

# ADMET PROPERTY PREDICTION



SMILES

CONTINUOUS TRANSLATIONAL  
CDDD DESCRIPTOR



ADAPTIVE  
LEARNING  
AND  
PREDICTING  
UNIT

24 —  
✓/ —  
✓ —  
✓ —  
✓ —  
✓ —  
✓ —

24 ENDPOINTS

PREDICTS 24 ADMET PROPERTIES

## Absorption



HIA



OB



P-gp  
inhibitor



LogD



P-gp  
substrate



CaCO<sub>3</sub>  
perm.

## Distribution



BBB



PPB



CL (Clearance)

## Metabolism



ESOL



Half-Life



CYP12



CYP18



CYP39



CYP66

Cytochrome  
P450 (CYP450)



Respiratory  
toxicity



Hepatotoxicity



Cardiotoxicity



Acute oral  
toxicity (LD50)

IGC50