

Review Article

Artificial intelligence in precision pharmacotherapy: Transforming drug selection, dose optimization, and patient safety

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Abstract

Precision pharmacotherapy is focused on achieving maximum therapeutic effectiveness while minimizing adverse effects by using individualized treatment approaches. The current way of prescribing does not consider the differences between individuals in their ability to metabolize drugs, respond to medications, have genetic factors that influence their response to medications, have other medical conditions that may affect their response to medications, or have environmental influences that might affect their response to medications. The use of Artificial Intelligence (AI) through machine learning, deep learning, natural language processing, and predictive analytics to enhance personalized pharmacotherapy through decision-making based on large volumes of data is continuing to evolve. AI applications are used for drug selection, optimizing drug dosage, monitoring for adverse drug reactions, predicting adverse drug reactions, and monitoring patient safety by combining many different types of data including Electronic Health Records (EHRs), pharmacogenomics, biomarker data, and real-world evidence of patient outcomes. Although AI has become a valuable tool in the delivery of precision pharmacotechnology, barriers to implementing AI tools include algorithmic bias, privacy concerns, ethical issues, lack of transparency, and regulatory hurdles. This review will discuss the use of AI in the areas of drug selection, optimizing drug doses, and improving patient safety as well as other implementation-related challenges and future innovations in precision pharmacotherapy.

Keywords: Artificial intelligence, Precision pharmacotherapy, Personalized medicine, Machine learning, Dose optimization, Drug selection, Pharmacogenomics, Patient safety, Pharmacovigilance, Clinical decision support systems.

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1. Introduction

Precision pharmacotherapy is an emerging trend in clinical medicine that aims to develop treatment interventions tailored to the characteristics of each patient such as genetics, heterogeneity of disease, physiological characteristics, lifestyle factors, and environmental exposure.¹ This approach differs from the classic approach of prescribing “one size fits all” to each patient because it takes into account how individuals may respond to medications differently, which allows health care providers to provide personalized medications, recommend the proper dose, and maximize therapeutic benefits while minimizing side effects/effects caused by medications and treatment failures.² An increase in the number of chronic conditions, polypharmacy, and variability from patient to patient with their response to treatment has led to an increased need for specific pharmacological treatment for individuals.³ Variability in response to medications between individuals continues to present a broad problem for clinical pharmacology and health care services worldwide.

Major sources of variability between patients in response to medication result from differences between patients with regards to pharmacokinetics and pharmacodynamics. These differences greatly influence treatment outcome, frequently leading to non-therapeutic effectiveness or

adverse drug reactions.⁴ Polymorphisms in genes associated with drug biotransformation enzymes, transporters, and receptors, especially the cytochrome P450 enzyme system, have a far-reaching effect on the degree of therapeutic effectiveness that a patient receives from a prescribed medication, as well as the potential for a patient receiving an adverse effect from taking that medication.⁵ In addition to genetic polymorphisms affecting the pharmacokinetics and pharmacodynamics of medications, other factors affecting variability include patient age, sex, organ dysfunction, additional co-morbidities affecting the patient, individual dietary patterns, composition of their microbiome, and adherence to their prescribed medications.⁶

New advancements in precision medicine now allow physicians to use developments in all of these disciplines (i.e., genomics, transcriptomics, proteomics, and metabolomics) to make decisions when prescribing medication for their patients.⁷ Unfortunately, due to the rapid growth in biomedical data and the increasing complexity of analyzing it, there are currently not enough people with the requisite skills and training necessary to analyze this information effectively using traditional clinical methods, thus creating opportunities for more advanced computational methods to be developed.⁸ Artificial Intelligence (AI), with its many branches (e.g., Machine Learning [ML], Deep

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Learning [DL], Natural Language Processing [NLP], and predictive modeling using neural networks), is emerging as a new, destructive force that will revolutionize the delivery of precision pharmacotherapy via advanced methods of analyzing and interpreting large amounts of data.⁹ AI-based systems are able to analyze massive amounts of multidimensional data from sources including electronic health records, pharmacogenomic profiles, lab results, wearable devices, medical imaging systems, and real-world evidence to determine appropriate treatment therapies for patients.¹⁰

Using computational models driven by AI, prescribers will be able to select the most appropriate medication for their patient; provide individualized doses of medications; monitor patients for therapeutic drug levels and/or side effects; and, use data collected on patients from the aforementioned sources to predict the likelihood of patients developing side effects from medications.¹¹ AI-based clinical decision support systems will provide physicians with the information needed to determine the best treatment option for their patients based on the latest available medical research and studies, as well as various patient characteristics that change on a daily basis.¹²

Over the last few years, there has been considerable evidence supporting the use of AI technologies to improve the precision of pharmacotherapy in various therapeutic areas, including oncology, cardiovascular medicine, psychiatry, infectious diseases (HIV, etc.), diabetes management, and critical care pharmacology.¹³ Machine learning models have been developed for predicting individualized warfarin dosing regimens; insulin adjustment guidelines; antimicrobial stewardship programs; and predicting the efficacy of chemotherapeutic regimens, among other applications.^{14,15} Moreover, AI-based pharmacovigilance systems have significantly improved the early detection of medication-related adverse events through automated analyses of electronic databases and real-world patient data.¹⁶ However, despite these advances, there are several clinical barriers that limit the routine use of AI technologies in clinical pharmacotherapy. Challenges include transparency of algorithms, reproducibility of models, data privacy and security of patient records, ethical considerations of using AI to make treatment decisions, bias within training datasets, and lack of regulation of AI-assisted therapeutic decision-making.^{17,18}

