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# Pharmacoinformatics and Drug Discovery Technologies

Theories and Applications

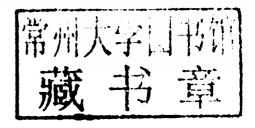


**Tagelsir Mohamed Gasmelseid** 

## Pharmacoinformatics and Drug Discovery Technologies:

Theories and Applications

Tagelsir Mohamed Gasmelseid King Faisal University, Saudi Arabia





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### **Preface**

The question of healthcare reform and the improvement of the pharmaceutical care services have gained momentum attention over the last decade in response to the expansion of drug-related problems. Such problems have been complicated by the challenges that limit the capacity of Healthcare institutions to improve the safety, accessibility and reliability of evidence-based healthcare services. Especially in developing countries, the improvement of pharmaceutical care processes has been challenged by the inability to control the development of chronic conditions, prevent life threatening conditions, develop healthcare support systems, build partnerships with stakeholders (including patients), and manage costs. Such challenges originate from internal inefficiencies and external change agents such as change in demography and disease patterns, increasing costs of technologies, workforce problems, lack of public funding, the changing context of urban planning, and its impacts on maintaining health equality. In response to such challenges healthcare institutions are investing in implementing some organizational, institutional and technological interventions. Institutionally, there have been a shift in terms of the sites that provide healthcare services by migrating from acute inpatient hospitals (providing episodic care) to outpatient configurations (providing ongoing care) in response to the change of disease patterns from acute infectious diseases to chronic conditions. In addition, there has been some emphasis on the introduction of new healthcare and pharmaceutical providers and a considerable diffusion of Pharmacoinformatics applications and technologies to improve the functionality of pharmaceutical care core processes.

Pharmacoinformatics, as an emerging discipline, has the potential of making quantum leaps in the quality of pharmaceutical care services through the deployment of information systems for provision of pharmacy related decision support tools. Such tools are essential for the improvement of drug management, use and administration processes and the solution of drug-related problems. They are also necessary for improvement of patients' knowledge about drugs administration and the consequences of adverse drug events. However, despite the successes here and there, many issues concerning the context of Pharmacoinformatics and its applications require additional analysis, experimental examination and research.

Firstly, there is still a need to theorize, crystallize and conceptualize the term itself and provide answers for questions like: "What is Pharmacoinformatics?" "What constitutes Pharmacoinformatics?" and "Is it Pharmacoinformatics or Pharmacy Informatics?" Little has been to focus of Pharmacoinformatics or "pharmacy informatics" with the aim of understanding its role in improving the efficiency and effectiveness of pharmaceutical care processes and patient-oriented outcomes and enhancing decision making at the operational, tactical and strategic levels in healthcare organizations. Over years, the have been some emphasis on the use of information systems in drug manufacturing processes such as drug analysis, testing and production. This orientation focuses more on the concepts of computer based manufacturing

that drive organization-wide "production information systems" but it provides a limited description of pharmacy management and pharmacy decision making. Considering the concept under the umbrella of biomedical and/or medical informatics moves the term closer to its decision support domain.

Secondly, there has been limited emphasis on understanding the context of Pharmacoinformatics in terms of its infrastructures, information processing environment, and the type of Pharmacoinformatics applications to be used. As a result, there has been some "selectivity" in the deployment of Pharmacoinformatics applications mainly for reporting and analyzing adverse drug events. The emphasis on the development of selected "evolutionary" pharmacy-related models has also been accompanied with a considerable failure to understand the roles and attitudes of "users" (such as physicians, pharmacists, nurses, laboratory personnel, and other healthcare professionals) and maximize the benefits from the emerging technology-driven business models.

This publication has been arranged into five parts with the aim of contributing to the abovementioned considerations. The first part is dedicated to the presentation of the contextual analysis of the domain of Pharmacoinformatics with emphasis on pharmacy management and pharmaceutical care systems and paradigms, analysis, definitions, methodologies, and interconnections. This part includes four chapters. In his work on the context of Pharmacoinformatics, Gasmelseid emphasized the centrality of the role of Pharmacoinformatics applications and technologies in the improvement of Pharmaceutical care processes. Stergachis et al used a case study approach to introduce a framework for using informatics for medicines management systems in resource-limited settings. Hugman examined communications in healthcare and proposed a number of strategies for addressing the shortcomings in areas such as information for patients and healthcare professionals, physician and pharmacist consultations, and the avoidance of medicinal and vaccination errors and crises. Postma and Hubben investigated the role of Pharmacoinformatics in enhancing the Pharmacoeconomics context of decision-making through the use of generalisable, transferable and accessible computer models for drugs management.

