Zoology and Allied Sciences Letters
Content Available at www.lapinpress.com ISSN (O): 3139-5155
(An online peer reviewed Referred Journal)

Review Article
OPEN ACCESS

AI-DRIVEN SYSTEMS PHARMACOLOGY AND DIGITAL TWINS IN PRECISION MEDICINE: TRANSFORMING DRUG RESPONSE PREDICTION, TOXICITY PROFILING, AND THERAPEUTIC OPTIMIZATION

NERELLA MOUNIKA

Assistant Professor, Department of Pharmacology, School of Pharmacy, Anurag University, Venkatapur, Ghatkesar, Hyderabad, Telangana, India-500 088.

***Corresponding Author**
Dr. Nerella Mounika

Article History: Received: 24 Jan 2026, Revised: 19 Feb 2026, Accepted: 14 Mar 2026

Abstract: AI-driven systems pharmacology combined with digital twin technology is emerging as a transformative framework in precision medicine, enabling highly accurate prediction of drug response, toxicity profiling, and therapeutic optimization. Traditional pharmacological approaches often fail to account for inter-individual variability in genetics, environment, and disease heterogeneity, leading to unpredictable therapeutic outcomes and adverse drug reactions. Systems pharmacology integrates multi-scale biological data, including genomic, proteomic, metabolomic, and clinical datasets, to model complex drug–target–disease interactions. The incorporation of Artificial Intelligence (AI), particularly machine learning, deep learning, and network-based modeling, enhances the predictive capacity of these systems by identifying nonlinear relationships within high-dimensional biological datasets. Digital twins-virtual, dynamic representations of individual patients-extend this paradigm by simulating patient-specific biological systems in silico. These models enable continuous monitoring and prediction of drug efficacy, toxicity risks, and disease progression in real time. AI-powered digital twins integrate real-world patient data with mechanistic and statistical models to optimize therapeutic strategies before clinical application. This review explores the convergence of AI, systems pharmacology, and digital twin technology in modern precision medicine. It highlights their applications in pharmacokinetics/pharmacodynamics (PK/PD) modeling, adverse drug reaction prediction, oncology, cardiovascular disease, and neuropharmacology. Additionally, it discusses challenges such as data heterogeneity, model interpretability, computational demands, and ethical concerns surrounding patient-specific digital modeling. The integration of AI-driven systems pharmacology with digital twins represents a paradigm shift from population-based medicine to individualized predictive therapeutics, paving the way for next-generation intelligent healthcare systems.

Keywords: *Artificial Intelligence; Systems Pharmacology; Digital Twins; Precision Medicine; Drug Response Prediction; Toxicity Profiling.*

This article is licensed under a Creative Commons Attribution-Non-commercial 4.0 International License.
Copyright © 2026 Author(s) retains the copyright of this article.

1. INTRODUCTION

Precision medicine aims to tailor therapeutic interventions based on individual variability in genes, environment, and lifestyle. Despite advancements in pharmacogenomics and biomarker discovery, clinical outcomes remain inconsistent due to the complexity of biological systems and drug interactions.

Systems pharmacology has emerged as a holistic discipline that integrates pharmacology, systems biology, and computational modeling to understand drug actions at multiple biological scales. However, classical models are limited in handling nonlinear interactions and large-scale heterogeneous datasets.

Artificial Intelligence (AI) enhances systems pharmacology by enabling:

- Pattern recognition in complex biological networks
- Prediction of drug–target interactions
- Simulation of pharmacological responses
- Integration of multi-omics datasets

Digital twins further extend this framework by creating **real-time, patient-specific computational replicas** that simulate biological behavior under different therapeutic scenarios [1].

Together, AI-driven systems pharmacology and digital twins are redefining precision medicine as a predictive, adaptive, and continuously learning system.

2. EVOLUTION OF SYSTEMS PHARMACOLOGY TO AI-DRIVEN PRECISION MEDICINE

The evolution of this field can be categorized into four stages:

2.1 Classical Pharmacology Era

- Single-target drug hypothesis
- Population-based clinical trials
- Empirical dose optimization

2.2 Systems Biology Era

- Network modeling of biological pathways
- Multi-target drug understanding

2.3 Computational Systems Pharmacology Era

- PK/PD modeling
- Mathematical simulation of drug response

2.4 AI and Digital Twin Era

- Machine learning-based prediction
- Real-time patient simulation
- Adaptive therapeutic optimization [2].

