

• 论著 •

基于机器学习决策树模型对急性百草枯中毒患者预后的预测价值

吕广卫 冯顺易 李勇 王剑

沧州市中心医院急诊医学部,河北沧州 061000

通信作者:王剑,Email:15103173507@163.com

【摘要】目的 探讨基于机器学习的决策树模型对急性百草枯(PQ)中毒(APP)患者预后的预测价值。**方法** 采用回顾性研究方法。收集 2012 年 5 月至 2021 年 8 月沧州市中心医院急诊医学部救治的 APP 患者的临床数据,包括性别、年龄、服毒至洗胃的时间、血液灌流比例、血 PQ 浓度、生化指标[白细胞计数(WBC)、丙氨酸转氨酶(ALT)、血肌酐(SCr)、血淀粉酶及血钾]以及血气指标[动脉血乳酸(Lac)、剩余碱和动脉血氧分压(PaO₂)]。根据中毒后 90 d 预后将患者分为生存组(56 例)和死亡组(74 例),比较不同预后两组患者临床指标的差异。通过多因素 Logistic 回归分析影响 APP 患者预后的危险因素,将危险因素作为变量构建含血 PQ 浓度及不含血 PQ 浓度的两种决策树模型。绘制受试者工作特征曲线(ROC 曲线)评估决策树模型对 APP 患者预后的预测价值,通过 Hanley & McNeil 法对两种决策树模型的 ROC 曲线下面积(AUC)进行比较。**结果** 患者 90 d 的生存率为 43.1%(56/130)。与死亡组比较,生存组 WBC [$\times 10^9/L$: 8.9(7.0, 11.6) vs. 17.4(11.9, 23.1)], ALT[U/L: 25.3(21.2, 31.8) vs. 29.3(23.2, 40.3)], SCr[$\mu\text{mol}/L$: 64.0(53.0, 74.0) vs. 91.0(72.5, 141.5)], Lac[mmol/L: 2.5(1.4, 4.0) vs. 7.1(3.7, 11.0)]和血 PQ 浓度[ng/L: 0.3(0.1, 0.9) vs. 2.9(1.9, 8.1)]均较低,差异均有统计学意义(均 $P < 0.05$),剩余碱[mmol/L: -2.5(-4.2, -1.1) vs. -7.2(-10.9, -4.7)]和血钾[mmol/L: 3.7(3.5, 4.0) vs. 3.2(2.8, 3.7)]均较高,差异均有统计学意义(均 $P < 0.05$),患者更年轻[岁: 33.5(26.0, 47.8) vs. 42.5(26.0, 58.0), $P < 0.05$]。单因素 Logistic 回归分析结果显示,年龄、WBC、ALT、SCr、血钾、Lac、剩余碱和血 PQ 浓度是影响 APP 患者 90 d 预后的独立危险因素[优势比(OR)和 95% 可信区间(95%CI)分别为 1.03(1.01~1.05)、1.30(1.18~1.44)、1.04(1.01~1.07)、1.02(1.01~1.04)、7.59(3.25~17.70)、1.64(1.35~1.99)、1.51(1.29~1.76)、7.00(3.41~14.37), P 值分别为 0.018、<0.001、0.011、<0.001、<0.001、<0.001、<0.001]。含血 PQ 浓度的多因素 Logistic 回归分析结果显示,WBC、血钾和血 PQ 浓度是影响患者 90 d 生存的独立危险因素[OR 和 95%CI 分别为 1.17(1.03~1.33)、7.29(1.66~32.01)、5.49(2.48~12.13), P 值分别为 0.014、0.008、<0.001]。不含血 PQ 浓度的多因素 Logistic 回归分析显示,年龄、WBC、血钾和剩余碱是影响患者 90 d 生存的独立危险因素[OR 和 95%CI 分别为 1.05(1.01~1.08)、1.20(1.07~1.34)、3.12(1.01~9.66)、1.41(1.16~1.72), P 值分别为 0.008、0.002、0.049、0.001]。基于血 PQ 浓度和血钾决策树模型的 AUC 为 0.94, 95%CI 为 0.89~0.98, 敏感度为 91.9%, 特异度为 89.3%, 准确率为 90.0%。基于 WBC、剩余碱和年龄决策树模型的 AUC 为 0.89, 95%CI 为 0.84~0.95, 敏感度为 86.5%, 特异度为 91.1%, 准确率为 88.5%。Hanley & McNeil 法比较显示,两种决策树模型的 AUC 差异无统计学意义($Z=1.34$, $P=0.180$)。**结论** 基于机器学习的决策树模型可为临床早期评估 APP 患者的预后提供定量、直观的预测工具。