In addition, the lack of transparency inherent in many machine learning models may decrease clinicians' confidence in these systems and may affect their acceptance of using AI systems in their practices.¹⁹ As computational intelligence becomes more integrated into the overall healthcare system, it is important to understand how AI will change the way drugs are selected, optimized, and made safe. Therefore, the purpose of this review is to review critically the evolving role of AI in advancing the precision of drug selection, optimizing dosing, and increasing patient safety while discussing current issues and limitations to AI's clinical application.²⁰

2. Overview of Artificial Intelligence Technologies in Pharmacotherapy

AI technologies represent a wide variety of computational technologies used for simulating cognitive abilities in humans, including the ability to learn, reason, make predictions, and develop a course of action appropriately.⁹ Today, the healthcare and drug-related uses of AI are receiving tremendous amounts of attention because these types of technologies are capable of processing complex, multidimensional sets of data from millions of sources, in order to deliver actionable clinical insights.³ As a result, precision pharmacotherapy is heavily reliant on sophisticated computational frameworks that can accommodate the increased volume of patient-specific information (e.g., pharmacogenomic data, clinical histories, laboratory results, and real-world therapeutic outcomes).⁸ The most proliferative form of AI used in pharmacotherapy is the use of Machine Learning (ML) to develop algorithms capable of discovering previously unknown relationships and predictive patterns within both structured and unstructured healthcare datasets without human programming.¹⁰ The continual improvement of the ML-based systems results in better accuracy for therapeutic recommendations by developing algorithms through an iterative process of exposure to the data.¹¹ Supervised ML models are typically employed for the prediction of therapeutic responses, adverse drug reactions, and individual drug dosages, while unsupervised learning methods are primarily used for patient stratification and disease classification/phenotyping purposes.¹²

Deep Learning (DL) refers to a specific type of machine learning that relies on and learns from artificial neural networks, and it has been proven to provide superior performance in terms of analyzing complex biomedical datasets.⁹ For instance, Deep Learning (DL) models are useful for analyzing imaging, genomic, and multidimensional clinical data sets because they can find subtle therapeutic patterns that traditional statistical tools cannot detect.¹³ In addition to predicting drug response variability and optimizing treatment plans, deep learning has been used in the area of pharmacotherapy by assessing risks associated with toxicities caused by medications.¹⁴ Natural Language Processing (NLP) is another form of Artificial Intelligence (AI) that allows computers to collect meaningful clinical data elements from unstructured text (e.g., physician notes, discharge summaries, pharmacovigilance reports, etc.) for the purposes of automation, such as automatically extracting medication-related data, identifying adverse drug events, and improving pharmacovigilance from real-world patient records.¹⁶ This type of automation not only enhances clinical decision-making but also reduces the documentation workload for healthcare providers.⁵ Furthermore, Clinical Decision Support Systems (CDSSs) that utilize AI technology are playing an increasingly large role in precision pharmacotherapy.¹¹ CDSSs use patient demographics, laboratory results, medication history, disease state, and pharmacogenomic factors to generate recommendations for evidence-based therapies.¹⁷ Clinicians can use AI-enabled CDSS platforms to identify potential drug interactions, contraindications, inappropriate prescriptions

and dosing modifications. This leads to improvement in medication safety and therapeutic outcomes.¹⁸

The efficacy of AI technologies applied to pharmacotherapy is highly reliant on the acquisition of large-scale, high-quality datasets. Collected datasets from electronic health records (EHRs), genomic repositories, wearables, biomedical imaging and real-world clinical evidence provide significant material for predictive modeling.⁷ The synchronization of multi-modal data sources has allowed for a more comprehensive understanding of variability in disease and individual responses to treatment.¹⁰ Moreover, cloud computing and high-performance computational capability have significantly expedited the practical application of AI-assisted therapeutic systems in healthcare settings.⁹

Although tremendous advancements have been made, the application of AI technologies for pharmacotherapy remains limited due to issues related to data quality; interoperability; model transparency; and, reproducibility.¹⁷ Most predictive algorithms behave as “black-boxes” — making clinical interpretation of results difficult.¹⁹ Therefore, there has been more emphasis placed on providing AI explainability models and algorithms to enhance clinician confidence in the use of these technologies and make it easier to implement them into clinical practice.¹⁸ AI technologies are rapidly transforming precision pharmacotherapy through the use of advanced data analytics, predictive therapeutic modeling, and tailored patient care techniques. By being incorporated into everyday clinical workflows, AI may improve the accuracy of therapy, decrease the likelihood of complications from medication use, and provide safer approaches to pharmacological interventions.^{9,11}

3. Artificial Intelligence in Drug Selection and Personalized Therapeutics

The selection of a medication is an important part of determining how well that medication works. Modern healthcare providers typically rely on standardized guidelines for prescribing, as well as science-based population data about treatment effects. However, this often masks the differences that exist between individuals when they take the same medication to treat the same medical condition.¹ Consequently, patients receiving the same medication often experience markedly different degrees of response in terms of overall effectiveness, side effects, and tolerability of the drugs.⁴ Artificial intelligence can be a useful avenue to address the limitations listed above and facilitate the selection of individualized drugs for a patient by using predictive analytical tools and precision medicine approaches.⁹

