Supplementary

Table S1 Definitions for postoperative pulmonary complications

Outcomes	Definition and diagnostic criteria
Respiratory infection	Antibiotic treatment for suspected respiratory infection plus at least one of the following: new or altered sputum, fever (> 38°C), white blood cell count >12 × 10^9/L, or new/progressive pulmonary infiltrates on chest imaging.
Pneumonia	New or progressive infiltrate, consolidation, or cavitation on chest imaging together with clinical evidence of infection, including fever (>38°C), abnormal white blood cell count (<4 or >12 × 10^9/L), purulent sputum, worsening cough or dyspnea, abnormal breath sounds, or impaired gas exchange.
Aspiration pneumonitis	Acute lung injury caused by aspiration of gastric contents.
Bronchospasm	Newly detected expiratory wheezing requiring bronchodilator therapy.
Pleural effusion	Pleural fluid accumulation on chest imaging counted as PPC only when accompanied by respiratory symptoms, oxygen requirement, therapeutic intervention such as diuretic therapy or drainage, or documented clinical management. Incidental small effusions without symptoms or treatment were not counted.
Atelectasis	Radiographic evidence of pulmonary opacity with volume loss counted as PPC only when associated with respiratory symptoms, impaired oxygenation, need for respiratory physiotherapy/airway clearance, or other clinical intervention. Minor asymptomatic atelectasis detected only on imaging was not counted.
Pneumothorax	Air in the pleural space on chest imaging, particularly when requiring oxygen therapy, drainage, monitoring, or other clinical management.
Respiratory failure	Postoperative PaO_2 <60 mm Hg on room air, PaO_2/FiO_2 ratio ≤ 300 mm Hg, oxygen saturation <90%, or requirement for noninvasive or invasive ventilatory support.
ARDS	Bilateral pulmonary infiltrates on chest imaging, PaO_2/FiO_2 ratio ≤ 300 mm Hg, and respiratory failure not fully explained by cardiac failure or fluid overload within 30 days after surgery.

ARDS, acute respiratory distress syndrome; FiO_2, fraction of inspired oxygen; PaO_2, partial pressure of arterial oxygen.

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Table S2 Incidence of postoperative pulmonary complications in development cohort

Type	**Number of patients**	**Incidence rate (%)**
Total number of patients with one or more PPCs	131	/
Respiratory infection	32	24.4
Pneumonia	27	20.6
Aspiration pneumonitis	6	4.58
Bronchospasm	17	13.0
Pleural effusion	45	34.4
Atelectasis	13	9.9
Pneumothorax	19	14.5
Respiratory failure	7	5.3
ARDS	1	0.8

ARDS, acute respiratory distress syndrome; PPCs, postoperative pulmonary complications.

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Table S3 Missing proportion of candidate predictors before multiple imputation

Candidate predictor	Missing proportion (%)
Intraoperative temperature	12.5
Colloid administration	10.8
Estimated blood loss	10.5
Cirrhosis	9.2
HBV/HCV infection	8.6
Smoking history	8.4
Serum creatinine (SCr)	8
Alanine aminotransferase (ALT)	7.8
Hemoglobin (Hgb)	7.7
Uric acid (UA)	7.7
Crystalloid administration	7.1
Previous abdominal surgery history	7
Drinking history	6.9
Aspartate aminotransferase (AST)	6.8
Intraoperative urine volume	6.6
Prothrombin time	5.9
White blood cell count (WBC)	5.8
Surgical duration	5.7
Cerebrovascular disease	5.6
Dyslipidemia	5.4
Hypertension	5
Total bilirubin (TBIL)	4.6
Chronic respiratory disease	4.6
Coronary heart disease	4.3
Intraoperative blood transfusion	3.6
Diabetes mellitus	3.6
Blood urea nitrogen (BUN)	3.3

Note: Missing proportions were calculated before multiple imputation.

