

Working Model of Skin Permeability Prediction

Integrating Stochastic Differential Equations and Machine Learning Approaches

STAGE 1: Input Parameters (Molecular Descriptors)

The following six molecular descriptors serve as input features for predicting skin permeability coefficients:

Molecular Weight	Log Kow	Balaban Index	Harary Index	Ramification Index	Forgotten Index
Mass of molecule	Partition coefficient	Topological index	Topological index	Branching descriptor	Degree-based index

Dataset: Curated collection of 87 chemical compounds with experimentally determined permeability coefficients.

STAGE 2: Sources of Experimental Variability

Traditional QSPR models underestimate the following sources of variability:

Skin Shape Variations	Experimental Circumstances	Measurement Noise	Biological Variability
Regional anatomical differences	Temperature, humidity, protocols	Instrument precision limits	Hydration, lipid composition

STAGE 3: Predictive Modeling Approaches

A. Stochastic Differential Equation Methods

Capable of modeling random noise and inherent biological variability in experimental data.

Method	R ² Value	MSE Value	Rank
Euler–Maruyama Algorithm	0.81	0.5259	2nd 🥈
Milstein Scheme	0.74	0.634	4th
Heston Model	0.72	0.66	5th

B. Machine Learning Methods

Pattern recognition and nonlinear relationship mapping for predictive modeling.

Method	R ² Value	MSE Value	Rank
Gradient Boost Regression	0.84	0.45	1st 🥇

Support Vector Regression	0.78	0.62	3rd 🏅
Levenberg-Marquardt Algorithm	0.58	0.94	6th

STAGE 4: Comprehensive Model Performance Comparison

Method	Category	R ² Value	MSE Value	R ² Rank	MSE Rank
Gradient Boost Regression	Machine Learning	0.84	0.45	1st	1st
Euler-Maruyama Algorithm	Stochastic	0.81	0.5259	2nd	2nd
Support Vector Regression	Machine Learning	0.78	0.62	3rd	3rd
Milstein Scheme	Stochastic	0.74	0.634	4th	4th
Heston Model	Stochastic	0.72	0.66	5th	5th
Levenberg-Marquardt	Machine Learning	0.58	0.94	6th	6th

STAGE 5: Model Output

<p>Predicted Skin Permeability Coefficient (log Kp) Accounting for biological variability and experimental noise</p>

STAGE 6: Pharmaceutical Applications

Transdermal Patch Design	Drug Loading Optimization	Dosing Regimen Design	Excipient Selection
Lead Compound Screening	Permeation Enhancer Selection	Formulation Optimization	Risk Assessment