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# Chemoinformatics: Directions Toward Combating Cancer in the Future

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**Abstract**

Cancer remains one of the leading causes of mortality worldwide, demanding the continuous development of more effective and personalized therapies. The discovery of new antineoplastic drugs is a complex, costly, and time-consuming process. In this context, Chemoinformatics emerges as an essential tool, integrating computational methods to analyze chemical data, predict molecular interactions, and optimize drug candidates. Supported by machine learning, molecular modeling, and big data analysis, Chemoinformatics accelerates the identification of novel bioactive compounds as well as the repositioning of already approved drugs, contributing to the advancement of targeted therapies and precision medicine. This opinion article highlights the role of Chemoinformatics in addressing cancer and its relevance to the future of computational oncology.

**Keywords:**Cancer; Chemoinformatics; Drug Repositioning; Artificial Intelligence; Computational Oncology

**Abbreviations:** CADD: Computer-Aided Drug Design; QM: Quantum Mechanical

## Introduction

Cancer has a significant contribution to new or reemerging public health challenges worldwide [1]. Thus, every action, activity, and strategy for the surveillance, prevention, and control of cancer must be preceded by a survey of the context of impact on public health, through evaluation of the magnitude, potential for dissemination, severity, and vulnerability related to the epidemiological process of development, progression, and maintenance of cancer, considering the affected population, the genetic and environmental factors involved, and the affected regions in a given period of time. Evidence-based prevention strategies are nowadays a global priority, especially in cancer-affected areas. A current example is the increasing incidence of cancers associated with genetic mutations, environmental exposure, and lifestyle factors, such as lung, breast, and colorectal cancer [2]. In this context, research is important to better understand the behavior of these different cancer types, to develop ways to prevent their onset and progression, as well as avoiding the spread of metastases.

Thus, Chemoinformatic has played an important role in comprehending the molecular mechanisms and drug interactions involved in these diseases. Computational chemistry techniques can provide new clues to help combat cancer, assisting in the development of novel ways for diagnosis, prevention, and treatment. Due to the complex and multifactorial nature of cancer, which involves genetic, epigenetic, and environmental components, tumor development and progression occur through intricate molecular pathways. The current scenario shows that, despite our knowledge of oncogenic processes-for instance, those related to breast, lung, and colorectal cancers-it is difficult to prevent tumor recurrence and resistance to therapies. Even with improvements in national and global cancer surveillance and early detection systems, the development of efficient ways to treat and prevent cancer remains a challenge.

In view of this scenario, it is necessary to re-evaluate potential molecular targets and signaling pathways involved in tumor initiation and progression, and to examine whether we can minimize the risk for therapeutic resistance and disease recurrence. Thus, we should recommend more studies about important molecular interfaces and biological pathways that drive cancer development and metastasis, as well as the feasibility of

reducing the risks of treatment failure at these interfaces [3]. The rise in global cancer incidence has boosted research surrounding all aspects of oncology [4]. There have been many works in the field of Chemoinformatics that attempt to address the discovery of novel therapeutics against different cancer types [5-8]. For instance, numerous virtual screening publications have proposed potential drug candidates and inhibitors to combat the molecular targets associated with cancer [9].

The growing interest in cancer research brought a range of challenges for the computational chemistry and informatics research community. Note that the current challenge is to identify novel therapeutics in a rapid but rigorous fashion [10]. Computational methods are indeed useful to accelerate the long and costly drug discovery process [6,7]. Commonly, the drug discovery for a determined target is divided as the following: (i) identification of chemical compounds with promising activities toward the target; (ii) compounds improvement in potency against the target; and (iii) compounds optimization to generate drug-like molecules capable of exerting beneficial therapeutic effects in patients [11]. Artificial Intelligence (AI) and Machine Learning (ML), especially in conjunction with molecular modeling techniques, have been gaining enormous visibility and success in the modern computational drug discovery process [12-14].