3. FOUNDATIONS OF SYSTEMS PHARMACOLOGY

Systems pharmacology integrates multiple biological layers:

- Molecular interactions (drug–target binding)
- Cellular signaling pathways
- Tissue-level responses
- Organ-level pharmacodynamics
- Whole-body pharmacokinetics

This multi-scale integration is essential for understanding complex drug effects Table 01.

Table 01: Multi-Scale Structure of Systems Pharmacology

Biological Level	Data Type	Modeling Approach	Outcome
Molecular	Protein–ligand interactions	Docking + ML	Binding prediction
Cellular	Gene expression	Network models	Pathway regulation
Tissue	Metabolic flux	Differential equations	Functional response
Organ	PK/PD data	Compartment models	Drug distribution
Whole body	Clinical data	AI systems	Treatment outcome

4. ARTIFICIAL INTELLIGENCE IN SYSTEMS PHARMACOLOGY

AI enhances systems pharmacology through advanced computational techniques.

4.1 Machine Learning in Drug Response Prediction

Machine learning models predict:

- Drug efficacy
- Dose-response relationships
- Patient-specific sensitivity

Algorithms used include:

- Random Forest
- Support Vector Machines
- Gradient Boosting Machines

4.2 Deep Learning for Biological Network Analysis

Deep learning enables:

- Identification of hidden pathway interactions
- Prediction of gene–drug associations
- Modeling nonlinear pharmacological responses

Graph Neural Networks (GNNs) are especially effective in biological network representation [3].

4.3 Reinforcement Learning in Therapeutic Optimization

Reinforcement learning (RL) is used to:

- Optimize drug dosing strategies
- Adapt treatments dynamically
- Simulate clinical decision-making

4.4 Natural Language Processing (NLP)

NLP extracts knowledge from:

- Clinical records
- Biomedical literature
- Electronic health records (EHRs)

This supports continuous learning in systems pharmacology models [4].

5. DIGITAL TWIN CONCEPT IN PRECISION MEDICINE

A digital twin is a computational replica of a physical patient system that evolves in real time using incoming data.

5.1 Architecture of Digital Twins

Digital twin systems consist of:

- Data acquisition layer (wearables, EHRs)
- Modeling layer (AI + mechanistic models)
- Simulation engine
- Feedback optimization loop

5.2 Functional Capabilities

Digital twins enable:

- Real-time disease monitoring
- Drug response prediction
- Toxicity risk simulation
- Treatment personalization

5.3 Types of Digital Twins in Healthcare

- Patient-level digital twins
- Organ-level twins (heart, liver, brain)
- Disease-specific twins
- Population-level twins Table 02 [5].

Table 02: Digital Twin Applications in Medicine

Type	Application	AI Role	Outcome
Cardiac twin	Heart failure prediction	ML + simulation	Risk reduction
Oncology twin	Tumor progression modeling	Deep learning	Therapy optimization
Liver twin	Drug metabolism prediction	PK modeling	Toxicity prevention
Brain twin	Neurodegenerative diseases	Network AI	Cognitive decline prediction

6. INTEGRATION OF AI AND DIGITAL TWINS IN SYSTEMS PHARMACOLOGY

AI and digital twins are interconnected in modern precision medicine.

6.1 Data Integration Pipeline

1. Patient data collection
2. AI-based preprocessing
3. Systems pharmacology modeling
4. Digital twin simulation
5. Treatment recommendation
6. Continuous feedback learning

6.2 AI-Enhanced Simulation Models

AI improves simulation accuracy by:

- Learning from real-world data
- Updating predictive parameters dynamically
- Reducing computational uncertainty

6.3 Closed-Loop Therapeutic Systems

Digital twins enable closed-loop medicine where:

- Treatment is continuously optimized
- Drug dosage is dynamically adjusted

- Adverse effects are predicted before occurrence

7. DRUG RESPONSE PREDICTION USING AI SYSTEMS

Drug response variability is one of the major challenges in clinical pharmacology [6].

7.1 Genetic Influence Modeling

AI models incorporate:

- SNP variations
- Gene expression profiles
- Epigenetic markers to predict drug sensitivity.

7.2 Disease-Specific Response Prediction

AI systems classify patients into:

- Responders
- Non-responders
- Toxic responders

based on biological signatures.