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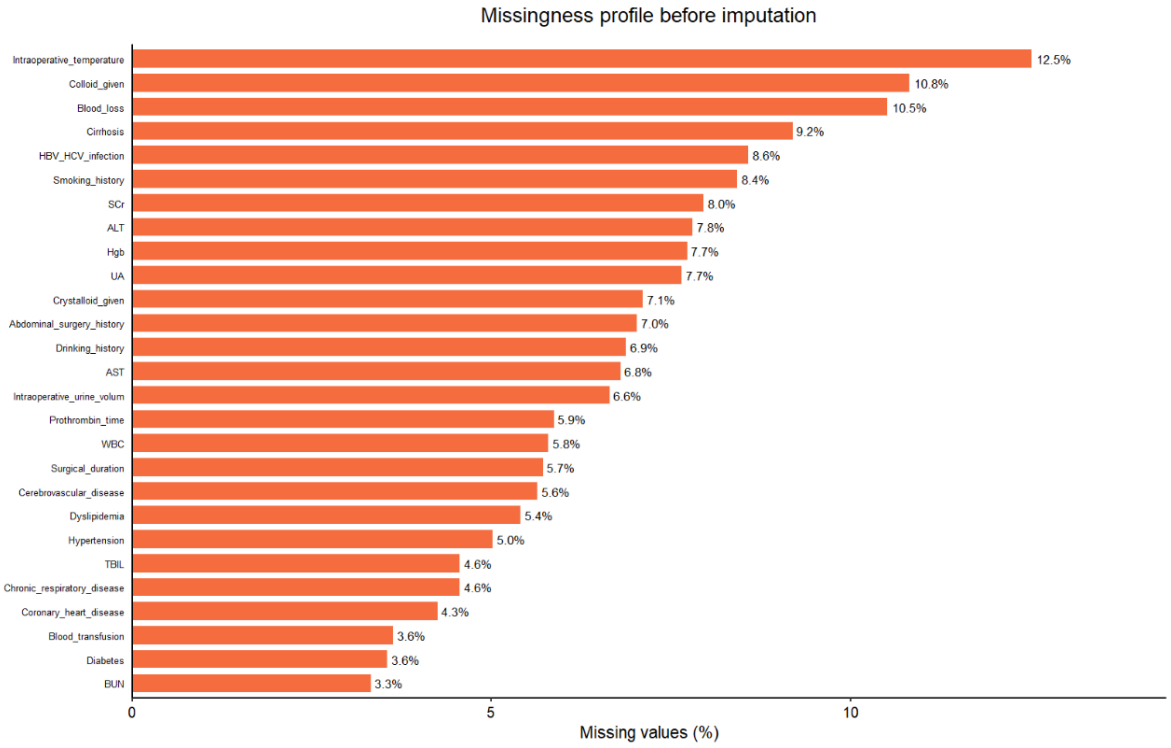


Figure S1 Proportion of missing values among candidate predictors before imputation.

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Table S4 Hyperparameters and optimization settings for the machine-learning algorithms

Model	Package	Hyperparameters evaluated (search space)	Other settings
Logistic Regression (LR)	glm	No hyperparameter tuning required	Family = quasibinomial; class weights applied; optimization metric = PR-AUC
Random Forest (RF)	ranger	mtry: √p, p/2, p splitrule: gini min.node.size: 5, 10, 20	Number of trees = 500; impurity-based variable importance; class weights applied
Decision Tree (DT)	rpart	complexity parameter (cp): 0.001, 0.005, 0.01, 0.02, 0.05	Case weights applied; optimization metric = PR-AUC
Naïve Bayes (NB)	Naïve_bayes	laplace smoothing: 0, 0.25, 0.5, 1, 2 usekernel: TRUE/FALSE kernel bandwidth adjustment: 0.5, 0.75, 1, 1.25, 1.5, 2, 2.5, 3 (when usekernel = TRUE)	Optimization metric = PR-AUC; class imbalance adjustment applied after probability estimation
K-Nearest Neighbors (KNN)	knn	number of neighbors (k): 5, 11, 21, 31, 41	Predictor centering and scaling; optimization metric = PR-AUC
Support Vector Machine (SVM)	svmRadial	sigma: 0.001, 0.01, 0.05, 0.1 cost parameter (C): 0.25, 1, 4	Radial basis function kernel; predictor centering and scaling; class weights applied
Extreme Gradient Boosting (XGBoost)	xgbTree	nrounds: 200 max_depth: 2, 3 eta: 0.03, 0.05 gamma: 0 colsample_bytree: 0.8 min_child_weight: 5, 10 subsample: 0.8	Scale positive weight = class imbalance ratio; optimization metric = PR-AUC
Light Gradient Boosting Machine (LightGBM)	lightgbm	max_depth: 2, 3 num_leaves: 3, 7 learning_rate: 0.01, 0.03	min_data_in_leaf = 15; feature_fraction = 0.8; bagging_fraction = 0.8; bagging_freq = 1; scale_pos_weight applied

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Table S5 Baseline characteristics of patients in the training and internal testing cohorts

