Blocker/Non-blocker |
| Toxic Myopathy | Binary Classification | Positive/Negative |
| Phospholipidosis | Binary Classification | Positive/Negative |
| hERG Cardiotoxicity | Binary Classification | Positive/Negative |
| Haemolytic Toxicity | Binary Classification | Positive/Negative |
| Myelotoxicity | Binary Classification | Positive/Negative |
| Urinary Toxicity | Binary Classification | Positive/Negative |
| Hepatic Steatosis | Binary Classification | Positive/Negative |
| Respiratory Toxicity | Binary Classification | Yes/No |
| Phototoxicity human/in vitro | Binary Classification | Yes/No |
| Mitochondrial Toxicity | Binary Classification | Inactive: non-toxic; Active: induce mitochondrial toxicity |
| Cytotoxicity HepG2/NIH cell line | Binary Classification | P: cytotoxic ; N: non-toxic |
| Cytotoxicity (HEK-293/NIH-3T3/CRL-7250/HaCat) cell line | Binary Classification | Inactive: non-toxic; Active: cytotoxic |
| T1/2 Human/Mouse/Rat | Multiclass | High/Medium/Low |