7.3 Multi-Drug Interaction Prediction

AI identifies:

- Synergistic drug effects
- Antagonistic combinations
- Metabolic competition risks

8. AI IN TOXICITY PROFILING AND SAFETY PREDICTION

One of the most critical challenges in drug development is the early prediction of toxicity. Nearly 30–40% of drug failures in clinical trials are due to unexpected toxic effects. AI-driven systems pharmacology significantly improves safety assessment by integrating molecular, cellular and clinical toxicity signals [6].

8.1 Computational Toxicology Frameworks

AI-based toxicity prediction models typically integrate:

- Chemical structure descriptors
- Biological pathway data
- Gene expression profiles
- Clinical adverse event records

Machine learning models identify toxicity signatures before experimental validation.

8.2 Types of Toxicity Predicted by AI

(a) Hepatotoxicity

AI models simulate liver metabolism using enzyme interaction networks, particularly cytochrome P450 pathways.

(b) Cardiotoxicity

Deep learning systems predict QT interval prolongation and ion channel disruption.

(c) Nephrotoxicity

Systems pharmacology models assess renal clearance and tubular accumulation risk.

(d) Immunotoxicity

AI detects cytokine storm risk and immune overactivation.

8.3 Deep Learning for Toxicity Classification [7].

Deep neural networks analyze:

- SMILES molecular representations
- Protein interaction networks
- Transcriptomic toxicity signatures

Graph Neural Networks (GNNs) are especially effective in predicting structural toxicity patterns.

8.4 Predictive Toxicology Pipeline

1. Compound encoding
2. Multi-omics integration
3. Toxicity scoring model
4. Pathway disruption analysis
5. Risk classification Table 03.

Table 03: AI-Based Toxicity Prediction Models

Toxicity Type	AI Method	Biological Marker	Outcome
Hepatotoxicity	ML + PK modeling	ALT/AST elevation pathways	Early liver risk detection
Cardiotoxicity	Deep learning	Ion channel genes	Arrhythmia prediction

Nephrotoxicity	Systems pharmacology	Renal transporter proteins	Kidney injury risk
Immunotoxicity	Network AI	Cytokine signaling	Immune overactivation

9. DIGITAL TWINS IN ORGAN-SPECIFIC MODELING

Digital twins enable organ-level simulation of drug effects with high biological fidelity [8].

9.1 Cardiac Digital Twins

Cardiac twins simulate:

- Electrical conduction
- Myocardial contraction
- Blood flow dynamics

Applications:

- Arrhythmia prediction
- Heart failure progression modeling
- Drug-induced QT prolongation detection

AI continuously updates cardiac behavior using ECG and imaging data.

9.2 Liver Digital Twins

The liver is central to drug metabolism [9].

Functions of liver twins:

- Predict first-pass metabolism
- Simulate enzyme induction/inhibition
- Assess hepatotoxicity risk

Machine learning models simulate CYP450 enzyme interactions for precise metabolic prediction [10].

9.3 Kidney Digital Twins

Kidney twins model:

- Glomerular filtration rate (GFR)
- Tubular secretion
- Drug clearance dynamics

They are critical in nephrotoxic drug dose adjustment.

9.4 Brain Digital Twins

Brain twins are used in:

- Neurodegenerative disease modeling
- Blood–brain barrier permeability prediction
- Neuropharmacological response simulation

They integrate EEG, MRI, and molecular data.

9.5 Multi-Organ Digital Twin Systems

Advanced systems integrate multiple organ twins into a **whole-body physiological model**, enabling:

- Systemic drug interaction simulation
- Whole-body toxicity prediction
- Multi-organ disease modelling [11].

10. AI IN PHARMACOKINETICS AND PHARMACODYNAMICS (PK/PD)

PK/PD modeling is central to drug response prediction.

10.1 AI-Enhanced Pharmacokinetics

AI models predict:

- Absorption rates
- Distribution volumes
- Metabolic pathways
- Excretion kinetics

Machine learning improves parameter estimation from sparse clinical data [12].

10.2 Pharmacodynamics Modeling

AI assists in:

- Dose-response curve prediction
- Receptor occupancy modeling
- Therapeutic window estimation

10.3 Reinforcement Learning in Dose Optimization

Reinforcement learning systems:

- Adjust dosage dynamically

- Minimize toxicity risk
- Maximize therapeutic efficacy

This creates adaptive treatment systems.