Parameters	Total (n = 906)	Training set (n = 635)	Testing set (n = 271)	Statistics	*p*-value
PPCs	131 (14.5%)	93 (14.6%)	38 (14.0%)	0.060	0.807
Age (year)	58.00 [46.00–72.00]	58.00 [46.00–73.00]	57.00 [44.00–70.00]	1.605	0.108
Sex					
Male	533 (58.8%)	377 (59.4%)	156 (57.6%)	0.256	0.613
Female	373 (41.2%)	258 (40.6%)	115 (42.4%)		
BMI (kg/m^2)	23.40 [19.80–29.10]	23.70 [20.00–29.20]	22.70 [19.30–28.40]	1.619	0.105
Smoking history	274 (30.2%)	189 (29.8%)	85 (31.4%)	0.231	0.631
Drinking history	377 (41.6%)	273 (43.0%)	104 (38.4%)	1.666	0.197
Prior anticancer therapy[a]	84 (9.3%)	53 (8.3%)	31 (11.4%)	2.160	0.142
Comorbidities					
Hypertension	245 (27.0%)	163 (25.7%)	82 (30.3%)	2.027	0.154
Diabetes	162 (17.9%)	116 (18.3%)	46 (17.0%)	0.216	0.642
Dyslipidemia	121 (13.4%)	84 (13.2%)	37 (13.7%)	0.030	0.863
Chronic respiratory disease	78 (8.6%)	56 (8.8%)	22 (8.1%)	0.119	0.731
Coronary heart disease	60 (6.6%)	40 (6.3%)	20 (7.4%)	0.359	0.549
Abdominal surgery history	297 (32.8%)	215 (33.9%)	82 (30.3%)	1.117	0.291
Cerebrovascular disease	107 (11.8%)	77 (12.1%)	30 (11.1%)	0.203	0.652
HBV/HCV·infection	677 (74.7%)	483 (76.1%)	194 (71.6%)	2.015	0.156
Cirrhosis	376 (41.5%)	268 (42.2%)	108 (39.9%)	0.433	0.511
Child-Pugh stage					
A	676 (74.6%)	481 (75.7%)	195 (72.0%)	1.442	0.230
B	230 (25.4%)	154 (24.3%)	76 (28.0%)		
Pathology					
HCC	781 (86.2%)	556 (87.6%)	225 (83.0%)	3.282	0.070
ICC/cHCC-CCA	125 (13.8%)	79 (12.4%)	46 (17.0%)		
Maximum tumor size (≥5 cm)	410 (45.3%)	283 (44.6%)	127 (46.9%)	0.404	0.525
Tumor multiplicity					

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Single	583 (64.3%)	410 (64.6%)	173 (63.8%)	0.044	0.834
Multiple	323 (35.7%)	225 (35.4%)	98 (36.2%)		
Vascular invasion	199 (22.0%)	129 (20.3%)	70 (25.8%)	3.371	0.066
ASA classification					
I-II	732 (80.8%)	511 (80.5%)	221 (81.5%)	0.142	0.706
III-IV	174 (19.2%)	124 (19.5%)	50 (18.5%)		
Surgical approach					
Laparoscopic	241 (26.6%)	173 (27.2%)	68 (25.1%)	0.450	0.502
Open	665 (73.4%)	462 (72.8%)	203 (74.9%)		
Hepatectomy scope					
Partial hepatectomy	766 (84.5%)	536 (84.4%)	230 (84.9%)	0.031	0.860
Hemihepatectomy or more	140 (15.5%)	99 (15.6%)	41 (15.1%)		
Concomitant extrahepatic procedures	164 (18.1%)	116 (18.3%)	48 (17.7%)	0.040	0.842
Hepatectomy type					
Segment resection in VII/VIII	295 (32.6%)	215 (33.9%)	80 (29.5%)	1.628	0.202
Other segments	611 (67.4%)	420 (66.1%)	191 (70.5%)		
Portal triad clamping duration (min)	17.00 [9.00–28.00]	17.00 [9.00–28.00]	16.00 [7.00–29.00]	0.695	0.487
Blood loss (mL)	679.50 [439.00–999.75]	684.00 [441.00–1013.00]	661.00 [415.00–946.00]	1.528	0.127
Crystalloid given (L)	2.40 [1.60–3.30]	2.30 [1.60–3.30]	2.50 [1.70–3.40]	1.140	0.254
Colloid given (L)	1.90 [1.00–2.60]	1.90 [1.00–2.60]	2.00 [1.00–2.70]	0.650	0.516
Blood transfusion	364 (40.2%)	245 (38.6%)	119 (43.9%)	2.244	0.134
Surgical duration (min)	183.00 [109.00–261.25]	184.00 [109.00–263.00]	174.00 [111.00–260.00]	0.095	0.925
Intraoperative urine volume (mL)	651.00 [396.00–942.00]	646.00 [396.00–930.00]	651.00 [408.00–962.00]	0.323	0.747
Intraoperative temperature (°C)	36.40 [34.80–37.82]	36.40 [34.90–37.80]	36.20 [34.60–37.90]	0.713	0.476
Preoperative laboratory tests					
Hgb (g/L)	141.00 [122.00–161.00]	141.00 [122.00–163.00]	141.00 [122.00–159.00]	0.021	0.983

