

Complementary data

Table S1: Demographic and clinical data for the 22 renal transplant patients

Age (years), median (range)	57.5 (25 – 76)	
Male/female, n/n	18/4	
Mycophenolate mofetil yes/no, n/n	12/10	
Creatinine clearance (mL/min), median (range)	45.7 (18.8 – 95.7)	
CMV serology +/-2, n/n	10/12	
	First blood sample after drug introduction	Blood sample at PK sampling
Hemoglobin concentration (g/L), median (range)	11.55 (7.85–13.7)	12.05 (9.29–15.6)
Platelets (10^9 /L), median (range)	198 (117–532)	204 (139 –337)
Lymphocytes (10^9 /L), median (range)	1.63 (0.35–5.44)	1.51 (0.28–3.59)
Neutrophils (10^9 /L), median (range)	5.31 (1.78–8.88)	3.85 (0.6 –8.04)

Table S2: Performance Analysis of ML Algorithms

ML algorithms	RMSE, mg.h/L	R ²	Relative MPE, %	Relative RMSE, %
XGBoost	0.83	0.99	0.032	1.30
Random forest	1.56	0.99	3.51	2.18
glmnet	4.23	0.96	-0.434	7.97
MARS	3.89	0.97	0.325	6.56
SVM	0.77	0.99	0.063	1.48

Values obtained after 10-fold cross-validation

Figure F1: Scatterplots of bias as a function of reference AUCss in the validation set