The core principle behind the AI-driven selection of therapies is multidimensional patient data used to create integrated databases. These data can include demographic information, disease severity, genomic data, metabolic sufficiency, comorbid conditions, previous medications taken, and biochemical characteristics of the patient.⁷ By applying machine learning methods to this diverse pool of patient data, researchers can better recognize shared characteristics between successful and unsuccessful responses to therapies and better identify the most appropriate

drug therapy for a given patient.¹⁰ The result of taking this individualized approach is higher rates of successful treatment while minimizing unnecessary exposure to ineffective or adverse medications.¹⁴ A large part of the advances in AI-assisted decision-making for drug therapies has come from incorporating pharmacogenomics into that decision-making process. Genetic variations (polymorphisms) are responsible for much of the variation in how patients respond to drugs after they are metabolized, transported, bind to receptors, or exert their pharmacological effects.⁵ Polymorphisms in cytochrome P450 enzymes (CYP2D6, CYP2C19, and CYP3A4) are responsible for much of the overall variability seen in patient responses to drug therapy.⁶

With the use of AI systems, pharmacogenomic information along with clinical information have allowed for the prescription of customized medication regimens based on the predicted direction that a patient will metabolize the medication, as well as how well the medication will work for the patient.²⁰ In oncology, using AI to guide the development of individualized treatment strategies or precision treatment has advanced rapidly.¹³ Utilizing machine learning, researchers have developed models to predict how well a tumour will respond to targeted therapies, immunotherapies, and chemotherapy based on the gene and biomarker analysis.¹⁴ These models allow for precision selection of medications while reducing the amount of toxicity associated with the empirical method of treating the individual.⁷

In addition, the use of AI in psychiatric pharmacotherapy has resulted in improved individualized selection of antidepressants and antipsychotics.¹⁵ Traditional methods of prescribing psychotropic medications are based on a trial-and-error approach, which leads to delayed response to treatment and an increased number of adverse effects.³ AI predictive modelling can evaluate clinical characteristics, genetic predisposition, and prior treatment responses assisting in optimizing drug selection and improving patient outcomes.¹⁶ In the area of infectious disease care, AI-assisted antimicrobial stewardship programs greatly enhance the use of precision therapeutics through the ability to predict pathogen susceptibility and antibiotic resistance patterns.¹¹ Researchers have developed machine learning models that quickly process microbiological, epidemiological, and clinical data to recommend the most appropriate antimicrobial regimen for a patient while simultaneously reducing inappropriate antibiotic use and the development of antimicrobial resistance.¹²

Additionally, AI can help with discovering new uses for old drugs through drug repurposing involving the identification of novel therapeutic indications for existing drugs.⁹ The use of AI to study molecular interactions, disease pathways, and real-world clinical data allows the identification of candidate drugs that may be repurposed for new therapeutic uses in clinical settings.¹⁰ This has the potential to decrease the time and expense associated with developing new drugs, while also enhancing therapeutic innovation.¹⁷ However, there are limitations associated with

the use of AI-assisted methods to select drugs. In particular, predictive models may have less predictive power when used with different patient populations than those used to train them, because of dataset bias and inadequate representation of patient populations in the training datasets.¹⁸ Patient consent, algorithmic transparency and fairness are also important ethical and practical issues associated with the use of AI in drug selection and discovery.¹⁹ The reliance upon computational recommendations for drug selection without appropriate clinical oversight can negatively impact clinical judgment by clinicians and limit their ability to provide patient-centered care.¹⁷

Despite these challenges, there is great promise for the use of AI-based personalized therapeutics to improve pharmacotherapy decisions. AI-based systems that incorporate information about an individual patient's biological and clinical characteristics could result in more effective, safer and individually tailored selection of drugs, thereby helping to advance the goals of precision pharmacotherapy.^{9,14}

4. AI-Assisted Dose Optimization in Precision Pharmacotherapy

In terms of pharmacotherapy, one of the most fundamental problems that exist with prescribing the correct dose to a patient arises from the fact that there are significant interindividual differences in how drugs are absorbed, distributed, metabolized and eliminated.⁴ Many standardized dosage regimens do not account for differences in physiology, genetics, pathology and environmental exposure; as a consequence, they expose patients to the possibility of treatment failure or adverse drug reactions.¹ At the same time, precision pharmacotherapy is attempting to address these issues by developing individualized dosing protocols; in addition, Artificial Intelligence (AI) has emerged as an extremely useful tool in providing better dose prediction and improved accuracy in delivering therapeutics.⁹ Dose optimization with AI tools is accomplished by developing a predictive computer model that will determine individualized medication doses based on patient-related characteristics.¹⁰ The computer models evaluate many different factors including age, weight, organ function, disease severity, PGx profile, concomitant medications, and laboratory parameters in order to create a personalized dosing recommendation for each individual patient.¹¹