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ALB (g/L)	34.00 [25.00–44.00]	34.00 [25.00–43.00]	35.00 [26.00–45.00]	1.444	0.149
TBIL (μmol/L）	15.00 [9.00–41.25]	15.00 [9.00–41.00]	16.00 [9.00–43.00]	0.927	0.354
AST (U/L)	35.00 [21.00–186.25]	35.00 [21.00–214.00]	38.00 [22.00–157.00]	0.423	0.673
ALT (U/L)	28.60 [15.57–53.40]	28.70 [16.10–52.60]	28.50 [14.10–56.20]	0.055	0.956
BUN (mmol/L)	5.00 [3.80–6.10]	5.00 [3.80–6.10]	5.00 [3.80–6.20]	0.334	0.738
UA (μmol/L）	318.00 [235.75–379.25]	316.00 [235.00–381.00]	318.00 [236.00–374.00]	0.495	0.620
SCr (μmol/L）	77.00 [57.00–97.00]	77.00 [57.00–97.00]	78.00 [58.00–96.00]	0.362	0.718
Prothrombin time (s)	11.30 [9.20–13.10]	11.40 [9.40–13.10]	11.20 [9.00–12.70]	1.576	0.115
WBC ($\times10^9$/L)	6.45 [4.90–8.20]	6.30 [4.90–8.30]	6.70 [5.20–8.20]	0.745	0.456
PLT ($\times10^9$/L)	188.00 [137.00–239.25]	187.00 [135.00–237.00]	191.00 [140.00–243.00]	1.255	0.210
LYM ($\times10^9$/L)	1.50 [1.10–2.10]	1.50 [1.10–2.20]	1.50 [1.10–2.10]	0.888	0.375
NEU ($\times10^9$/L)	4.20 [3.00–5.60]	4.30 [3.00–5.60]	4.10 [2.80–5.60]	0.740	0.459
PLR	117.64 [82.17–170.00]	116.00 [80.53–167.27]	125.26 [87.89–173.33]	1.780	0.075
NLR	2.70 [1.79–4.29]	2.68 [1.85–4.25]	2.73 [1.63–4.55]	0.075	0.940
PNI	42.50 [33.50–51.50]	42.00 [33.00–51.00]	43.00 [34.50–53.50]	1.115	0.265

Data are presented as median (IQR) or frequencies (%). [a]Preoperative anticancer therapy was defined as any prior history of radiotherapy–systemic chemotherapy–targeted or immunotherapy–or liver-directed interventional therapy before hepatectomy. ALB, albumin; ALT, alanine aminotransferase; ASA, American Society of Anesthesiologists; AST, aspartate aminotransferase; BMI, body mass index; BUN, blood urea nitrogen; cHCC-CCA, combined hepatocellular-cholangiocarcinoma; HBV, hepatitis B virus; HCC, hepatocellular carcinoma; HCC-ICC, mixed hepatocellular-cholangiocarcinoma; HCV, hepatitis C virus; Hgb, hemoglobin; ICC, intrahepatic cholangiocarcinoma; LYM, lymphocytes; NEU, neutrophils; NLR, neutrophil-to-

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lymphocyte ratio; PLT, platelets; PLR, platelet-to-lymphocyte ratio; PNI, prognostic nutritional index; SCr, serum creatinine; TBIL, total bilirubin; UA, uric acid; WBC, white blood cells; PPCs, postoperative pulmonary complications.

