

Table S1 Performance metrics and hyperparameter settings of machine learning models

Model	AUC (95% CI)	Accuracy (95% CI)	Precision	Recall	F1 score	Hyperparameters and search range
Random Forest (RF)	0.98 (0.96–0.99)	0.92 (0.89–0.95)	0.91	0.91	0.91	n_estimators: [100, 200, 300]; max_depth: [5, 10, 15]; min_samples_split: [2, 5]
Light Gradient Boosting Machine (LightGBM)	0.97 (0.95–0.99)	0.94 (0.91–0.96)	0.95	0.93	0.94	learning_rate: [0.01, 0.05, 0.1]; n_estimators: [100, 200, 300]; max_depth: [3, 5, 7]
Support Vector Machine (SVM)	0.84 (0.82–0.86)	0.62 (0.60–0.64)	0.62	1.00	0.77	kernel: [linear, rbf]; C: [1, 5, 10]; gamma: [0.01, 0.1, 1]
Decision Tree (DT)	0.90 (0.88–0.92)	0.90 (0.84–0.96)	0.89	0.89	0.89	max_depth: [3, 5, 7, 9]; min_samples_split: [2, 5, 10]; min_samples_leaf: [1, 2, 3]
Gradient Boosting (GB)	0.98 (0.97–0.99)	0.94 (0.92–0.96)	0.87	0.93	0.94	learning_rate: [0.01, 0.05, 0.1]; n_estimators: [100, 200, 300]; min_samples_split: [2, 5]
Artificial Neural Network (ANN)	0.93 (0.90–0.96)	0.87 (0.86–0.88)	0.86	0.86	0.86	hidden_neurons: [32, 64, 128]; activation: [ReLU, sigmoid]; learning_rate: [0.001, 0.01, 0.1]
CatBoost	0.98 (0.97–0.99)	0.91 (0.88–0.94)	0.92	0.90	0.91	learning_rate: [0.01, 0.05, 0.1]; n_estimators: [100, 200, 300]; l2_leaf_reg: [1, 3, 5]
Extreme Gradient Boosting (XGBoost)	0.97 (0.96–0.98)	0.91 (0.90–0.92)	0.92	0.90	0.91	learning_rate: [0.01, 0.05, 0.1]; n_estimators: [100, 200, 300]; subsample: [0.7, 0.8, 0.9]
Logistic Regression (Baseline Model)	0.89 (0.85–0.93)	0.84 (0.80–0.88)	0.66	0.80	0.74	—