【关键词】 百草枯; 中毒; 机器学习; 决策树

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Predictive value of decision tree-based machine learning model for prognosis in acute paraquat poisoning

Lyu Guangwei, Feng Shunyi, Li Yong, Wang Jian

Department of Emergency, Cangzhou Central Hospital, Cangzhou 061000, Hebei, China

Corresponding author: Wang Jian, Email: 15103173507@163.com

【Abstract】Objective To investigate the predictive value of a decision tree-based machine learning model for prognosis in acute paraquat (PQ) poisoning (APP) patients. **Methods** A retrospective study was conducted. The clinical data of APP patients from Cangzhou Central Hospital between May 2012 and August 2021 were collected, including gender, age, time from ingestion to gastric lavage, proportion of hemoperfusion, serum PQ concentration, biochemical indicators [white blood cell count (WBC), alanine aminotransferase (ALT), serum creatinine (SCr), serum amylase, and serum potassium], and blood gas indicators [arterial blood lactic acid (Lac), base excess (BE), and arterial partial pressure of oxygen (PaO₂)]. Patients were divided into a survival group ($n = 56$) and a death group ($n = 74$) based on 90-day prognosis, and the clinical data between the two groups were compared. The multivariate Logistic regression analysis was conducted to analyze the risk factors of prognosis in APP patients, and two decision tree models (i.e., with/without serum PQ concentration) were constructed based on the risk factors. The predictive value was evaluated by the receiver operator characteristic (ROC) curve, and the area under the ROC curve (AUC) of two decision tree models was compared by Hanley & McNeil method. **Results** The 90-day survival rate of the patients was 43.1% (56/130). Compared with death group, patients in the survival group had lower WBC [$\times 10^9/L$: 8.9 (7.0, 11.6) vs. 17.4 (11.9, 23.1)],

ALT [U/L: 25.3 (21.2, 31.8) vs. 29.3 (23.2, 40.3)], SCr [$\mu\text{mol}/\text{L}$: 64.0 (53.0, 74.0) vs. 91.0 (72.5, 141.5)], Lac [mmol/L: 2.5 (1.4, 4.0) vs. 7.1 (3.7, 11.0)], and serum PQ concentration [ng/L: 0.3 (0.1, 0.9) vs. 2.9 (1.9, 8.1)], the difference were statistically significant (all $P < 0.05$), higher BE [mmol/L: -2.5 (-4.2, -1.1) vs. -7.2 (-10.9, -4.7)] and serum potassium [mmol/L: 3.7 (3.5, 4.0) vs. 3.2 (2.8, 3.7)], the difference were statistically significant (all $P < 0.05$), and patients were younger [years: 33.5 (26.0, 47.8) vs. 42.5 (26.0, 58.0), $P < 0.05$]. Univariate Logistic regression analysis showed that age, WBC, ALT, SCr, serum potassium, Lac, BE and serum PQ concentration were independent risk factors of 90-day survival [odds ratio (*OR*) and 95% confidence interval (95%CI) were 1.03 (1.01–1.05), 1.30 (1.18–1.44), 1.04 (1.01–1.07), 1.02 (1.01–1.04), 7.59 (3.25–17.70), 1.64 (1.35–1.99), 1.51 (1.29–1.76), 7.00 (3.41–14.37), P values were 0.018, < 0.001, 0.011, < 0.001, < 0.001, < 0.001, < 0.001, < 0.001]. Multivariate Logistic regression analysis with serum PQ concentration showed that WBC, serum potassium, and serum PQ concentration were independent risk factors for 90-day survival [*OR* and 95%CI were 1.17 (1.03–1.33), 7.29 (1.66–32.01), 5.49 (2.48–12.13), P values were 0.014, 0.008, < 0.001]. Multivariate Logistic regression analysis without serum PQ concentration showed that age, WBC, serum potassium and BE were independent risk factors for 90-day survival [*OR* and 95%CI were 1.05 (1.01–1.08), 1.20 (1.07–1.34), 3.12 (1.01–9.66), 1.41 (1.16–1.72), P values were 0.008, 0.002, 0.049, 0.001]. The decision tree model based on serum PQ concentration and serum potassium showed an AUC of 0.94 (95%CI was 0.89–0.98), along with 91.9% sensitivity, 89.3% specificity, and 90.0% accuracy. The decision tree model based on WBC, BE, and age showed an AUC of 0.89 (95%CI was 0.84–0.95), with 86.5% sensitivity, 91.1% specificity, and 88.5% accuracy. Pairwise comparison of the AUC using Hanley & McNeil method demonstrated that no statistical difference between the two decision tree models ($Z = 1.34$, $P = 0.180$). **Conclusion** The decision tree-based models can provide quantitative and intuitive prediction tools for the early detection of prognosis in APP patients in clinical practice.