The second part includes four chapters that provide information about Pharmacoinformatics-oriented business models. Lin and Jalleh examined the key issues and challenges for managing and evaluating B2B E-Commerce projects within the Australian Pharmaceutical supply chains and their roles in setting up an infrastructure, which supports complex, multiparty Internet-based trading and transactions. Frattini et al. conducted an exploratory analysis on the role of platform biotech firms to examine the context of collaborations for innovation in the bio-pharmaceutical industry. In his work on cost-effectiveness analysis and the value for money of health technologies, Simoens reviewed and presented different approaches about cost effectiveness that enable decision making with regards to pharmacoinformatics technologies. Lin et al. used a multi-case study approach to investigate the practices and processes of B2B e-commerce evaluation and benefits realization and their impact on B2B e-commerce benefits and user satisfaction in Taiwanese hospitals.

The third part of this publication is devoted to the description of some of the methodologies, technologies and applications of pharmacoinformatics in pursuit of improving pharmaceutical care and patient-oriented outcomes. It includes nine chapters. Kevin Yap investigated the evolving role of Pharmacoinformatics in targeting drug-related problems in clinical oncology practice. His work also sheds light on the use of Pharmacoinformatics applications by healthcare practioners and patients. Claudia and Hilgarth examined the context of clinical pharmacists' intervention documentation in Germany using DokuPIK databases to demonstrate the improvement of drug therapy and the applicability of alternative strategies that can be used to reduce medication errors. Gasmelseid, proposed (in two chapters) a multi agent reference Pharmacoinformatics decision support model for the improvement of hospital management. In their

work entitled the healthcare factory, Cazzola et al. proposed a highly integrated system designed with the aim of improving the overall healthcare process management and of obtaining a flexible and deeper understanding of the patient treatment mechanisms. Col described the applications and challenges associated with the use of personalized decision support tools and models for the enhancement of patient choice. Chhanabhai examined the roles, benefits and disadvantages of social network sites in sharing health information by focusing on their corresponding privacy; security and ethical considerations. Butler addressed data integrity concepts and their use in pharmacy by highlighting relational models and relational database management systems. Chakraborty analyzed and interpreted the statistical methods used for analysis of safety issues within drug event combination.

The fourth pat of this publication includes three chapters which reflect on the multidisciplinary context of Pharmacoinformatics and its linkages with other sciences. Muneer, Abdullah, and Zaman proposed an optimization methodology to identify protein coding regions in Eukaryotes. Shahid et al. linked the context of Pharmacoinformatics through the analysis of Pharmaco-EcoMicrobiology concepts and their potential role in medical and environmental sciences. Sridhar et al emphasized the role of informatics in biology and drug discovery by describing in silico pharmaco-gene-informatics identification of insulin like proteins in plants. Pharmacovigilance issues and concepts are covered in the fifth part of this publication. Pharmacovigilance—basic concepts and application of pharmacoinformatics are presented by Jose. Elkhawad examined the role of Pharmacovigilance Center in Sudan in reporting adverse drug reactions by focusing on its functionalities and challenges.

Tagelsir Mohamed Gasmelseid King Faisal University, Saudi Arabia

### Section 1 Contextual Analysis of the Domain of Pharmacoinformatics

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### Section 1 Contextual Analysis of the Domain of Pharmacoinformatics

### Chapter 1

Healthcare organizations are facing serious internal and external challenges that affect their ability to provide quality pharmaceutical care and maintain patient safety. The dynamics of such challenges are affecting pharmaceutical processes, organizational and operating efficiencies, and patient outcomes. Pharmacoinformatics has been used as a term to reflect upon the use of information system technologies in the improvement of pharmaceutical care. However, despite its growing importance, it has been deployed in a limited scale. This chapter sheds light on the context of pharmacoinformatics, its conceptualization within the domain of decision support tools, and its role in the improvement of pharmaceutical care.

### Chapter 2

Improved access to information is necessary to ensure achievement of the potential benefits of medicines in resource-limited countries. The scaling up of treatment and prevention programs involving medicines in resource-limited regions with high disease burdens requires proper and urgent attention to the development and use of information technologies. Areas of need for medicines management systems informatics include prescribing, dispensing, pharmaceutical care, administration, patient monitoring, education and training, supply chain management, and monitoring and evaluation of program performance. Such information systems should strive to collect and manage data that are a standardized, compiled, and made easily accessible for use by key stakeholders, including ministries of health, medicines regulators, pharmaceutical industry, public health programs, academic researchers, donor organizations, the health care delivery sector, and ultimately the public and patients. A framework is described for medicines management systems informatics in resource-limited settings.