$p < 0.05$ indicate statistically significant

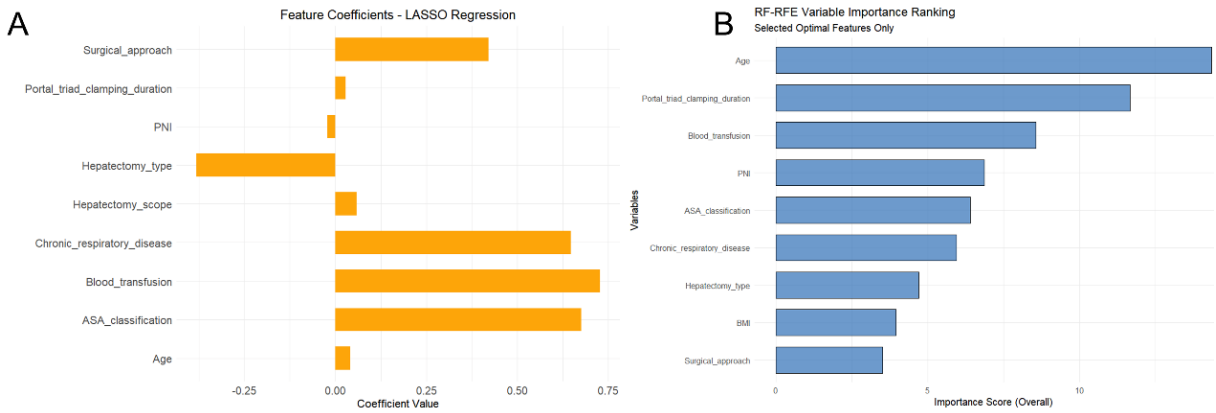


Figure S2 Variable retention and importance ranking from feature selection. (A) Final variable retention and coefficient distribution under the optimal LASSO regularization parameter (λ at 1-SE). (B) Feature importance ranking of the clinical variables evaluated by the RF-RFE algorithm–sorted from highest to lowest predictive contribution.

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Table S6 Comprehensive predictive performance metrics of the eight machine learning models evaluated in the training and internal testing cohorts

Algorithms	Youden threshold	AUC (95% CI)	PR-AUC (95% CI)	Accuracy	Balanced accuracy	Sensit-ivity	Specifi-city	NPV	Precision	F1-score	Brier score	Calibra-tion slope	Calibration intercept
LR_Train	0.084	0.893 (0.862–0.924)	0.638 (0.538–0.725)	0.734	0.822	0.946	0.697	0.987	0.349	0.510	0.082	0.869	-1.794
RF_Train	0.136	0.864 (0.826–0.902)	0.597 (0.493–0.692)	0.757	0.796	0.849	0.742	0.966	0.361	0.506	0.087	1.354	0.003
DT_Train	0.183	0.790 (0.736–0.844)	0.426 (0.328–0.541)	0.739	0.762	0.796	0.729	0.954	0.335	0.471	0.109	0.197	-1.671
NB_Train	0.221	0.889 (0.855–0.923)	0.667 (0.575–0.748)	0.855	0.817	0.763	0.871	0.955	0.504	0.607	0.079	0.971	0.589
KNN_Train	0.204	0.856 (0.815–0.898)	0.610 (0.509–0.700)	0.819	0.778	0.720	0.836	0.946	0.429	0.538	0.087	1.512	-1.499
SVM_Train	0.132	0.839 (0.796–0.881)	0.537 (0.434–0.632)	0.751	0.774	0.806	0.742	0.957	0.349	0.487	0.094	0.890	-3.492
XGBoost_Train	0.141	0.888 (0.855–0.922)	0.640 (0.538–0.730)	0.797	0.810	0.828	0.792	0.964	0.405	0.544	0.082	0.952	-1.379
LightGBM_Train	0.154	0.868 (0.833–0.904)	0.524 (0.423–0.629)	0.786	0.803	0.828	0.779	0.963	0.391	0.531	0.094	1.605	-0.912
LR_Test	0.084	0.858 (0.775–0.942)	0.697 (0.534–0.820)	0.753	0.790	0.842	0.738	0.966	0.344	0.489	0.073	0.883	0.070
RF_Test	0.136	0.826 (0.743–0.908)	0.615 (0.432–0.759)	0.793	0.770	0.737	0.803	0.949	0.378	0.500	0.081	0.782	0.056
DT_Test	0.183	0.792 (0.699–0.884)	0.539 (0.374–0.695)	0.738	0.738	0.737	0.738	0.945	0.315	0.441	0.104	0.821	0.174
NB_Test	0.221	0.851 (0.767–0.934)	0.668 (0.485–0.798)	0.878	0.808	0.711	0.906	0.950	0.551	0.621	0.075	0.821	-0.019
KNN_Test	0.204	0.820 (0.731–0.909)	0.611 (0.436–0.746)	0.823	0.765	0.684	0.845	0.943	0.419	0.52	0.084	0.372	-0.101
SVM_Test	0.132	0.843 (0.759–0.928)	0.666 (0.498–0.790)	0.860	0.819	0.763	0.876	0.958	0.500	0.604	0.076	0.908	0.248
XGBoost_Test	0.141	0.845 (0.764–0.927)	0.627 (0.445–0.780)	0.815	0.783	0.737	0.828	0.951	0.412	0.528	0.078	0.810	0.036
LightGBM_Test	0.154	0.857 (0.780–0.934)	0.656 (0.477–0.796)	0.756	0.781	0.816	0.747	0.961	0.344	0.484	0.080	1.338	-0.196

