An AI-based Application for Personalized Pharmacokinetic Modeling and Adverse Effect Prediction

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***Abstract*— Conventional pharmacokinetic models often fail to account for significant inter-individual variability in drug response. This project proposes a system to address this limitation by integrating four key data sources: (1) traditional pharmacokinetic data, (2) user-provided biometric profiles, (3) subjective feedback on drug efficacy and adverse effects, and (4) bio-signals from wearable devices. Utilizing a machine learning model, the system aims to generate a personalized, time-series graph visualizing predicted drug effects and side effects. This will empower users to optimize medication timing and proactively manage their treatment. Furthermore, the aggregated, anonymized data holds significant potential to contribute to future pharmaceutical research and development.**

I. Introduction

A. Motivation

A significant challenge for individuals taking common medications, such as allergy relief, pain relievers, or antidepressants is the difficulty in predicting the onset, peak, and duration of therapeutic effects and side effects. For instance, an individual preparing for a critical task may need to precisely time their medication for peak cognitive performance, while a person with allergies must plan outdoor activities around the drug's effective window.

An individual's response to medication is highly dependent on a multitude of factors, including metabolism, physical condition, and other unique physiological traits. Consequently, standard dosage guidelines are often insufficient for optimizing an individual's quality of life. This project is motivated by the need to bridge this informational gap. We aim to develop a tool that leverages modern technology to provide users with a means for intelligent self-management of medication, tailored specifically to their bodies.

B. Problem Statement

The primary objective of this project is to develop a software solution that provides personalized predictions of drug efficacy and adverse effects. The core problems to be addressed are:

- The inability of generalized pharmacokinetic models to accurately predict drug responses for a specific individual.
- The lack of accessible tools for patients to track and anticipate their subjective experience with medication over time.
- The difficulty for patients in optimizing their dosing schedules to maximize therapeutic benefits while minimizing adverse effects.

C. Related Works

The existing landscape of digital health applications includes several categories of tools, though none fully address the problem stated above.

1. *Medication Reminder Applications:* Apps like MyTherapy and Medisafe are effective scheduling tools that help improve medication adherence. However, their functionality is limited to static reminders and they do not incorporate or predict the user's dynamic physiological response to the medication.
2. *Symptom Tracking and Health Monitoring Applications:* Tools such as Bearable allow users to manually log symptoms and moods, providing a retrospective view of their health. While valuable for tracking, they lack the integration of pharmacokinetic data and sensor-based bio-signals to offer predictive insights.
3. *AI-Driven Drug Response and Pharmacokinetic Modeling Tools:* Recent research and commercial platforms have explored the use of AI for drug response prediction. Some advanced research software, like Simcyp®, GastroPlus®, and Phoenix NLME, can model how drugs move through the body using detailed scientific equations; meanwhile, AI tools like pkCSM and Deep-PK that predict how drugs behave or whether they might cause toxicity. However, these solutions are research-oriented and designed primarily for scientists rather than for everyday use.

Our proposed system differentiates itself by creating a novel synthesis of these areas: it combines the scheduling utility of reminder apps, the subjective data logging of symptom trackers, and a predictive AI model powered by objective sensor data to deliver a forward-looking, personalized medication management tool.

D. Regulations of Health Apps in place, in Korea and the United State

South Korea and the United States have established regulatory systems for mobile health applications that incorporate AI, focusing particularly on those classified as Software as a Medical Device (SaMD). In both countries, software that performs clinical functions, such as diagnosis or treatment independently qualifies as a medical device and falls under the oversight of the national health authority (the Ministry of Food and Drug Safety [MFDS] in South Korea and the Food and Drug Administration [FDA] in the U.S.). While lower-risk apps, such as simple medication reminders or wellness trackers, may be exempt from strict regulation, tools that influence clinical decisions like AI models for pharmacokinetics or symptom forecasting typically require formal approval. In South Korea, the 2025 Digital Medical Products Act introduced clearer distinctions between digital therapeutic devices and wellness software, while in the U.S., the FDA continues to refine its AI/ML framework to accommodate adaptive algorithms that evolve post-deployment.

Both countries emphasize the importance of clinical validation, algorithmic transparency, and explainability, especially for higher-risk applications. The FDA has proposed mechanisms like predetermined change protocols and Good Machine Learning Practices (GMLP), and South Korea is similarly adjusting its policies to address AI-specific safety considerations. Despite structural differences, both regulatory environments aim to ensure that AI-based health applications are safe, effective, and appropriately classified based on their intended use and clinical impact.

Given the current regulatory landscapes in South Korea and the United States, our health application centered on AI-based personalized pharmacokinetic modeling and adverse effect prediction would likely be considered a Software as a Medical Device if it is intended to influence clinical decision making or guide treatment. While initial versions of the app that provide general wellness information, symptom tracking, or adherence support may fall into a lower risk category and be exempt from formal regulatory approval, any future versions that offer dose optimization, predictive alerts with clinical implications, or decision support functionality would require rigorous certification. This includes demonstrating clinical safety, effectiveness, and transparency of the AI model. In both countries, preparing for such certification entails early integration of Good Machine Learning Practices, explainability features, secure data management, and robust clinical validation protocols. Therefore, the app should be developed with a modular architecture, separating wellness oriented features from clinically influential components, allowing incremental deployment, and enabling a clear regulatory pathway for future expansion into medical grade functionality.