11. SYSTEMS PHARMACOLOGY NETWORKS [13].

Systems pharmacology relies heavily on biological network modeling.

11.1 Drug–Target Networks

AI constructs networks linking:

- Drugs
- Proteins
- Genes
- Diseases

This enables identification of multi-target therapies.

11.2 Disease Module Identification [15].

AI detects clusters of genes associated with specific diseases, allowing:

- Target prioritization
- Drug repositioning
- Pathway-level intervention

11.3 Multi-Layer Biological Networks

These include:

- Protein–protein interaction networks
- Gene regulatory networks
- Metabolic networks

Graph-based AI models integrate these layers Table 04.

Table 04: Systems Pharmacology Network Components

Network Type	Nodes	AI Role	Application
Drug–target network	Drugs + proteins	Link prediction	Drug discovery
Gene network	Genes	Clustering AI	Disease modeling
Metabolic network	Metabolites	Graph AI	Pathway analysis
Disease network	Diseases	Pattern recognition	Drug repositioning

12. CASE STUDIES IN AI-DRIVEN SYSTEMS PHARMACOLOGY

12.1 Oncology Precision Modeling

AI systems have been used to:

- Predict chemotherapy response
- Optimize immunotherapy combinations
- Model tumor heterogeneity

Digital twins simulate tumor evolution under treatment pressure [16].

12.2 Cardiovascular Disease Modeling

AI-driven heart twins predict:

- Myocardial infarction risk
- Drug-induced arrhythmias
- Long-term cardiac remodeling

12.3 COVID-19 Drug Response Modeling

During the pandemic, AI systems pharmacology was used to:

- Predict antiviral drug combinations
- Model cytokine storm pathways
- Simulate patient-specific immune responses

12.4 Neurological Disorder Simulation

Applications include:

- Alzheimer's disease progression modeling
- Parkinson's disease dopaminergic pathway simulation
- Personalized neurodrug response prediction

13. ADVANCED AI ARCHITECTURES IN SYSTEMS PHARMACOLOGY AND DIGITAL TWINS

The evolution of AI has introduced highly sophisticated architectures that significantly enhance systems pharmacology modeling and digital twin development [17].

13.1 Transformer Models in Biomedical Systems

Transformer architectures, originally developed for natural language processing, are now widely applied in precision medicine.

Applications:

- Drug–target interaction prediction
- Protein structure-function modeling
- Clinical text mining from EHRs
- Multi-omics integration

Transformers excel at capturing long-range dependencies in biological sequences, enabling superior predictive performance compared to traditional ML models.

13.2 GRAPH NEURAL NETWORKS (GNNS)

GNNs are fundamental in modeling biological systems because:

- Genes, proteins, and drugs form network structures
- Biological pathways are inherently graph-based

Applications:

- Drug repurposing
- Disease module detection
- Toxicity pathway analysis
- Multi-target drug prediction [18].

13.3 Federated Learning in Precision Medicine

Federated learning enables AI model training without sharing sensitive patient data.

Key Advantages:

- Preserves patient privacy
- Enables multi-hospital collaboration
- Reduces data security risks

This is particularly important for digital twin ecosystems that rely on real patient data.

13.4 Generative AI for Drug Optimization

Generative AI systems (GANs, VAEs, diffusion models) are used to:

- Design novel drug candidates
- Optimize pharmacokinetic properties
- Reduce toxicity profiles
- Generate personalized drug molecules

This allows **on-demand therapeutic design** tailored to digital twin predictions [19].

14. CLINICAL TRANSLATION OF DIGITAL TWINS

The transition from computational models to clinical practice is a critical step in precision medicine.

14.1 Real-Time Clinical Decision Support

Digital twins integrate with hospital systems to provide:

- Treatment recommendations
- Risk alerts for toxicity
- Dynamic dosage adjustments

14.2 Integration with Electronic Health Records (EHRs)

AI systems continuously update digital twins using:

- Laboratory reports
- Imaging data
- Medication history
- Genomic profiles

14.3 Wearable Device Integration [20].

Real-time physiological data is collected using:

- Smartwatches
- ECG patches
- Glucose monitors
- Blood pressure sensors

This enables continuous digital twin updating.