AUC, area under the receiver operating characteristic curve; CI, confidence interval; PR-AUC, area under the precision-recall curve; Accuracy, overall classification accuracy; Balanced accuracy, mean of sensitivity and specificity; Specificity, true negative rate; NPV, negative predictive value; Precision, positive predictive value; F1-score, harmonic mean of precision and recall; LR, Logistic Regression; RF, Random Forest; DT, Decision Tree; NB, Naïve Bayes; KNN, *k*-Nearest Neighbors; SVM, Support Vector Machine; XGBoost, Extreme Gradient Boosting; LightGBM, Light Gradient Boosting Machine.

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Table S7 Baseline characteristics of patients in the external validation cohort

Parameters	**Total (n = 388)**	**PPCs (n = 66)**	**None-PPCs (n = 322)**	**Statistics**	***p*-value**
Age (year)	59.00 [46.00–73.00]	70.00 [62.50–78.25]	56.50 [46.00–70.00]	4.927	<0.001
Sex					
Male	219 (56.4%)	36 (54.5%)	183 (56.8%)	0.117	0.733
Female	169 (43.6%)	30 (45.5%)	139 (43.2%)		
BMI (kg/m^2)	23.20 [20.00–28.17]	24.00 [20.50–30.98]	22.90 [19.90–28.00]	1.553	0.120
Smoking history	131 (33.8%)	22 (33.3%)	109 (33.9%)	0.007	0.935
Drinking history	173 (44.6%)	36 (54.5%)	137 (42.5%)	3.192	0.074
Prior anticancer therapy[a]	39 (10.1%)	5 (7.6%)	34 (10.6%)	0.539	0.463
Comorbidities					
Hypertension	103 (26.5%)	17 (25.8%)	86 (26.7%)	0.025	0.873
Diabetes	72 (18.6%)	12 (18.2%)	60 (18.6%)	0.007	0.931
Dyslipidemia	49 (12.6%)	7 (10.6%)	42 (13.0%)	0.295	0.587
Chronic respiratory disease	23 (5.9%)	9 (13.6%)	14 (4.3%)	8.474	0.004
Coronary heart disease	29 (7.5%)	4 (6.1%)	25 (7.8%)	0.230	0.632
Abdominal surgery history	115 (29.6%)	19 (28.8%)	96 (29.8%)	0.028	0.868
Cerebrovascular disease	46 (11.9%)	5 (7.6%)	41 (12.7%)	1.394	0.238
HBV/HCV infection	318 (82.0%)	56 (84.8%)	262 (81.4%)	0.449	0.503
Cirrhosis	170 (43.8%)	29 (43.9%)	141 (43.8%)	0.001	0.982

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Child-Pugh stage					
A	282 (72.7%)	47 (71.2%)	235 (73.0%)	0.086	0.769
B	106 (27.3%)	19 (28.8%)	87 (27.0%)		
Pathology					
HCC	331 (85.3%)	53 (80.3%)	278 (86.3%)	1.590	0.207
ICC/cHCC-CCA	57 (14.7%)	13 (19.7%)	44 (13.7%)		
Maximum tumor size (≥5 cm)	193 (49.7%)	32 (48.5%)	161 (50.0%)	0.050	0.823
Tumor multiplicity					
Single	270 (69.6%)	50 (75.8%)	220 (68.3%)	1.431	0.232
Multiple	118 (30.4%)	16 (24.2%)	102 (31.7%)		
Vascular invasion	98 (25.3%)	21 (31.8%)	77 (23.9%)	1.813	0.178
ASA classification					
I-II	314 (80.9%)	44 (66.7%)	270 (83.9%)	10.479	0.001
III-IV	74 (19.1%)	22 (33.3%)	52 (16.1%)		
Surgical approach					
Laparoscopic	91 (23.5%)	9 (13.6%)	82 (25.5%)	4.269	0.039
Open	297 (76.5%)	57 (86.4%)	240 (74.5%)		
Hepatectomy scope					
Partial hepatectomy	320 (82.5%)	49 (74.2%)	271 (84.2%)	3.728	0.053
Hemihepatectomy or more	68 (17.5%)	17 (25.8%)	51 (15.8%)		
Concomitant extrahepatic procedures	74 (19.1%)	18 (27.3%)	56 (17.4%)	3.465	0.063