The use of these types of technologies can improve therapeutic efficacy and reduce the risk of drug toxicity or medication-related complications.¹⁸ One of the most excellent examples of an application of AI tools in supporting dose optimization training is in the management of patients receiving warfarin; this drug is complicated by the fact that there is greater than normal inter-patient variability in the administration of this drug.¹⁴ The amount of warfarin that is required for each patient to achieve effective anticoagulation (or balance between preventing clots and causing bleeding) is largely influenced by factors such as age, diet, liver function, and the presence of genetic polymorphisms affecting CYP2C9 and VKORC1.⁵ Models using Machine Learning (ML) that include genetic and clinical data have outperformed

traditional methods of determining individualized warfarin (Coumadin) doses.²⁰

AI has provided extensive assistance for optimized insulin dosing in the management of diabetes as well.¹³ Those same AI-enabled systems using continuous glucose monitoring can estimate when there will be increases or decreases in blood sugar and suggest the need for dynamic adjustments in insulin dosages using real-time patient information.¹⁵ These types of technology can help decrease the chances of both hypoglycemia and hyperglycemia and help achieve improved glycemic control and compliance with treatment.¹⁶

For patients being treated with chemotherapy, AI-assisted dose optimization has allowed for safer delivery by utilizing toxicity risk, organ function, and treatment response data for individual patients.⁷ Predictive algorithms may assist the provider with optimizing the dosage of chemotherapeutic agents while minimizing adverse side effects.¹⁴ In addition, AI models have shown promise for the optimization of dosing of antimicrobials in critical care settings by employing Pharmacokinetic (PK) and Pharmacodynamic (PD) modeling.¹² AI integration has significantly impacted Therapeutic Drug Monitoring (TDM) as well.¹⁸ The use of traditional TDM is based on the use of laboratory data obtained intermittently via blood draws for the purpose of adjusting the dosage of the medication based on those data points. In contrast, AI-enabled TDM provides the ability to monitor the patient continuously, thus allowing the provider to make real-time adjustments to dosage based on predictive analytics.¹⁰ Therefore, the integration of AI to TDM increases dosage precision for medications with narrow therapeutic indices such as immunosuppressants, antiepileptics, and anticoagulants.¹¹

AI-guided dose optimization offers great promise but faces obstacles to implementation including limited standardization of datasets, the complexity of algorithms and a lack of clinical validation.¹⁷ The predictive accuracy of models may diminish significantly when applied, based on non-representative patient data, across the breadth of diverse healthcare environments.¹⁹ As well, both regulatory concerns and the reluctance of clinicians to utilize automated decision-making tools are barriers to wider-reaching implementation of AI-based dose optimization.¹⁸ Even so, advancements in AI-assisted dose optimization play a critical role in improving pharmacotherapy's efficacy/safety profile. AI systems can leverage and interpret rich, individual-level information about patients from clinical (direct and electronic health record), genomic and physiological sources to dramatically improve the precision of therapeutic drug use and reduce occurrence of negative drug effects as well as increase levels of patient safety.^{9,20}

5. Role of Artificial Intelligence in Pharmacogenomics and Biomarker-Guided Therapy

Pharmacogenomics is rapidly becoming an essential part of precision pharmacotherapy. It looks at how variations in genes influence responses to drugs, the efficacy of drugs, and intolerances to drugs.⁵ Overall, the differences between people regarding their gene encoding for drug

metabolizing enzymes, transporters, and receptors create a high degree of interpatient variability in the outcomes of drug therapies.⁶ When genetics is not considered when prescribing and/or treating, there is a greater chance of not achieving purposely prescribed therapy, experiencing adverse drug effects, or select an incorrect drug.¹ More and more, Artificial Intelligence (AI) is being added into pharmacogenomics so that the interpretation of large complex genomic information can be completed more efficiently and allow for personalized therapeutic interventions.⁹

AI-assisted pharmacogenomics apply machine or deep learning approaches to analyze multidimensional genomic data associated with predicting how an individual will respond to a drug.¹⁰ Computational models will analyze a tremendous amount of genomic data, far beyond the analytic capability of clinical professional or conventional statistical methods, and will identify patterns related to pharmacological responses.¹³ An integrated approach, combining genomic markers with clinical, biochemical, and environmental variables will allow AI systems to make personalized therapeutic recommendations and optimize therapeutic outcomes.²⁰ Polymorphisms in CYP450 enzymes (cytochrome P450) are one of the most important areas of pharmacogenomics that have a clinical impact.⁵ Variants of CYP2D6, CYP2C19, and CYP3A4 can greatly affect how drugs are metabolised and their bioavailability.⁶ AI algorithms that utilise genetic information can also divide patients into multiple different categories of metaboliser (i.e., poor, intermediate, extensive or ultra-rapid) to assist in finding the best drug, as well as find the appropriate dose to give.¹⁰ By using this approach, it is possible to reduce the incidence of adverse drug reactions and improve the efficacy of drugs, particularly for those with narrow therapeutic indices.¹⁸

In cardiovascular medicine, AI-assisted pharmacogenomic assessments have been used to optimise anticoagulant and antiplatelet therapy.¹⁴ Genetic differences in metabolism of warfarin and differences in activation of clopidogrel can account for significant variability in patient response.²⁰ Machine learning algorithms that incorporate both genomic and clinical data have the potential to improve personalised treatment choices and decrease drug-related complications.¹¹ Similarly, oncological pharmacogenomics has benefited significantly from AI-assisted guidance in selecting treatments based on biomarker-guided therapy.⁷ Tumour heterogeneity and molecular complexity complicate the determination of how best to treat an individual with cancer.¹³ AI models are capable of evaluating genomic sequencing information, molecular biomarkers, and tumour expression profiles to identify targeted therapies and predict their effectiveness.¹⁴ In this review we discuss AI-assisted pharmacogenomics that provides personalized treatment options with decreased toxicity levels associated with non-effective therapies.⁹ Psychotropic medications are representative of an application of AI-assisted pharmacogenomics.¹⁵ The response to antidepressants and antipsychotics is often affected by genetic differences that affect the mechanisms of neurotransmitter receptors and

drug metabolic enzymes.³ By utilizing machine learning systems to incorporate pharmacogenomic knowledge along with clinical data, clinicians may be aided in their medication selection by choosing medications that will have the greatest therapeutic effect while minimizing adverse side effects.¹⁶