14.4 Hospital-Based Digital Twin Platforms

Hospitals are developing integrated platforms that:

- Simulate patient response before treatment
- Predict ICU deterioration risk
- Optimize drug regimens in real time

15. ETHICAL, LEGAL, AND REGULATORY CHALLENGES

Despite its promise, AI-driven systems pharmacology raises significant ethical concerns [22].

15.1 Patient Data Privacy

Digital twins require continuous patient data flow, raising concerns about:

- Data confidentiality
- Unauthorized access
- Cybersecurity threats

15.2 Algorithmic Bias

AI systems may inherit bias from training datasets, leading to:

- Unequal treatment predictions
- Reduced accuracy in underrepresented populations

15.3 Accountability in AI-Driven Decisions

Key issue:

- Who is responsible if AI-based recommendations fail?

This includes clinicians, developers, or institutions.

15.4 Regulatory Framework Gaps

Current regulatory systems are not fully adapted for:

- Self-learning AI models
- Continuously evolving digital twins
- Autonomous decision systems

Table 05: Ethical Challenges and Mitigation Strategies

Challenge	Risk	Mitigation Strategy
Data privacy	Breach of patient records	Federated learning + encryption
Algorithm bias	Unequal predictions	Balanced datasets + fairness algorithms
Lack of transparency	Black-box models	Explainable AI (XAI)
Regulatory gaps	Approval delays	AI-specific guidelines
Liability issues	Legal uncertainty	Shared accountability frameworks

16. FUTURE PERSPECTIVES OF AI-DRIVEN SYSTEMS PHARMACOLOGY [23].

The future of this field is highly transformative and will redefine healthcare systems globally.

16.1 Autonomous Digital Twin Ecosystems

Future systems will:

- Self-learn from real-time patient data
- Automatically adjust treatment protocols
- Predict disease progression continuously

16.2 Fully Integrated Multi-Organ Simulations

Whole-body digital twins will simulate:

- Cardiovascular system
- Nervous system
- Metabolic pathways
- Immune responses in a unified computational model.

16.3 AI-Driven Preventive Medicine

Instead of treating diseases, AI systems will:

- Predict disease onset years in advance
- Recommend preventive interventions
- Monitor risk continuously

16.4 Global Health Digital Twin Networks

Population-scale digital twins will:

- Simulate disease outbreaks
- Model drug response variability across populations
- Optimize public health strategies

16.5 Quantum AI in Systems Pharmacology

Future integration may include:

- Quantum computing for molecular simulation
- Ultra-fast biological network modeling
- Complex protein folding prediction

17. CONCLUSION

AI-driven systems pharmacology combined with digital twin technology represents a fundamental paradigm shift in precision medicine. Unlike traditional pharmacological models that rely on static population averages, this integrated approach enables dynamic, patient-specific modeling of drug response, toxicity risk, and therapeutic outcomes. By incorporating machine learning, deep learning, graph-based modeling, and reinforcement learning, systems pharmacology evolves into a predictive science capable of decoding complex biological interactions across multiple scales. Digital twins further extend this capability by providing continuously updated virtual replicas of individual patients, enabling real-time therapeutic optimization. Despite significant progress, challenges such as data heterogeneity, interpretability limitations, regulatory gaps, and ethical concerns must be addressed before widespread clinical adoption. However, ongoing advancements in explainable AI, federated learning, and multi-omics integration are rapidly overcoming these barriers. Ultimately, AI-driven systems pharmacology and digital twin technology are expected to transform healthcare from reactive treatment-based medicine to proactive, predictive, and personalized precision medicine, fundamentally reshaping the future of global healthcare systems.

18. FUNDING

Nil

19. ACKNOWLEDGEMENT

Not Declared.

20. CONFLICT OF INTEREST

Nil

21. INFORMED CONSENT

Not applicable

22. ETHICAL STATEMENT

Not Applicable.

23. REFERENCES

1. Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. Nature medicine. 2019 Jan;25(1):44-56.
2. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, Li B, Madabhushi A, Shah P, Spitzer M, Zhao S. Applications of machine learning in drug discovery and development. Nature reviews Drug discovery. 2019 Jun;18(6):463-77.
3. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, Li B, Madabhushi A, Shah P, Spitzer M, Zhao S. Applications of machine learning in drug discovery and development. Nature reviews Drug discovery. 2019 Jun;18(6):463-77.
4. Schneider G. Automating drug discovery. Nature reviews drug discovery. 2018 Feb;17(2):97-113.
5. Zhu H. Big data and artificial intelligence modeling for drug discovery. Annual review of pharmacology and toxicology. 2020 Jan 6;60(1):573-89.
6. i Sunyer AP. Series Title Methods in Pharmacology and Toxicology Chapter Title Application of Tracer-Based Metabolomics and Flux Analysis in Targeted Cancer Drug Design Chapter SubTitle Copyright Year 2011 Copyright Holder Humana Press.
7. Barabási AL, Gulbahce N, Loscalzo J. Network medicine: a network-based approach to human disease. Nature reviews genetics. 2011 Jan;12(1):56-68.

