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From Pharmacological Informatics to Informational Pharmacology: A Conceptual Shift in Therapeutics

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ABSTRACT: This article offers a conceptual analysis of AI within information pharmacology, exploring its role as both a supportive tool and an autonomous therapeutic factor. It distinguishes between pharmacological informatics (instrumental level) and information pharmacology (ontological level) and proposes criteria for classifying AI systems as information-based medicinal products, focusing on dose-dependent, reproducible, and clinically meaningful effects. The study examines the relationship between material (molecular) and informational therapeutics, highlighting their conceptual connections and ontological distinctions. Comparative analysis of pharmacodynamics and pharmacokinetics elucidates therapeutic windows, dosing, efficacy, and risk for information-based interventions. The role of formal models in standardization, prediction, and regulatory evaluation is discussed. Finally, legal and ethical considerations for digital medicine and increasingly autonomous therapeutic systems are addressed, emphasizing the emerging framework for safely integrating AI into clinical practice.

KEYWORDS: information pharmacology; pharmacological informatics; digital therapeutics.

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Introduction

Over the past decades, pharmacology has been profoundly transformed by the rapid development of computational methods, large-scale biomedical data, and artificial intelligence. These advances have given rise to pharmacological informatics—an instrumental discipline focused on applying data-driven tools to classical pharmacological objects such as molecules, receptors, and pharmacokinetic processes (Wishart, 2018). Within this framework, information primarily serves to optimize the discovery, design, and evaluation of material therapeutic agents.

At the same time, emerging therapeutic practices increasingly challenge the traditional view of drugs as exclusively material entities. Digital therapeutics, adaptive treatment algorithms, neurocognitive interventions, and closed-loop regulatory systems suggest that information itself can act as a therapeutic agent (Lipsky & Sharp, 2019). These developments point toward a deeper conceptual transformation, one that cannot be fully captured by extending existing pharmacological informatics methods.

This article proposes the notion of informational pharmacology as an ontological shift in how therapeutic action is understood. Rather than treating information solely as a tool for studying drugs, informational pharmacology considers information, interpretation, and regulatory feedback as core pharmacological objects. In this perspective, therapeutic efficacy arises not only from molecular interactions but also from structured informational processes operating within biological, cognitive, and socio-technical systems.

By contrasting pharmacological informatics with informational pharmacology, we aim to clarify the distinction between an instrumental expansion of pharmacology and a fundamental redefinition of its subject matter. We argue that recognizing the distinction between material and informational agents is essential to understanding contemporary and future therapeutic paradigms (Hollis et al., 2017). This conceptual framework provides a foundation for integrating digital therapeutics, systems medicine, and cognitive models into a coherent pharmacological theory.

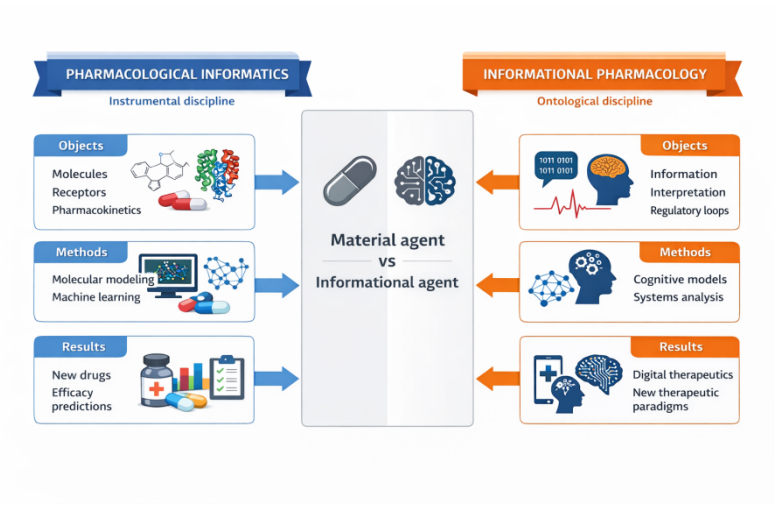
The study is based on an interdisciplinary approach that combines pharmacology, informatics, systems analysis, and the philosophy of science. Given the theoretical nature of the work and its focus on the conceptualization of information pharmacology, the study employs a set of theoretical, systemic, and comparative methods that provide a holistic understanding of the interaction between AI and pharmacology. The work uses theoretical methods of scientific knowledge aimed at generalization and conceptual analysis of existing knowledge, including the analysis and synthesis of scientific sources in pharmacology, pharmacometrics, bioinformatics, and artificial intelligence to identify key trends, methodological gaps, and points of integration between disciplines (Meadows, 1972).

Pharmacological informatics, as an analogue of chemoinformatics and bioinformatics, is an instrumental discipline whose main goal is to apply informatics methods, computational modeling, and data analysis to the study of material pharmacological systems (Ekins, 2007). Its object remains such

classical elements of pharmacology as chemical and biological compounds, receptors, signaling pathways, pharmacokinetic and pharmacodynamic processes. Information in this context performs a representational and analytical function, serving as a means of describing, predicting and optimizing the action of material therapeutic agents (Testa & van de Waterbeemd, 2001). Thus, pharmacological informatics does not rethink the nature of treatment but instead increases the efficiency of working with the existing pharmacological reality. Instead, informative pharmacology offers an ontologically distinct approach to understanding therapeutic action. The ontological approach in informative pharmacology holds that information is a real therapeutic agent, not just a means of communication. It is not a method, tool or technology, but a way of thinking about treatment. Within this scientific direction, information is considered an independent therapeutic agent, capable of initiating physiological changes through the processes of interpretation and regulation. The object of analysis here is not molecules or biochemical reactions, but information signals, cognitive structures, neural and behavioral regulatory circuits. Methodologically, information pharmacology is based on systems analysis, information theory, cognitive and neuroscientific models, and a philosophical understanding of causality and regulation in biological systems. Its task is to formalize information therapy by analogy with classical pharmacology, including the concepts of information dose, target, efficacy and side effects. The conceptual distinction between pharmacological informatics and information pharmacology, as two levels of scientific analysis of therapeutic action, is visually depicted in the compositional scheme (Fig. 1). The illustration compares the two disciplines, presenting them as complementary yet distinct.