Biomarkers using proteomics, metabolomics, transcriptomics, and inflammatory profiles also aid in the precision of pharmacotherapy.⁷ The ability to use AI technologies can be beneficial in interpreting complex biomarker data sets and identifying predictive treatment signatures for disease progression and response to treatment.¹⁰ In the management of chronic diseases such as diabetes, autoimmune disorders, and neurodegenerative disorders, the optimization of therapies using a biomarker-guided approach has the potential to improve treatment precision and long-term clinical outcomes.¹² However, there are major challenges that must be addressed prior to the implementation of AI-assisted pharmacogenomics into the clinic. Some limitations include barriers to access for genomic testing, the lack of standardized genomic databases, concerns regarding privacy of patient data, and a lack of representation of ethnic groups within training datasets.^{17,19} Additionally, there are ethical concerns associated with genetic discrimination and the process of obtaining informed consent which create further barriers to the clinical implementation of AI-assisted pharmacogenomics.¹⁸ However, integrating AI with pharmacogenomics and biomarker-guided treatment marks a major step forward in the movement toward personalized medicine. AI has the potential to interpret genomic and molecular information precisely, thereby providing safer and more effective treatment options and able to provide much more targeted approaches to treatment in pharmacology today than ever before.^{9,20}

6. Artificial Intelligence in Patient Safety and Pharmacovigilance

This has become increasingly important in light of the rise in complexity of medication regimens, polypharmacy, and ADRs.¹ Medication-related complications cause substantial morbidity, hospitalization, and costs to the global healthcare system.⁴ Conventional pharmacovigilance relies on spontaneous reporting systems to capture medication-related complications; however, these systems have limitations in terms of underreporting, delayed detection, and incomplete datasets.¹⁶ AI provides a new model for improving the safety of medications through enhanced pharmacovigilance, earlier detection of medication-related complications, and real-time monitoring of therapy.⁹ AI-based pharmacovigilance utilizes machine learning, natural language processing, and predictive analytics to detect ADRs from multiple types of data, including EHRs, insurance claims, biomedical literature, social media, and spontaneous reporting.¹⁵ By streamlining the process for identifying drug safety signals, these technologies can help improve the ability to conduct post-marketing surveillance.¹⁰

Natural Language Processing (NLP) has proven to have specific advantages in extracting medication-related information from unstructured narratives in clinical

documents and physician notes.¹⁶ Pharmacovigilance that uses traditional methods may miss clinically relevant information stored in free-text medical records.⁵ NLP techniques can automate identifying adverse drug reactions, medication errors, and treatment-related problems, which helps clinicians by automatically reducing their number of manual reviews and increasing their efficiency when reporting.¹⁵ Additionally, machine learning techniques have demonstrated effectiveness in forecasting patient-specific Adverse Drug Reaction (ADR) risk.¹¹ By utilizing a patient's demographic characteristics, laboratory results, medication history, pharmacogenomic profile(s), and coexisting medical condition(s), predictive algorithms can assist providers in identifying high-risk patients for developing toxicity before visible signs of toxicity present; thus, allowing timely interventions, alterations to dosing, and/or safe therapeutic management of these patients.²⁰

Examples of polypharmacy complications among older adults or critically ill patients further illustrate the importance of AI-based medication safety systems.³ AI-enabled decision support systems in clinical practice assist clinicians to identify potential drug-drug interactions, duplicate therapies, contraindicated medications, and inappropriate medication prescriptions.¹⁷ Alerts that automatically notify clinicians of safety-related issues may help clinicians reduce the number of medication errors and improve their prescribing practices through improved information flow.¹¹ Using AI-based systems in prescribing antimicrobials can support safe prescribing through the identification of trends in antibiotic resistance and applying antimicrobial stewardship.¹² Through predictive modeling, evidence-based antimicrobial classes are suggested while reducing the prevalence of inappropriate antibiotic prescriptions and minimizing the complications associated with the development of antimicrobial resistance.¹⁴

In oncology, the use of AI is expected to improve the safety of delivering chemotherapy by predicting treatment-related toxicity and helping the oncologist individualize the therapeutic monitoring for the patient.⁷ Through the integration of AI-enabled wearable technologies and remote patient monitoring systems, medication safety will be further enhanced by allowing for the ongoing monitoring of a patient's physiologic response to treatment.¹³ Real-time monitoring for useful information on a patient's vital signs, glucose concentration, cardiovascular indicators, and perceived compliance with their medication will allow for early identification of any adverse events and could lead to improving treatment outcomes.¹⁵

While much progress has been made in the use of AI in both Pharmacovigilance and Patient Safety, there continue to be challenges regarding the implementation of this technology due to the issues of heterogeneous data sources, lack of interoperability, algorithm transparency, and regulatory ambiguity.¹⁷ Additionally, false-positive safety signals, lack of proper validation, and undue reliance by healthcare providers on automated processes may negatively impact the reliability of AI technologies if not properly addressed.¹⁹ In addition to the issues mentioned above,

confidentiality and computer security are other factors that are impacting the greater adoption of AI technologies.¹⁸ Overall, there is great promise that AI Pharmacovigilance and Patient Safety systems will reduce the incidence of medication-related harm and improve treatment outcomes. Through real-time monitoring, predictive risk assessment, and automated safety detection, AI technologies could lead to improved quality and safety of pharmaco-therapeutic practice.^{9,20}

