

Table S1 Baseline characteristics of the training dataset

Characteristics	Pyonephrosis group (n=52)	Non-pyonephrosis group (n=173)	P value
Age (year), median (IQR)	51 (44–57)	53 (46–59)	0.237
Sex, n (%)			<0.001
Male	16 (30.8)	117 (67.6)	
Female	36 (69.2)	56 (32.4)	
UTI within 3 months, n (%)			<0.001
Yes	34 (65.4)	16 (9.2)	
No	18 (34.6)	157 (90.8)	
Renal colic, n (%)			0.116
Yes	29 (55.8)	117 (67.6)	
No	23 (44.2)	56 (32.4)	
Fever, n (%)			<0.001
Yes	25 (48.1)	14 (8.1)	
No	27 (51.9)	159 (91.9)	
Coexisting chronic diseases			
Hypertension (n/N)	15/52	60/173	0.434
Diabetes (n/N)	5/52	13/173	0.572
Hyperuricemia, n (%)			0.644
Yes	18 (34.6)	66 (38.2)	
No	34 (65.4)	107 (61.8)	
Stone size (mm), median (IQR)	14 (9–23)	13 (9–19)	0.228
Stone density (HU), median (IQR)	1,338.5 (1,193–1,558.25)	1,219 (1,009–1,433)	0.032
CT value of hydronephrosis (HU), median (IQR)	15.85 (11.5–21.5)	6.0 (2.0–12.7)	<0.001
Staghorn calculi, n (%)			0.428
Yes	4 (7.7)	20 (11.6)	
No	48 (92.3)	153 (88.4)	
Serum creatinine (μmol/L), median (IQR)	100.5 (75.0–185.5)	94.0 (73.0–131.0)	0.150
Hydronephrosis, n (%)			<0.001
Mild/Moderate	21 (40.4)	156 (90.2)	
Severe	31 (59.6)	17 (9.8)	
SHACK, n (%)			<0.001
Yes	16 (30.8)	13 (7.5)	
No	36 (69.2)	160 (92.5)	
Congenital renal malformation, n (%)			0.738
Yes	2 (3.8)	10 (5.8)	
No	50 (96.2)	163 (94.2)	

IQR, interquartile range; UTI, urinary tract infection; HU, Hounsfield unit; SHACK, severe hydronephrosis or atrophy of the contralateral kidney.

Table S2 Laboratory test results of the training dataset

Variables	Pyonephrosis group (n=52)	Non-pyonephrosis group (n=173)	P value
WBC ($\times 10^9/L$)	10.4 (7.3–17.0)	6.0 (5.1–7.3)	<0.001
Neutrophils ($\times 10^9/L$)	7.8 (5.4–14.1)	3.4 (2.9–4.3)	<0.001
Serum CRP (mg/L)	73.7 (47.7–133.9)	2.6 (1.1–6.8)	<0.001
Urine leukocyte ($/\mu L$)	201.3 (56.4–1733.6)	73.8 (25.0–180.0)	<0.001
Urinary nitrite, n (%)			0.120
Positive	10 (19.2)	19 (11.0)	
Negative	42 (80.8)	154 (89.0)	
Urine culture, n (%)			<0.001
Positive	23 (44.2)	22 (12.7)	
Negative	29 (55.8)	151 (87.3)	

WBC, white blood cell; CRP, C-reactive protein.

Table S3 Baseline characteristics of the testing dataset

Characteristics	Pyonephrosis group (n=24)	Non-pyonephrosis group (n=73)	P value
Age (year), median (IQR)	44.5 (39.75–53.75)	55.5 (48.5–66.25)	0.055
Sex, n (%)			0.001
Male	8 (33.3)	52 (71.2)	
Female	16 (66.7)	21 (28.8)	
UTI within 3 months, n (%)			<0.001
Yes	16 (66.7)	10 (13.7)	
No	8 (33.3)	63 (86.3)	
Renal colic, n (%)			0.588
Yes	15 (62.5)	50 (68.5)	
No	9 (37.5)	23 (31.5)	
Fever, n (%)			<0.001
Yes	11 (45.8)	6 (8.2)	
No	13 (54.2)	67 (91.8)	
Coexisting chronic diseases			
Hypertension (n/N)	10/24	22/73	0.297
Diabetes (n/N)	3/24	8/73	> 0.99
Hyperuricemia, n (%)			0.499
Yes	8 (33.3)	30 (41.1)	
No	16 (66.7)	43 (58.9)	
Stone size (mm), median (IQR)	15.5 (10–18.25)	11 (8–17)	0.132
Stone density (HU), median (IQR)	1,497 (1,286.75–1,668.50)	1,205 (925–1,380)	0.004
CT value of hydronephrosis (HU), median (IQR)	13.85 (11.675–22.10)	7.3 (2.4–12.9)	<0.001
Staghorn calculi, n (%)			0.444
Yes	1 (4.2)	8 (11.0)	
No	23 (95.8)	65 (89.0)	
Serum creatinine (μmol/L), median (IQR)	83.0 (64.5–212.5)	93.0 (75.0–116.0)	0.716
Hydronephrosis, n (%)			<0.001
Mild/Moderate	11 (45.8)	62 (84.9)	
Severe	13 (54.2)	11 (15.1)	
SHACK, n (%)			<0.001
Yes	10 (41.7)	5 (6.8)	
No	14 (58.3)	68 (93.2)	
Congenital renal malformation, n (%)			>0.99
Yes	1 (4.2)	4 (5.5)	
No	23 (95.8)	69 (94.5)	

IQR, interquartile range; UTI, urinary tract infection; HU, Hounsfield unit; SHACK, severe hydronephrosis or atrophy of the contralateral kidney.

Table S4 Laboratory test results of the testing dataset

Variables	Pyonephrosis group (n=24)	Non-pyonephrosis group (n=73)	P value
WBC ($\times 10^9/L$)	8.85 (7.65–13.20)	6.20 (5.30–7.90)	<0.001
Neutrophils ($\times 10^9/L$)	6.60 (5.225–10.325)	3.60 (2.80–4.60)	<0.001
Serum CRP (mg/L)	68.7 (35.825–123.225)	2.80 (1.20–7.30)	<0.001
Urine leukocyte ($/\mu L$)	434.2 (95.775–4126.95)	79.60 (30.60–200.50)	<0.001
Urinary nitrite, n (%)			0.003
Positive	8 (33.3)	5 (6.8)	
Negative	16 (66.7)	68 (93.2)	
Urine culture, n (%)			<0.001
Positive	15 (62.5)	5 (6.8)	
Negative	9 (37.5)	68 (93.2)	

WBC, white blood cell; CRP, C-reactive protein.

Table S5 DeLong P values resulting from the pairwise comparison of the area under the receiver operator characteristic (ROC) curve (AUC) between ML (machine learning)-based models

Variables	P value	
	Training dataset	Testing dataset
Lasso-LR vs. LR	0.032	0.314
SVM vs. LR	0.007	0.056
RF vs. LR	0.596	0.233
XGBoost vs. LR	0.035	0.513

LR, logistic regression; Lasso, least absolute shrinkage and selection operator; SVM, support vector machine; RF, random forest; XGBoost, extreme gradient boosting.