【Key words】 Paraquat; Poisoning; Machine learning; Decision tree

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百草枯(paraquat, PQ)是一种高效广谱的季铵盐类除草剂,其毒性强,病死率高^[1]。目前尚缺乏救治急性PQ中毒(acute PQ poisoning, APP)患者的有效方法,临幊上常采用洗胃、导泻、血液净化、抗炎、对症支持等综合疗法^[2-3]。血PQ浓度被认为是评估APP患者预后的一个强有力预测指标^[4]。虽然液相色谱法检测血PQ浓度是“金标准”^[5-6],但绝大多数医院无法开展此项技术。机器学习可通过分析大型数据集,并基于危险因素构建预测模型,从而快速准确地进行疾病诊断及预后评估^[7]。鉴于这一优势,在医学诊疗中使用机器学习模型作为决策支持系统的情况正逐渐增加。本研究构建并评估基于机器学习决策树模型对APP患者预后的预测价值,以期为APP的诊断提供参考。

1 资料与方法

1.1 研究对象:回顾性分析2012年5月至2021年8月本院急诊医学部救治的APP患者的临床数据。

1.1.1 纳入标准:①年龄≥14岁;②口服20%PQ溶液;③服毒至就诊时间<12 h。

1.1.2 排除标准:①血PQ浓度资料不全;②既往存在严重心肺和肝肾等器官功能障碍;③合并其他药物或农药中毒;④有近期感染史;⑤有恶性肿瘤;⑥孕妇或哺乳期女性。

1.1.3 伦理学:本研究遵循临床医学伦理准则,并经本院伦理委员会批准(审批号:2017-094-01),所有检测及治疗措施均获得患者或家属的知情同意。

1.2 数据收集:通过医院电子病历系统收集APP患者的人口学资料及临床数据,包括:①性别、年龄;②服毒至洗胃时间;③血PQ浓度;④生化指标,包括白细胞计数(white blood cell count, WBC)、丙氨酸转氨酶(alanine transaminase, ALT)、血肌酐(serum creatinine, SCr)、血钾及血淀粉酶;⑤血气指标,包括动脉血乳酸(lactic acid, Lac)、剩余碱和动脉血氧分压(arterial partial pressure of oxygen, PaO₂)。

1.3 分组:根据患者中毒后90 d的存活情况分为生存组和死亡组。

1.4 统计学方法:应用R 4.0.5软件分析数据。采用Kolmogorov-Smirnov法对计量资料进行正态性检验,符合正态分布的定量资料以均数±标准差($\bar{x} \pm s$)表示,组间比较采用两组独立样本t检验;非正态分布的定量资料以中位数(四分位数)[$M(Q_L, Q_U)$]表示,组间比较采用Mann-Whitney U检验。定性资料以例(百分比)表示,组间比较采用 χ^2 检验或秩和检验。采用Logistic回归分析筛选APP患者预后的危险因素,将危险因素作为模型变量通过rpart和ctree分析包构建并绘制含血PQ浓度及不含血PQ浓度的两种决策树模型,采用受试者工作特征曲线(receiver operator characteristic curve, ROC曲线)评估决策树模型的预测价值,通过Hanley & McNeil法对两种决策树模型的ROC曲线下面积(the area under the ROC curve, AUC)进行对比。 $P < 0.05$ 为差异有统计学意义。

2 结 果

2.1 一般资料(表1):通过医院电子病历系统初步筛查149例APP患者中10例资料不完整、6例随访失败、3例转院被排除,最终研究纳入130例。130例患者中,男性72例,女性58例;中位年龄[37.5(26.0, 53.0)]岁,从服毒至洗胃的中位时间1.0(0.5, 2.0)h,中位血PQ浓度1.6(0.4, 4.3)ng/L,96.2%的患者接受血液灌流治疗。56例(43.1%)患者生存,74例(56.9%)患者死亡。与死亡组比较,生存组WBC、ALT、SCr、Lac和血PQ浓度均降低,血钾和剩余碱水平均升高,患者更年轻(均P<0.05)。