The left part of the illustration shows pharmacological informatics as an instrumental discipline focused on the analysis of material objects (molecules, receptors and pharmacokinetic processes). The corresponding methods (molecular modeling and machine learning) and results (identification of new drugs and prediction of efficacy) emphasize its role in improving the accuracy and efficiency of classical pharmacotherapy without revising its ontological foundations.

Figure 1



The right part reflects the view of pharmacology as an ontological discipline that focuses on information as a therapeutic agent. Here, the objects are information signals, interpretation processes and regulatory circuits, and the methodological emphasis is on cognitive models and systems analysis. The result of such an approach is not the optimization of existing drugs but the development of new therapeutic paradigms, particularly digital therapeutic interventions.

The central element of the illustration depicts the opposition between the material and information agents, which plays a key conceptual role. He emphasizes that the difference between these areas is not in the use of digital technologies, but in different understandings of the nature of therapeutic action. Such a comparative analysis clearly demonstrates that pharmacological informatics and information pharmacology, despite the common use of information technologies, belong to different levels of scientific understanding of therapy.

The interaction between these two roles can be productive, as the instrumental AI can provide the therapeutic agent with the data, analytics, and contextual information needed to personalize the impact. In turn, the therapeutic agent can generate new data about the patient's condition, enriching the analytical models. In such a configuration, a closed feedback loop arises in which the instrumental and therapeutic functions reinforce each other, forming a holistic information-therapeutic system. At the same time, antagonism is also possible between them, since the instrumental approach involves control, predictability, and standardization, while the therapeutic agent operates under conditions of contextual variability and the patient's individual sensitivity. An excessive focus on instrumental efficiency can lead to ignoring the patient's subjective experience and cognitive limitations, while the autonomy of the therapeutic agent, without proper instrumental control, can create risks of excessive influence, cognitive overload, or even harm. Such antagonism has not only a technical but also an ethical dimension. An algorithm that simultaneously analyzes data and performs a therapeutic action requires clearly defined boundaries of autonomy, transparency, and the possibility of human intervention, because the absence of such distinctions creates a risk of a shift towards uncontrolled action.

Thus, the interaction and antagonism between the information tool and the information therapeutic agent of AI reflect a deeper transformation of medicine towards information-oriented models of treatment. Awareness of this duality is a necessary condition for developing theoretically sound and clinically safe approaches to AI use.

The introduction of the concept of information pharmacology inevitably raises a number of legal and ethical issues, since it concerns the use of information not only as a means of information, but also as a regulatory therapeutic factor. The dual nature of information interventions is both cognitive and clinical, which calls into question the traditional boundaries between medical intervention and communication with patients (Beauchamp & Childress, 2019). A key ethical challenge is the distinction between manipulation and therapeutic modulation. Both processes can lead to changes in behavior or emotional state, but differ in intention, transparency and direction. Manipulation involves covert

influence focused on the interests of the system or a third party, whereas therapeutic modulation should be open, voluntary, and aimed exclusively at the patient's benefit. Thus, the ethics of information pharmacology is determined not by the fact of influence itself, but by the architecture of the system: the level of transparency of algorithms, the possibility of user control and the absence of coercion. Ethically acceptable use of information systems occurs only when the patient is informed about their regulatory function, understands the limits of their capabilities, and has a real opportunity to refuse use without negative consequences for access to basic medical care (World Medical Association, 2013). Covert or implicit modulation of cognitive and emotional processes should be considered a violation of the principle of patient autonomy. The classic principle of informed consent assumes that the patient is aware of the nature, purpose and potential risks of medical intervention. In the case of information pharmacology, the difficulty lies in the fact that the therapeutic effect is achieved not through direct physiological action, but through cognitive and behavioral modulation. Under such conditions, information ceases to be neutral and becomes an intervention. The legal status of information pharmacological systems remains uncertain. Currently, there are no clear mechanisms for distributing responsibility among developers, medical institutions, and clinical specialists in the event of adverse consequences from their use. This requires the development of new regulatory approaches that recognize information interventions as a separate category of medical technologies, with appropriate standards for safety, effectiveness, and ethical oversight. Therefore, the use of information pharmacology is possible only if the principles of transparency, voluntariness, control, and orientation to the patient's benefit are observed. Information used as a therapeutic agent should be considered not as a neutral support for treatment, but as a form of regulatory intervention that requires a clear ethical and legal framework. It is their presence that will determine informationwhether possibility of pharmacology can be integrated into legitimate and safe clinical practice.

Conclusion

Thus, information pharmacology acts as a conceptual bridge between information-based medicine and the practice of digital therapeutic interventions. It allows us to describe informational influences in the language of therapeutic action, without reducing them to purely psychological effects or technical tools. This is precisely its contribution to the formation of a holistic model of medicine, in which treatment is understood as a guided information interaction, capable of complementing and reinforcing classical biomedical approaches

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