8. Forman V, Luo D, Geu-Flores F, Lemcke R, Nelson DR, Kampranis SC, Staerk D, Møller BL, Pateraki I. A gene cluster in Ginkgo biloba encodes unique multifunctional cytochrome P450s that initiate ginkgolide biosynthesis. Nature Communications. 2022 Sep 1;13(1):5143.
9. Esteva A, Robicquet A, Ramsundar B, Kuleshov V, DePristo M, Chou K, Cui C, Corrado G, Thrun S, Dean J. A guide to deep learning in healthcare. Nature medicine. 2019 Jan;25(1):24-9.
10. Rajkomar A, Loreaux E, Liu Y, Kemp J, Li B, Chen MJ, Zhang Y, Mohiuddin A, Gottweis J. Deciphering clinical abbreviations with a privacy protecting machine learning system. Nature communications. 2022 Dec 2;13(1):7456.
11. Zhou H. Predicting Moonlighting Proteins on the Protein-Protein Networks with Graph Neural Networks.
12. Miotto R, Li L, Kidd BA, Dudley JT. Deep patient: an unsupervised representation to predict the future of patients from the electronic health records. Scientific reports. 2016 May 17;6(1):26094.
13. De Domenico M, Allegri L, Caldarelli G, d'Andrea V, Di Camillo B, Rocha LM, Rozum J, Sbarbati R, Zambelli F. Challenges and opportunities for digital twins in precision medicine from a complex systems perspective. npj Digital Medicine. 2025 Jan 17;8(1):37.
14. De Domenico M, Allegri L, Caldarelli G, d'Andrea V, Di Camillo B, Rocha LM, Rozum J, Sbarbati R, Zambelli F. Challenges and opportunities for digital twins in precision medicine from a complex systems perspective. npj Digital Medicine. 2025 Jan 17;8(1):37.
15. De Domenico M, Allegri L, Caldarelli G, d'Andrea V, Di Camillo B, Rocha LM, Rozum J, Sbarbati R, Zambelli F. Challenges and opportunities for digital twins in precision medicine from a complex systems perspective. npj Digital Medicine. 2025 Jan 17;8(1):37.
16. De Domenico M, Allegri L, Caldarelli G, d'Andrea V, Di Camillo B, Rocha LM, Rozum J, Sbarbati R, Zambelli F. Challenges and opportunities for digital twins in precision medicine from a complex systems perspective. npj Digital Medicine. 2025 Jan 17;8(1):37.
17. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, Garcia-Fandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891.
18. Chakraborty C, Priya D, Chen L, Zhu H. Evaluating protein-protein interaction (PPI) networks for diseases pathway, target discovery, and drug-design using 'in silico pharmacology'. Current Protein and Peptide Science. 2014 Sep 1;15(6):561-71.
19. Paul Gleeson M, Hersey A, Hannongbua S. In-silico ADME models: a general assessment of their utility in drug discovery applications. Current topics in medicinal chemistry. 2011 Feb 1;11(4):358-81.
20. Paul Gleeson M, Hersey A, Hannongbua S. In-silico ADME models: a general assessment of their utility in drug discovery applications. Current topics in medicinal chemistry. 2011 Feb 1;11(4):358-81.
21. Collins FS, Varmus H. A new initiative on precision medicine. New England journal of medicine. 2015 Feb 26;372(9):793-5.
22. Hood L, Friend SH. Predictive, personalized, preventive, participatory (P4) cancer medicine. Nature reviews Clinical oncology. 2011 Mar;8(3):184-7.
23. Yurkovich JT, Tian Q, Price ND, Hood L. A systems approach to clinical oncology uses deep phenotyping to deliver personalized care. Nature Reviews Clinical Oncology. 2020 Mar;17(3):183-94.