2.2 APP患者90d预后影响因素的Logistic回归分析(表2~3):单因素Logistic回归分析显示,年龄、WBC、ALT、SCr、血钾、Lac、剩余碱和血PQ浓度均是影响APP患者90d生存的独立危险因素(均P<0.05)。含血PQ浓度的多因素Logistic回归分析显示,WBC、血钾和血PQ浓度是影响患者90d生存的独立危险因素,不含血PQ浓度的多因素Logistic回归分析显示,年龄、WBC、血钾和剩余碱是影响患者90d生存的独立危险因素(均P<0.05)。

2.3 决策树模型的构建:含血PQ浓度的决策树模型中,决策树共2层,4个终末节点,2个解释变量为血PQ浓度及血钾(图1)。树的首层根据血PQ浓

表3 130例APP患者90d预后的多因素
Logistic回归分析

项目	含血PQ浓度			项目	不含血PQ浓度		
	OR值	95%CI	P值		OR值	95%CI	P值
WBC	1.17	1.03~1.33	0.014	年龄	1.05	1.01~1.08	0.008
血钾	7.29	1.66~32.01	0.008	WBC	1.20	1.07~1.34	0.002
血PQ浓度	5.49	2.48~12.13	<0.001	血钾	3.12	1.01~9.66	0.049
剩余碱				剩余碱	1.41	1.16~1.72	0.001

度划分,提示血PQ浓度是患者90d预后的最佳预测因素。血PQ浓度≥1.6 ng/L时患者的生存概率为5.8%,<0.6 ng/L时患者的生存概率为97.3%。其次,血PQ浓度在0.6~1.6 ng/L时患者预后按血钾划分,血钾<3.4 mmol/L患者的生存概率为25.0%,血钾≥3.4 mmol/L时患者的生存概率为73.7%。不含血PQ浓度的决策树模型中,决策树共3层,4个终末节点,3个解释变量:WBC、剩余碱及年龄(图2)。树的首层根据WBC划分,WBC<10×10⁹/L时患者的生存概率为83.3%,≥10×10⁹/L时患者的生存概率为19.5%。其次,WBC≥10×10⁹/L的患者依据剩余碱划分,剩余碱<-4.1 mmol/L患者的生存概率为11.1%,≥-4.1 mmol/L时患者的生存概率为54.5%。再次,WBC≥10×10⁹/L且剩余碱≥-4.1 mmol/L的患者依据年龄划分,年龄≥52岁时患者的生存概率为11.1%,年龄<52岁时患者的生存概率为84.6%。

表1 不同预后两组APP患者一般资料的比较

组别	例数	性别(例)		年龄[岁, M(Q _L , Q _U)]	服毒至洗胃时间 [h, M(Q _L , Q _U)]	血液灌流 [例(%)]	WBC [×10 ⁹ /L, M(Q _L , Q _U)]	ALT [U/L, M(Q _L , Q _U)]
	(例)	女性	男性					
死亡组	74	31	43	42.5(26.0, 58.0)	1.0(1.0, 2.5)	71(95.9)	17.4(11.9, 23.1)	29.3(23.2, 40.3)
生存组	56	27	29	33.5(26.0, 47.8)	1.0(1.0, 1.5)	54(96.4)	8.9(7.0, 11.6)	25.3(21.2, 31.8)
χ^2/Z 值		0.520		2.260	0.640	0.020	6.780	2.780
P值		0.473		0.024	0.524	0.887	<0.001	0.005
组别	例数	SCr [μmol/L, M(Q _L , Q _U)]	血淀粉酶[U/L, M(Q _L , Q _U)]	血钾[mmol/L, M(Q _L , Q _U)]	PaO ₂ [mmHg, $\bar{x} \pm s$]	Lac [mmol/L, M(Q _L , Q _U)]	剩余碱[mmol/L, M(Q _L , Q _U)]	血PQ浓度[ng/L, M(Q _L , Q _U)]
(例)								
死亡组	74	91.0(72.5, 141.5)	97.5(67.5, 187.3)	3.2(2.8, 3.7)	91.1±11.1	7.1(3.7, 11.0)	-7.2(-10.9, -4.7)	2.9(1.9, 8.1)
生存组	56	64.0(53.0, 74.0)	98.5(69.0, 154.8)	3.7(3.5, 4.0)	94.5±9.2	2.5(1.4, 4.0)	-2.5(-4.2, -1.1)	0.3(0.1, 0.9)
Z/t值		5.520	0.380	5.440	1.900	6.450	6.560	8.670
P值		<0.001	0.702	<0.001	0.059	<0.001	<0.001	<0.001

