

A PICTURE STORY

Tacrolimus: A Picture Story

— Our study, in which AI predicts drug levels,
explained simply with pictures —

AIForALab · CHA University

SCENE ONE

This medicine is called Tacrolimus

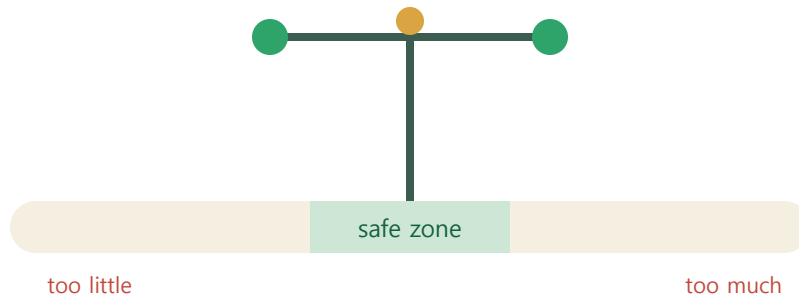


It is a medicine taken **every day** by people who have received an organ transplant (kidney, liver, and so on).

Our body mistakes the newly transplanted organ for a strange “**intruder**” and tries to attack it. Tacrolimus **calms** that attack so the new organ can settle in well.

SCENE TWO

The right amount is what matters



If there is **too much**, the kidneys can be harmed or side effects appear;
if there is **too little**, the body rejects the new organ.

So the drug level in the blood must be kept right inside a **narrow safe zone**.

SCENE THREE

But it differs from person to person

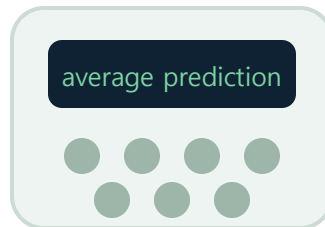


Even with the exact same dose, the blood level is **different for every person.**

Age, weight, genes, other medicines taken together... it varies for countless reasons. So **predicting “what will this patient’s level be next time?” in advance is very hard.**

SCENE FOUR

The method so far — the average calculator (PopPK)



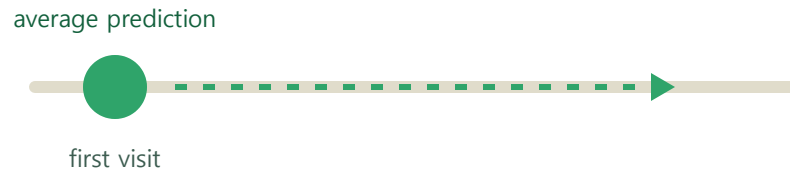
The traditional method (**population pharmacokinetics, PopPK**) calculates the level based on an “average patient.”

Upside: it can be used **right away, even for a brand-new patient.**

Downside: it **cannot capture that person’s individual differences** well.

SCENE FIVE

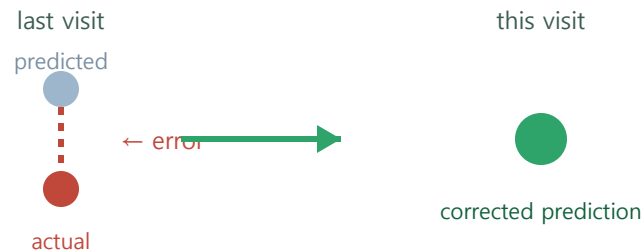
Our idea ① — start from the average



A brand-new patient **has no data of their own yet**. So we cannot build a personalized prediction.

So we took the **average prediction (DVI), which can be computed for anyone**, as a solid **starting point**.

Our idea ② — learning from the last error



From the second visit on, we get a clue: **“how far off was the prediction last time?”**

We look at this **last error (ERR_LAG1)** and gently nudge the next prediction. As visits pile up, it **gets closer to a personal fit.**

The key: there is no need to re-fit a complex model for each patient in advance. With just the past records, it personalizes itself.

SCENE SEVEN

Three AI friends lend a hand



LightGBM



RNN



LSTM

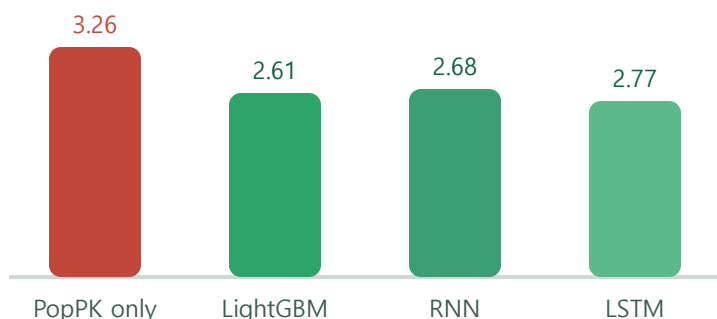
Three artificial-intelligence models read the patient's **past visit records** and predict the next level.

All of them use our idea — “average prediction + last error” — as their ingredients.

SCENE EIGHT

Result — combining the two fits better!

We compared **how far the predictions were off** from reality (the error — lower is better).



When we **combined the average prediction (PopPK) with AI**, all three models had **less error than PopPK alone**. Among them, **LightGBM** was the most accurate. 🏆

#1

LightGBM
most accurate

↓ 20%

error reduction
vs. baseline

109

outpatients
in the data

* Numbers are the prediction error (RMSE, ng/mL) — the lower the bar, the more accurate the prediction.

The most important clue? The last error!



★ #1

last error

When we opened up what the AI looked at to decide (a SHAP analysis), all three models picked **“the last error” as the most important clue.**

Remarkably, that error was on average **about a month old** — and it still mattered. This suggests a person’s “habit” can be **relatively stable between visits.**

So, what is good about it?

- ✓ It can be **applied right away**, even to a brand-new patient.
- ✓ As visit records pile up, it **gets closer to a personal fit**.
- ✓ It works **without** any complex per-patient re-computation.

A future we dream of: that one day, when a doctor decides the dose at the next visit, this prediction stands beside them as a **smart guide**.

Tacrolimus: A Picture Story · The End

Model-Informed AI for Tacrolimus Concentration Prediction Using Outpatient Data

Gyu Seong Lee · On Hu Park · Mi Kyong Shim* · Dae Keun Park* | CHA University · Seoul
National University Hospital data

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dkpark@cha.ac.kr · pharmsuni@cha.ac.kr