II. REQUIREMENTS

A. Functional Requirements

The system shall:

- **FR1. User Account Registration and Auth:** The system shall allow users to securely register, authenticate, and manage their account using email/password or third-party OAuth (e.g., Google, Apple) with multi-factor authentication support.
- **FR2. Medication Management:** Enable users to add, edit, and remove medications, including dosage and schedules.
- **FR3. Wearable Device Integration:** Interface with standard health data APIs (e.g., Google's Health Connect, Apple's HealthKit) to automatically sync sensor data such as heart rate, sleep patterns, and physical activity.
- **FR4. Subjective Feedback Logging:** Provide an intuitive interface for users to periodically log the perceived intensity of drug effects and side effects (e.g., on a 1-5 scale).
- **FR5. AI-Powered Prediction:** Process the integrated data through a machine learning model to generate a personalized time-series forecast of drug efficacy.
- **FR6. Data Visualization:** Display the prediction as an easy-to-understand graph showing the expected rise and fall of drug effects and side effects over time. Render an interactive, zoomable time-series graph displaying predicted efficacy, side-effect likelihood, and key events (e.g., dose intake, peak plasma time, alert thresholds).
- **FR7. Smart Notifications:** Provide users with intelligent alerts, such as recommending the optimal time for the next dose or providing a warning before a period of predicted high side effects.
- **FR8. Historical Data Import and Backup:** The system shall allow users to import prior medication logs, symptom data, or wearable health history from compatible formats (CSV, JSON, or API-based import) and back up all local data to a secure cloud repository.
- **FR9. Anonymized Research Data Export:** The system shall allow anonymized user data export to secure research servers, ensuring removal of personally identifiable information (PII) while retaining relevant pharmacological metrics.
- **FR10. Data Access and consent management:** The system shall include a dashboard for users to review, modify, or revoke data-sharing consents at any time, with clear visibility into which data categories are being used for model training or external research.
- **FR11. Emergency and safety alert:** The system shall detect and notify the user (and optionally a designated contact) in cases of abnormally high

predicted toxicity levels, anomalous vital signs, or adherence lapses suggesting possible medical risk.

- **FR12. Multilingual and accessibility support:** The system shall support multiple languages and accessibility standards (WCAG 2.1), providing localization for interface elements and voice-based interactions for visually impaired users.
- **FR13. Medication catalog and Search:** The system shall provide a searchable medication database with detailed pharmacokinetic parameters (e.g., Tmax, Cmax, half-life, mechanism of action), enabling users to select drugs from a pre-defined catalog or manually add custom entries.
- **FR14. Biometric and Health Profile Setup:** The system shall enable users to input and update biometric and health-related data, including age, sex, height, weight, known allergies, medical conditions, and concurrent medications.
- **FR15. Continuous Multi-Source Data Integration:** Support real-time aggregation of user-reported inputs (e.g. medication intake, symptom logs, side effects) with biometric streams from wearables (heart rate, sleep, activity, etc.) and other connected health devices (e.g. blood pressure cuffs, glucometers). The system should seamlessly fuse these data into a unified timeline for modeling.
- **FR16. Customization of alert Thresholds:** Enable users and clinicians to personalize alert settings. For instance, a risk-averse user might want notification at even low side-effect probability, whereas another might only want to be alerted for high-severity or high-probability events. The app's alert logic should be tunable to individual preferences and clinical guidance.
- **FR17. Biometric Trend Analysis and Baseline Tracking:** Establish a baseline profile for each user's normal biometric readings and symptom levels when off medication or stable. The app tracks long-term trends in these metrics (resting heart rate, sleep quality, mood, etc.) to distinguish drug-related changes from background variability. It can highlight gradual shifts over weeks that might indicate developing tolerance or health changes, supporting timely interventions.
- **FR18. Explainable AI Feedback:** To build trust, the app provides explanations for its predictions. When presenting a predicted side effect risk, the interface might indicate contributing factors (for example: "High dizziness risk predicted due to elevated heart rate and rapidly rising drug level"). The underlying AI model should thus be designed with interpretability in mind, offering users and clinicians insight into why a prediction is made.
- **FR19. Integration with health platforms:** To build trust, the app provides explanations for its predictions. When presenting a predicted side effect risk, the interface might indicate contributing factors (for example: "High dizziness risk predicted due to elevated heart rate and rapidly rising drug level"). The underlying AI model should thus be designed with interpretability in mind, offering users and clinicians insight into why a prediction is made.
- **FR20. Future Clinical Integration and Audit Trails:** Although not a certified medical device yet, design the system with future clinical integration in mind. This means maintaining a detailed audit log of data inputs, model outputs, and any adjustments made, which can be invaluable for validation studies or regulatory review down the line. The app's architecture should allow a "clinical mode" where health professionals can review the patient's data trends or override certain settings. In the long term, this foundation will support compliance with regulatory standards (FDA, EMA, etc.) if the app seeks approval as a clinical decision support or therapy tool.

B. Non-Functional Requirements

- **NFR1. Security:** All user data, particularly sensitive health information, must be encrypted both in transit and at rest.
- **NFR2. Privacy:** Data used for model training or research must be strictly anonymized, and the system must obtain explicit user consent for data collection and usage.
- **NFR3. Usability:** The user interface must be simple, intuitive, and require minimal effort to encourage consistent daily use.
- **NFR4. Reliability:** The application must be stable and ensure that critical functionalities, such as notifications, operate with high availability.

III. Sources

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