注:1 mmHg≈0.133 kPa

表2 130例APP患者90d预后的单因素Logistic回归分析

项目	OR值	95%CI	P值	项目	OR值	95%CI	P值
年龄	1.03	1.01~1.05	0.018	血淀粉酶	1.00	0.99~1.00	0.107
男性	1.29	0.64~2.60	0.473	血钾	7.59	3.25~17.70	<0.001
服毒至洗胃时间	0.85	0.66~1.10	0.215	PaO ₂	0.97	0.94~1.00	0.062
血液灌流	0.88	0.14~4.43	0.887	Lac	1.64	1.35~1.99	<0.001
WBC	1.30	1.18~1.44	<0.001	剩余碱	1.51	1.29~1.76	<0.001
ALT	1.04	1.01~1.07	0.011	血PQ浓度	7.00	3.41~14.37	<0.001
SCr	1.02	1.01~1.04	<0.001				

注:OR为优势比,95%CI为95%可信区间

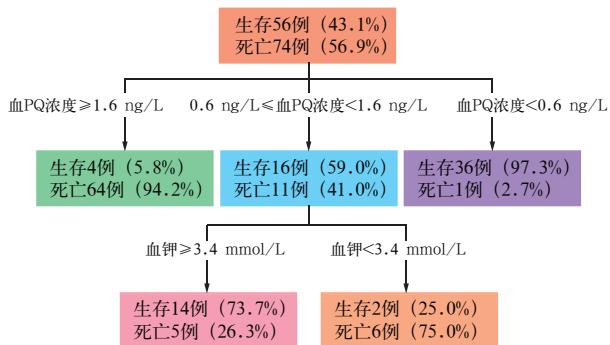


图 1 影响 APP 患者预后的决策树模型(含血 PQ 浓度)

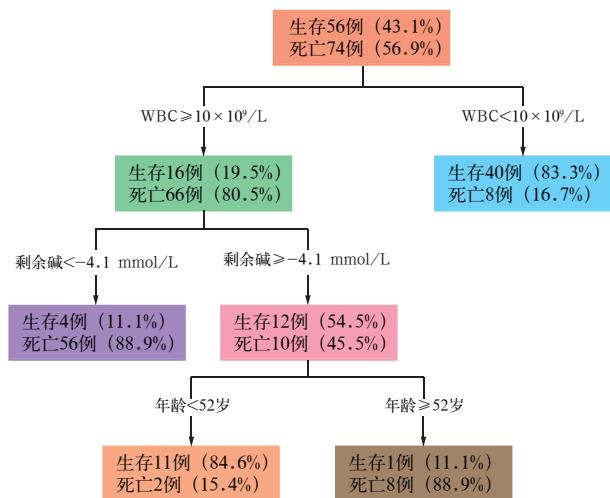


图 2 影响 APP 患者预后的决策树模型(不含血 PQ 浓度)

2.4 ROC 曲线分析(图 3): ROC 曲线分析显示,含血 PQ 浓度决策树模型的 $AUC=0.94$, $95\%CI$ 为 $0.89 \sim 0.98$, 敏感度为 91.9%, 特异度为 89.3%, 准确率为 90.0%。不含血 PQ 浓度决策树模型的 $AUC=0.89$, $95\%CI$ 为 $0.84 \sim 0.95$, 敏感度为 86.5%, 特异度为 91.1%, 准确率为 88.5%。Hanley & McNeil 法比较结果显示,两种决策树模型的 AUC 比较差异无统计学意义($Z=1.34$, $P=0.180$)。