7. Clinical Applications of AI in Precision Pharmacotherapy across Therapeutic Areas

Utilizing artificial intelligence (AI) to enhance precision pharmacotherapy has been shown to have significant value across various types of therapies (e.g., oncology, cardiology) and improve clinical outcomes via tailored treatment strategies.⁹ Different specialties are now using AI-based tools (e.g., precision oncology and individualized treatment planning; anticoagulation management; etc.) increasingly regularly to help clinicians make more sensible therapeutic decisions.¹³ In oncology, the introduction of AI-based technologies for identifying the best therapeutic options via biomarker-guided treatment, optimizing chemotherapy regimens, and predicting patient response has changed the landscape of cancer pharmacotherapy.⁷ High-throughput genomic and molecular tumor profiling data can help physicians discover possible targeted therapies and predict resistance to therapy using machine learning-based algorithms.¹⁴

In addition to potentially improving survival rates, AI-enabled personalized treatment plans may greatly reduce unnecessary treatment-induced adverse effects.¹³ The incorporation of AI in the management of cardiovascular pharmacotherapy has similarly yielded substantial improvements; for example, through more effective management of anticoagulants and improved prediction of cardiovascular risk.²⁰ In particular, AI-assisted platforms help create more effective warfarin dosing regimens that take into consideration genetic and clinical data thus limiting the risk of bleeding and variability in treatment.¹⁴ In addition, AI-based predictive algorithms can improve engagement with patients and physicians to optimize antihypertensive/ lipid lowering medication regimens.¹¹ Similarly, in psychiatry, use of AI-based algorithms is helping clinicians select the most beneficial antidepressant and/or antipsychotic medications based on patient characteristics and treatment history.¹⁵ This can reduce both the need for trial-and-error prescribing and increase medication adherence.¹⁶

AI-assisted Pharmacotherapy, including its use in diabetes management, has emerged as a significant new area of application for AI in Healthcare. The integration of continuous glucose monitors with AI-driven insulin dosing prediction methods provides improved glycemic control and increased options for dynamically adjusting insulin doses.¹³ These advances improve individualization of therapy and decrease risks of hypoglycemic incidents.¹⁵ In addition, AI-based antimicrobial stewardship programs for infection management provide clinicians with individualized recommendations for antibiotic therapy based upon specific

pathogen resistance and susceptibility forecasting.¹² These AI applications offer improved precision and contribute to efforts to mitigate the growing issue of antimicrobial resistance.¹⁴

AI is also providing meaningful enhancements to Critical Care Pharmacotherapy through optimized dosing of antimicrobials, management of sedation in the critically ill patient population, and monitoring patient condition in a critical care setting.¹¹ Predictive modeling patients and their clinical response can aid a clinician's ability to modify treatments rapidly to respond to frequently changing patient condition.¹⁸ Although the application of AI technology to therapeutics is currently highly variable across all health care settings, the increasing utilization of AI technology within multiple therapeutic specialties confirms that AI will have a meaningful impact on how precision pharmacotherapy is administered in the future.^{9,20}

8. Challenges, Ethical Issues, and Regulatory Considerations

The implementation of Artificial Intelligence (AI) systems for precision pharmacotherapy has the potential to transform medication management and patient outcomes. However, several barriers including scientific, technical, ethical, and regulatory will continue to impede the routine application of these advanced tools in clinical practice.¹⁷ Although AI-based solutions have demonstrated powerful capabilities for optimizing drug selection, individualizing dosing and improving medication safety, serious concerns remain regarding the standards of: (1) algorithms' reliability, interpretability, and fairness; (2) healthcare delivery system integration.⁹

One of the greatest challenges inhibiting AI applications in pharmacotherapy relates to the availability and quality of data. As predictive accuracy and model training rely heavily on access to large volumes of high-quality, standardized data sets,¹⁰ the widespread use of Electronic Medical Records (EMRs) and other electronic health information systems across health care organizations has too often resulted in poorly understood and inconsistent datasets. Problems associated with data quality exist within healthcare databases (e.g., incomplete or inconsistent data due to data fragmentation, inaccurate clinical documentation, nonstandard terminology) can directly impair the performance of algorithms.¹⁵ Examples of insufficient representation of diverse racial and ethnic groups in the healthcare databases can result in biased recommendations for treatment and reduce predictive validity of therapeutic interventions among diverse populations.¹⁹

Ethically, algorithmic bias in AI-assisted healthcare is ongoing issue.¹⁷ Model training utilizes non-representative samples will contribute to reinforcement of ongoing disparities, including those related to ethnicity, socioeconomic status, age, and location, which create negative consequences for treating patients through recommending therapies¹⁹ and should therefore focus on creating fair, transparent, and representative AI development models so that people have equitable access to precision medicine.¹¹