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Hepatectomy type					
Segment resection in VII/VIII	131 (33.8%)	41 (62.1%)	90 (28.0%)	28.598	<0.001
Other segments	257 (66.2%)	25 (37.9%)	232 (72.0%)		
Portal triad clamping duration (min)	18.00 [8.00–29.75]	26.50 [16.50–43.25]	16.00 [7.00–27.00]	4.766	<0.001
Blood loss (mL)	708.00 [463.25–1037.75]	697.50 [481.75–1041.50]	710.50 [460.75–1036.00]	0.120	0.904
Crystalloid given (L)	2.30 [1.60–3.30]	2.70 [1.85–3.30]	2.30 [1.50–3.30]	1.548	0.122
Colloid given (L)	1.90 [1.10–2.80]	1.70 [1.10–2.70]	1.90 [1.10–2.90]	0.531	0.595
Blood transfusion	147 (37.9%)	36 (54.5%)	111 (34.5%)	9.379	0.002
Surgical duration (min)	189.50 [112.25–253.75]	222.50 [124.00–275.50]	184.00 [108.75–250.25]	1.905	0.057
Intraoperative urine volume (mL)	698.50 [366.75–923.00]	802.00 [399.25–1146.25]	667.00 [353.00–899.25]	1.942	0.052
Intraoperative temperature (℃)	36.10 [34.70–37.48]	35.95 [35.05–37.65]	36.10 [34.70–37.42]	0.319	0.749
Preoperative laboratory tests					
Hgb (g/L)	143.00 [125.00–163.00]	146.00 [127.75–161.75]	141.00 [124.00–163.25]	0.998	0.318
ALB (g/L)	35.00 [25.25–44.00]	24.00 [20.00–37.00]	37.00 [28.00–45.00]	4.736	<0.001
TBIL (μmol/L）	15.00 [9.00–34.00]	15.00 [8.75–41.50]	15.00 [9.00–34.00]	0.259	0.796
AST (U/L)	39.00 [19.00–273.00]	65.50 [22.00–555.00]	36.00 [18.00–229.00]	1.913	0.056
ALT (U/L)	30.20 [17.35–58.00]	30.65 [16.38–70.50]	29.95 [17.50–57.55]	0.380	0.704
BUN (mmol/L)	4.80 [3.70–6.00]	4.85 [4.07–6.08]	4.80 [3.60–6.00]	1.051	0.293
UA (μmol/L）	314.00 [243.50–378.75]	327.50 [221.75–364.50]	311.00 [249.00–382.25]	0.200	0.841
SCr (μmol/L）	77.00 [59.25–94.00]	81.00 [66.75–95.25]	76.00 [58.75–94.00]	0.951	0.341

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Prothrombin time (s)	11.60 [9.43–13.00]	11.00 [9.28–12.60]	11.70 [9.50–13.20]	1.407	0.159
WBC ($\times 10^9$/L)	6.70 [5.20–8.40]	6.35 [5.08–8.33]	6.70 [5.18–8.43]	0.758	0.448
PLT ($\times 10^9$/L)	197.00 [145.25–246.00]	170.50 [128.00–218.75]	205.00 [147.00–250.25]	2.702	0.007
LYM ($\times 10^9$/L)	1.60 [1.10–2.10]	1.45 [1.10–1.92]	1.60 [1.10–2.10]	1.039	0.299
NEU ($\times 10^9$/L)	4.10 [3.00–5.50]	4.55 [3.18–5.93]	4.00 [2.90–5.50]	1.258	0.208
PLR	127.38 [83.42–182.50]	127.10 [74.30–181.67]	127.74 [85.88–182.72]	0.808	0.419
NLR	2.83 [1.79–4.42]	3.22 [2.00–4.48]	2.71 [1.76–4.41]	1.697	0.090
PNI	43.50 [33.50–53.38]	32.50 [28.50–45.25]	45.00 [36.50–54.12]	4.907	<0.001