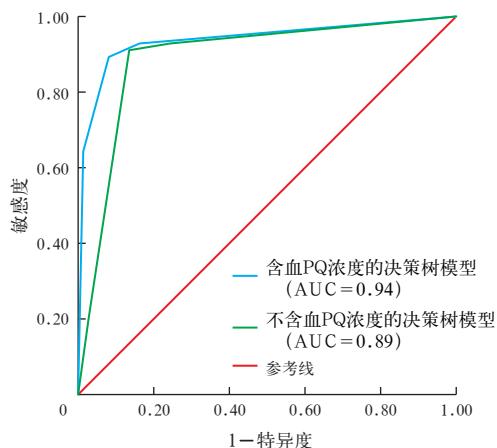


图 3 两种决策树模型预测 APP 患者预后的 ROC 曲线

3 讨论

决策树模型分析是一种分类和回归的计算机算法,决策过程以树状结构的图形呈现,并已应用于急诊中毒领域。Stoia 等^[8]报告决策树模型可预测制铅工人的职业性铅中毒风险。另一项研究表明,决策树模型预测成人血铅浓度升高的敏感度为 86.6%,特异度为 93.5%^[9]。此外,决策树模型可预测急性对乙酰氨基酚中毒患者的预后,其准确率为 84.8%^[10]。APP 患者的病死率高达 50%~80%^[11-13]。因此,早期准确预测患者预后对 APP 患者的临床决策非常重要。本研究旨在通过决策树分析为 APP 患者的预后评估开发一个易于使用的预测模型。

基于血 PQ 浓度及血钾的决策树模型显示,血 PQ 浓度是最重要的预测因子,并将血 PQ 浓度 $\geq 1.6 \text{ ng/L}$ 作为区分预后的阈值。既往研究显示,与血 PQ 浓度 $< 1.8 \text{ ng/L}$ 的患者相比,PQ 浓度 $\geq 1.8 \text{ ng/L}$ 的患者服毒量大,常伴代谢性酸中毒、少尿、纵膈气肿等^[14]。PQ 进入机体后迅速被吸收,血 PQ 浓度在服毒后 1 h 内达高峰后急剧下降^[15-16],PQ 的代谢特点符合 Gil 等^[17]研究的结论,高血 PQ 浓度预示患者死亡风险高,但低浓度并不预示患者生存,一些低血 PQ 浓度的患者仍存在死亡风险,这与本研究的模型特点一致。当血 PQ 浓度 $< 0.6 \text{ ng/L}$ 时,患者死亡风险低,而血 PQ 浓度在 $0.6 \sim 1.6 \text{ ng/L}$ 时,需要其他预测因素来评估患者的预后。低钾血症是 APP 患者常见的临床表现,其与钾离子肾小管重吸收减少、胃肠道流失增加及细胞内转移有关,在 APP 早期出现低钾血症的患者死亡风险高^[18]。

基于 WBC、剩余碱及年龄的决策树模型显示,WBC 是最重要的预测因子。Gao 等^[19]利用马尔可夫算法评估 APP 患者的危险因素与住院期间死亡风险的关联强度,WBC 有最强的关联强度值。最近一项包括 8 项研究纳入 980 例 APP 患者的 Meta 分析显示,WBC 高的患者死亡风险增加 18.6 倍^[20]。PQ 中毒后患者的炎症系统被激活^[21],白细胞是最早被释放并招募到损伤部位的免疫细胞。其次,PQ 中毒后机体的能量代谢受阻,体内无氧酵解导致酸性物质增多,约 50% 的患者在救治过程中出现代谢性酸中毒^[22]。Huang 等^[23]报告入院时剩余碱 $\leq -2.0 \text{ mmol/L}$ 的 PQ 中毒患者中,30.7% 的患者死亡;在 $-2.0 \sim -5.0 \text{ mmol/L}$ 的患者中,57.1% 的患者死亡;而 $\leq -5.0 \text{ mmol/L}$ 的患者中,病死率为 100%。虽然中毒严重程度是 PQ 中毒的主

要决定因素,但患者自身特点亦可影响PQ中毒患者的预后。老年患者血流量减少及肾功能下降可延迟PQ排泄,从而导致预后不良。一项以住院死亡为主要转归的研究结果显示,年龄每增加1岁,患者死亡风险增加1.04倍^[24]。

值得注意的是,除建立决策树模型的预测因素外,一些中毒症状、体征及实验室检查也与患者的预后相关。口服量在很大程度上决定PQ中毒的严重程度及临床预后^[25]。由于并非所有患者的电子病历均描述PQ的口服量,本研究未能提供患者PQ口服量的数据。PQ在肺内选择性积聚,产生氧自由基,造成膜损伤,最终导致呼吸窘迫^[26]。PQ可直接氧化损伤肾小管,伴急性肾损伤患者的死亡风险高于肾功能正常患者^[27-29]。Chen等^[30]研究的结果显示,Lac升高与APP患者的死亡风险升高有关,这与本研究的结果相似。

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