Another major limitation of some advanced machine

learning and deep learning types of AI is the lack of ability to explain the rationale for predictive algorithms.⁹ Many AI systems are referred to as "black-box" systems in that they produce predictive ability without ability to explain how they came to arrive at their conclusion.¹⁹ This can create issues with clinician confidence in adopting these types of systems into clinical practice when clinicians are expected to be accountable for their prescribing decisions.¹⁷ Development of explainable Artificial Intelligence (XAI) frameworks will be a way to create greater transparency and provide greater physician confidence in AI-prescribing recommendations.¹⁸

Barriers in implementing Artificial Intelligence (AI) technologies include concerns over data privacy and cybersecurity.¹⁰ There is an increasing amount of sensitive patient data that is used to personalize treatment plans for patients, such as genetic data, biomarker profiles, past medication history, and electronic health records.⁵ If someone were to gain unauthorized access to a patient's Protected Health Information (PHI), or if there were to be a cybersecurity breach or misuse of that information, it could greatly decrease trust among the general public and lessen the degree of confidentiality between patients and their providers using AI-powered solutions.¹⁸ To ensure responsible usage of PHI, secure data encryption, a robust cybersecurity framework, and ethical governance mechanisms must be implemented.¹⁷

The regulatory uncertainty surrounding the implementation of AI technologies into pharmacotherapy creates additional challenges for adoption of these technologies.¹¹ AI algorithms are continuously changing as they learn from data-driven sources as opposed to traditional therapeutic interventions; this will require further complexities with how AI technologies are evaluated.¹⁸ Although there are frameworks currently established for drug safety and medical devices, none of them provide guidance for validating, holding accountable, or approving an adaptive AI technology.¹⁷ Regulatory bodies have begun to emphasize validating algorithms, reproducing algorithms, and monitoring algorithms post-deployment as means of ensuring patient safety and efficacy of clinical outcomes.²⁰

Professional responsibility and clinician autonomy should be scrutinized to determine how ethical these issues are.¹⁹ Overreliance on automated recommendations with insufficient human supervision may result in the loss of individualized patient care.¹ For this reason, AI should be used to support clinical decision making and not act as a substitute for clinician judgment.¹¹ To fully implement AI into practice, there must be collaboration between clinical practitioners, pharmacists, data scientists, authorities overseeing regulation, and the healthcare delivery system so that each discipline can be integrated into the care system in an equitable manner.⁹

There are still many hurdles to overcome, but as these hurdles continue to lessen through advancements in explainable AI, data governance, algorithmic transparency, and regulatory harmonization, it is likely that the adoption of AI-assisted precision pharmacotherapy will continue to grow in the coming years.^{17,18}

9. Future Perspectives of Artificial Intelligence in Precision Pharmacotherapy

Advancements within AI, predictive analytics and personalized medicine could significantly influence the future of precision pharmacotherapy.¹⁰

Improvements in computational speed, access to biomedical data, and digital healthcare infrastructure could enhance integration of AI into the routine development of therapeutic decisions.⁹ Developing the capability to utilize AI-assisted pharmacotherapy will offer highly individualised treatment protocols that optimise efficacy, reduce toxicity and improve all clinical outcomes for patients.²⁰

Another exciting area of future development is the use of digital twins in healthcare. Digital twins are virtual representations of patients created from multidimensional data from across the biological, physiological and clinical domains that simulate an individualised therapeutic response.¹³ AI-enhanced digital twins have the potential to aid in predicting drug efficacy and adverse effects, as well as progression of disease prior to therapy initiation, thereby improving therapeutic precision and reducing the level of clinical uncertainty.¹⁴

The application of multi-omics (genomics, proteomics, transcriptomics, metabolic and microbiological) will also provide future improvements to pharmacotherapy through the integration of AI technology.⁷ Future predictive models will combine multidimensional biological data with environmental/lifestyle factors to develop highly personalised therapeutic regimens.¹⁰ Such approaches would lead to improved disease stratification, biomarker-directed therapy, and the prediction of individualised patient responses to medications.¹²

One area that is being developed is using wearable technology and remote healthcare to increase therapeutic monitoring in real-time.¹⁵ Using wearables with Artificial Intelligence (AI) to monitor physiological indicators would allow for dose adjustments and early identification of side effects in real time.¹³ This type of monitoring will be beneficial for managing patients with chronic illness, monitoring cardiovascular health, the management of diabetes, and monitoring oncology therapies.¹⁶

AI will also significantly speed up the processes of drug development and repurposing of existing drugs.⁹ It is possible to use predictive computational models to help identify new drug targets, optimise the molecules' design, and move already approved drugs to treat new indications.¹⁷ If successful, these advances will reduce the cost and duration of drug development while providing more options for people with effective treatments.¹⁰

Finally, it is expected that future clinical decision support systems will have enhanced explainability, transparency, and interoperability with the healthcare environment.¹⁸ By incorporating frameworks of explainable AI, clinicians will be more likely to trust and use the systems in practice.¹⁹ An ongoing partnership between health systems, regulatory agencies, and technology developers is required to develop the necessary standards and ethical safeguards to ensure that AI is implemented effectively in practice.²⁰

Incorporating generative AI as well as advanced conversational clinical models could facilitate furthering pharmacotherapeutic decision-making by providing rapid synthesis of medical evidence with patient-specific therapeutic recommendations.¹¹ However, it remains essential to maintain scientific validity and minimize the risk of hallucination, with human oversight in place to ensure safe deployment.¹⁷ Overall, future developments may indicate that AI-assisted precision pharmacotherapy will gradually move from supplemental to primary tools used in clinical practice as part of routine health care provision. Through personalized treatment optimization, predictive safety monitoring, and evidence-based therapeutic decisions, AI could have a significant impact on the future of pharmacological practice.^{9,20}