Data are presented as median (IQR) or frequencies (%). [a]Preoperative anticancer therapy was defined as any prior history of radiotherapy, systemic chemotherapy, targeted or immunotherapy, or liver-directed interventional therapy before hepatectomy. ALB, albumin; ALT, alanine aminotransferase; ASA, American Society of Anesthesiologists; AST, aspartate aminotransferase; BMI, body mass index; BUN, blood urea nitrogen; cHCC-CCA, combined hepatocellular-cholangiocarcinoma; HBV, hepatitis B virus; HCC, hepatocellular carcinoma; HCC-ICC, mixed hepatocellular-cholangiocarcinoma; HCV, hepatitis C virus; Hgb, hemoglobin; ICC, intrahepatic cholangiocarcinoma; LYM, lymphocytes; NEU, neutrophils; NLR, neutrophil-to-lymphocyte ratio; PLT, platelets; PLR, platelet-to-lymphocyte ratio; PNI, prognostic nutritional index; SCr, serum creatinine; TBIL, total bilirubin; UA, uric acid; WBC, white blood cells; PPCs, postoperative pulmonary complications. $p < 0.05$ indicate statistically significant.

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Table S8 Comprehensive predictive performance metrics of the eight machine learning models evaluated in the independent external validation cohort

Algorithm	Youden threshold	AUC (95% CI)	PR-AUC (95% CI)	Accuracy	Balanced accuracy	Sensitivity	Specificity	NPV	Precision	F1-score	Brier score	Calibration slope	Calibration intercept
LR	0.084	0.851 (0.800–0.902)	0.605 (0.471–0.720)	0.716	0.763	0.833	0.693	0.953	0.357	0.500	0.099	0.854	0.283
RF	0.136	0.852 (0.801–0.903)	0.597 (0.471–0.715)	0.763	0.779	0.803	0.755	0.949	0.402	0.535	0.101	0.956	0.328
DT	0.183	0.783 (0.718–0.849)	0.459 (0.333–0.589)	0.765	0.750	0.727	0.773	0.933	0.397	0.513	0.123	0.892	0.472
NB	0.221	0.861 (0.810–0.911)	0.650 (0.516–0.759)	0.822	0.748	0.636	0.860	0.920	0.483	0.549	0.094	0.898	0.217
KNN	0.204	0.857 (0.807–0.907)	0.585 (0.452–0.703)	0.832	0.779	0.697	0.860	0.933	0.505	0.586	0.100	0.852	0.243
SVM	0.132	0.856 (0.804–0.907)	0.618 (0.487–0.734)	0.812	0.784	0.742	0.826	0.940	0.467	0.573	0.099	0.980	0.515
XGBoost	0.141	0.847 (0.796–0.899)	0.614 (0.479–0.729)	0.776	0.756	0.727	0.786	0.934	0.410	0.525	0.099	0.853	0.279
LightGBM	0.154	0.849 (0.799–0.898)	0.614 (0.490–0.721)	0.711	0.760	0.833	0.686	0.953	0.353	0.495	0.102	1.333	0.001

AUC, area under the receiver operating characteristic curve; CI, confidence interval; PR-AUC, area under the precision-recall curve; Accuracy, overall classification accuracy; Balanced accuracy, mean of sensitivity and specificity; Specificity, true negative rate; NPV, negative predictive value; Precision, positive predictive value; F1-score, harmonic mean of precision and recall; LR, Logistic Regression; RF, Random Forest; DT, Decision Tree; NB, Naïve Bayes; KNN, *k*-Nearest Neighbors; SVM, Support Vector Machine; XGBoost, Extreme Gradient Boosting; LightGBM, Light Gradient Boosting Machine.

Table S9 Sensitivity analysis of Severe-PPC in NB model across three cohorts

Dataset	Model	N	Events	AUC (95% CI)	PR-AUC (95% CI)	Accuracy	Balanced accuracy	Sensitivity	Specificity	NPV	Precision	F1-score	Brier score	Calibration slope	Calibration intercept
Training	NB	635	55	0.844 (0.793–0.895)	0.403 (0.272–0.538)	0.753	0.774	0.800	0.748	0.975	0.232	0.359	0.064	0.877	0.112
Internal testing	NB	271	32	0.872 (0.791–0.953)	0.657 (0.476–0.794)	0.860	0.826	0.781	0.870	0.967	0.446	0.568	0.074	1.327	0.591
External validation	NB	388	45	0.838 (0.779–0.897)	0.511 (0.345–0.648)	0.771	0.706	0.622	0.790	0.941	0.280	0.386	0.082	1.161	0.509

AUC, area under the receiver operating characteristic curve; CI, confidence interval; PR-AUC, area under the precision-recall curve; Accuracy, overall classification accuracy; Balanced accuracy, mean of sensitivity and specificity; Specificity, true negative rate; NPV, negative predictive value; Precision, positive predictive value; F1-score, harmonic mean of precision and recall; NB, Naïve Bayes.

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