## Chemoinformatics

Chemoinformatics can assist for a deeper comprehension of drug activities, therapeutic mechanisms of action, drug target identification, commonly within a receptor or an enzyme, to the design and optimization of a new drug-like molecule. Usually, computational techniques for target identification depend on computational sciences, and in this context, it is to cite bioinformatics and computational genomics. Remarkably, there are different computational approaches available to search for promising drug candidates once the target has been identified [11]. In this line, we can cite computational drug repositioning. This technique is related to discovering new uses for existing drugs outside the scope of the original therapeutic indication and have a great potential for discovering new therapies for the treatment of diseases [15-22]. The present academic landscape should enable promising research programs for drug repositioning, by employing different techniques from computational chemistry, along with in vitro and in vivo experimental investigations [17-19]. High-throughput screening tools efficiently provide gains in speed and quickly screen large numbers of potential drug candidates for repositioning. In principle, this approach can be successfully applied in the search for novel therapies for the treatment of diverse diseases [23].

Due to the complex nature of pandemics epidemiology and virology, many questions are, in principle, difficult to answer. Chemoinformatics provides ways of getting better insights about the behavior of a pandemic, such as mutation mechanism of the virus and interaction modes with the host [14,24]. In this critical situation, computational modeling methods, specifically virtual screening, offers the fastest, cheapest, and most effective way for discovering effective drugs. Importantly, this research is accompanied by human clinical trials for testing vivo effectiveness and security [25]. The current pandemic has raised a global demand for fast and effective diagnosis, treatment and prevention of transmission. In this line, studies have also suggested that nanotechnology can be useful to help combat infectious diseases, and counter future pandemics [26-28].

Nanotechnology can introduce new disinfection protocols and enhance the barrier properties of personal protective equipment, to prevent the spread of the virus. For instance, nanotechnology-based solutions could support the development of safer masks or air filter devices, working through the immobilization and elimination of the virus. In addition to disease prevention and therapeutic potential, nanotechnology can play important roles in diagnostics, potentially supporting the development of simpler, faster and more cost-effective nanotechnology-based tools to monitor the presence of viruses and related biomarkers [28]. The Chemoinformatics has boosted the development of nanotechnology, the so-called “Computational Nanotechnology”, as detailed reported by Srivastava & Atluri [29]. Research in a wide range of applied sciences seeks to develop not only useful biomolecules and advanced materials, but also to understand, design, and control their functional properties [30-32].

These efforts may lead to new interpretations for carrying out experiments. In this context, it is well known that computational strategies have been widely applied to such specific chemical problems (e.g., proteins, DNA, and cell membranes) and have led to efficient approaches for analyzing the enzymatic activity [33-35]. Accurate models for the computing chemical properties of drug candidates and proteins are essential for drug discovery and design [36]. Thus, the notable use of computer-aided drug design (CADD) based quantum mechanical (QM) methods is fueled by present-day growth computing power; however, it is mainly because QM methods can provide higher accuracy in terms of computations and results [37-40]. In addition, the interest in the use of QM methods in CADD has boosted the development of further methodologies; for instance, the correlation of this approach with molecular docking, scoring, improvement of known lead compounds, and even the unraveling of reaction mechanisms [41].

With all exposed so far, it is important to mention that a fast detection, response and control of public health emergencies, mostly outbreaks of zoonotic diseases, are important measures to prevent global spread of diseases threats. These measures are crucial to ensure global health security. Due to the fact of zoonotic diseases can potentially affect animals and humans, diverse health agencies have a large interest in disease surveillance and control


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activities. Thus, collaboration among agencies is fundamental to have an efficient system for prevention and control of viral infectious diseases, aiming at the prevention of diseases outbreaks and pandemics. In conclusion, Chemoinformatics is an important approach when installing an effective implementation of disease prevention and control programs.

## Conclusion

With all exposures so far, it is important to mention that fast detection, response, and control of public health emergencies, most outbreaks of zoonotic diseases, are important measures to prevent the global spread of disease threats. These measures are crucial to ensure global health security. Due to the fact of zoonotic diseases can potentially affect animals and humans, diverse health agencies have a large interest in disease surveillance and control activities. Thus, collaboration among agencies is fundamental to having an efficient system for the prevention and control of viral infectious diseases, aiming at the prevention of disease outbreaks and pandemics. In conclusion, chemoinformatics is an important approach when installing an effective implementation of disease prevention and control programs.

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