10. Discussion

The advanced inclusion of AI in personalized medicines represents an important shift from the standard practice of prescribing based on the average characteristics of the entire population towards individualizing all aspects of pharmacotherapy.^{1,9} As cited throughout this review, current evidence indicates that AI applications like machine learning, artificial intelligence (AI), and natural language processing can greatly enhance accuracy in choosing medications, adjusting the dosage of those medications, and ensuring safe use of medications through the combination of complex, personalized information collected from each patient.^{10,11} In contrast to existing methods of prescribing medications, AI-assisted systems enable multidimensional analyses (using multiple dimensions) of the information generated from the following: pharmacogenomic profiling; patient history; biomarkers; and the patient's response to treatment, which increase both the precision with which we use medications and decrease the variability between patients in how they respond to medications.^{5,7}

A critical finding identified in the literature is the increasing application of AI to facilitate individualized medication selection and dosing when prescribing medications.^{14,20} The application of predictive computer models has been shown to have utility for individualized dosing of anticoagulants, insulin therapy, as well as for appropriate use of antibiotics, and for the use of chemotherapy.¹²⁻¹⁴ These examples demonstrate the capacity of AI technology to eliminate the trial-and-error approach to prescribing, to maximize the efficacy of medications, and to minimize the incidence of adverse drug effects, which continue to be a major concern in the practice of clinical pharmacology.^{4,16} A key area of emerging promise for precision medicines is the use of pharmacogenomics and biomarker-guided medicine.^{5,6} By exploiting the capabilities of AI, the interpretation of genomic and molecular datasets may lead to a greater understanding of the reasons for differences among patients in their response or adversely reacting to medication.¹⁰ Promising results have been seen in oncology and cardiology with the use of personalized biomarker-based and individualized dosing strategies.^{13,14} Those studies illustrate how increasing reliance on computational intelligence will enable patient-centered

pharmacological care.⁹

Nevertheless, there are still widespread barriers to implementing these advancements into actual practice according to the literature.¹⁷ Some of the main challenges to implementing AI in pharmacotherapy are the transparency of algorithms, bias in the training datasets used to develop the algorithms, concerns about patient's privacy, lack of interoperability between systems, and uncertainty regarding the regulatory landscape.^{18,19} The "black-box" nature of many of the algorithms creates uncertainty among clinicians as to the validity of the algorithms and as a result limits the potential of incorporating them into practice.¹⁷ The fact that many datasets do not accurately reflect the populations of patients being treated could also lead to injustice in drug delivery and create questions regarding the predictability of therapeutic results with real patient populations.¹⁸ This review indicates that AI should augment rather than replace clinician expertise in clinical decision-making.¹¹ For AI to be successfully integrated into practice, solid evidence of efficacy through validation studies, ethical safeguards, algorithm transparency, and collaboration among providers, pharmacologists, data scientists, and policymakers will all be required.^{17,20} Ongoing development of both explainable AI and real-time therapeutic monitoring technology may further improve the effectiveness of AI in providing precision pharmacotherapy and improving both patient safety and treatment outcome.¹⁸

The extensive body of evidence demonstrates that artificial intelligence (AI) has the potential to revolutionize modern pharmacotherapy by creating opportunities for personalized therapeutic optimization. Successful incorporation of AI into daily practice depends on balancing innovative technology with ethical dilemmas, regulatory management, and clinical judgement.^{9,17}

11. Conclusion

In conclusion, it is well documented that AI has become a major driver of precision pharmacotherapy by creating incredible opportunities for individual therapeutic interventions and improved outcomes.⁹ With the use of machine learning, deep learning, natural language processing, and predictive analysis, AI systems enable a variety of ways to personalize medications through: (1) selecting the optimal medication; (2) titrating the optimal dose; (3) using biomarkers to identify the best therapy; and (4) enhancing safety for patients.¹⁰ AI systems analyze large, multiple dimension datasets such as pharmacogenomics, electronic health records and real-world outcomes, to create the most accurate and evidence-based medical decisions.⁷ The use of AI across multiple therapy areas (e.g., oncology, cardiology, psychiatry, infectious disease and diabetes) exemplifies the broad applicability of AI for increasing the precision of therapy and decreasing the likelihood of adverse events.^{13,14} Additionally, AI pharmacovigilance and medication safety systems will facilitate early detection of adverse events, predict future risks, and optimize pharmacotherapeutic outcomes.¹⁶

While these benefits are clear there are still numerous challenges that impinge on the ability to achieve broader

application of clinically. There are many ethical considerations related to algorithmic bias, data privacy, interoperability, transparency, regulatory ambiguity and ethical considerations and all should be considered carefully.¹⁷⁻¹⁹ The successful incorporation of AI technology into pharmacotherapy will require proper validation, explicable computational models, standardized regulatory systems and cooperation among all stakeholders involved (clinicians, pharmacologists, policy makers and data scientists).²⁰ Ultimately, AI should serve an important role in the development of superior precision pharmacotherapy by enabling safer, more effective and highly individualised treatment options. As the evolution of computation technologies continues to evolve and is responsibly incorporated into clinical practice, it may change how we develop pharmacology services and contribute greatly towards patient-centred precision medicine.^{9,20}

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13. Conflict of Interest

None.

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