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All communications, especially those intended to influence attitudes and behaviour, depend on the empathy, creativity, and clarity of those responsible for them. Communications of all kinds, in healthcare and other sectors, can be greatly enhanced by the appropriate use of modern media and technology, but at the heart of effective communications are humane and compassionate purposes and values, which have the welfare of the recipient clearly in focus, whatever the chosen method or medium. This chapter examines ways in which communications in healthcare have often failed to meet the highest standards in protecting the welfare and safety of patients. It proposes a number of strategies for addressing the shortcomings in areas such as information for patients and healthcare professionals, physician and pharmacist consultations, and the avoidance of medicinal and vaccination errors and crises.

### **Chapter 4**

Maarten J. Postma, University of Groningen, The Netherlands Gijs A. A. Hubben, University of Groningen, The Netherlands

This chapter addresses the increasing role of pharmacoinformatics in enhancing the pharmacoeconomics context of decision-making. Notably, the role of pharmacoeconomics—i.e. cost per QALY calculations—is growing rapidly for decisions on reimbursement of new drugs. These pharmacoeconomic analyses often involve complex mathematical computer models requiring specific informatics techniques such as probabilistic simulations, bootstrapping, and discrete-event approaches. Transparancy of these complex models is crucial for decision makers to accept the model and its results. The authors argue that Web technology, Web-based access to models, international transferability of analyses, and decision-support systems may help in this respect. In particular, to allow decision makers and researchers to directly interact with transferable economic models and adapt a model to their region, efficient solutions have to be found to disseminate technically complex models to decision makers and researchers outside of the original setting. One such solution is through the use of Web technology and other pharmacoinformatics' techniques as explored in this chapter.

### Section 2 Pharmacoinformatics-Oriented Business Models

### Chapter 5

The use of Business-to-Business (B2B) e-commerce within the Australian pharmaceutical supply chain can potentially assist in setting up an infrastructure which supports complex, multiparty Internet-based trading and transactions among pharmaceutical manufacturers, wholesalers, hospitals, pharmacies, medical supply importers and exporters, and other players in the healthcare system. Effective use of B2B e-commerce can help these organizations reduce costs in supplying and distributing medicines and other medical-related products to the general public. However, despite high expectations for realizing

the benefits of B2B e-commerce in the pharmaceutical supply chain, issues surrounding its evaluation and management remain poorly understood and relatively under-researched. This chapter presents case study findings on key management and evaluation issues and challenges in adopting and utilizing B2B e-commerce systems on eight pharmaceutical organizations in Australia. The key objectives of this study are: (1) to establish current practices and norms in evaluating B2B e-commerce investments and projects in the pharmaceutical industry; and (2) to identify key B2B e-commerce management issues and challenges within the Australian pharmaceutical supply chain. A key contribution of this chapter is the identification and examination of key issues and challenges faced by the pharmaceutical organizations undertaking B2B e-commerce activities within their supply chain. The findings will guide senior executives in these organizations to develop their own approaches or strategies to manage the opportunities and threats that exist in the Australian pharmaceutical supply chain.

### Chapter 6

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The advent of biotechnology in the late '80s revolutionized the pharmaceutical industry and, in particular, caused a strong division of labour in the innovation process. As a result, the capability to master technological collaborations with external organizations has become a critical success factor for incumbent pharmaceutical firms as well as product biotech firms. This chapter investigates the phenomenon by using a rich and purposively collected empirical basis about the organisational forms (e.g., partnerships, in- and out-licensing, outsourcing, technology purchasing) through which inter-organizational collaborations are put into practice along the phases of the bio-pharmaceutical innovation process, and about the specific role played in these collaborations by platform biotech firms. Results are interpreted by drawing into two relatively novel streams of research in the innovation management literature, dealing with the Open Innovation paradigm and the role of Technical and Scientific Services (TSS).

### Chapter 7

Cost-effectiveness analysis serves as a tool to assess the value for money of a health technology. This chapter aims to review different approaches to assessing value for money of health technologies. First, the chapter discusses the methodological basis of the incremental cost-effectiveness ratio approach. Second, the chapter reviews alternative approaches such as the replacement approach, program budgeting and marginal analysis, the generalised optimisation framework, and multi-criteria decision analysis. This information will aid health care decision makers and researchers to interpret cost-effectiveness analyses and their results for the purpose of decision making.