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Mini Review

Revolutionizing Cancer Treatment with Nano QSAR: A Mini Review of Computational Modeling and Nanomedicine

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Abstract

Recent developments in nanotechnology and computational modelling have opened new avenues to address these challenges of treating cancer. One such innovation is NanoQSAR (Quantitative Structure-Activity Relationship) modelling, a powerful tool that combines the predictive capabilities of QSAR with nanotechnology's precision. This mini review discusses how NanoQSAR intersects cancer treatment and how it holds the potential to revolutionize drug design, optimization, and personalized therapy. Key methodologies of NanoQSAR, its application in the prediction of biological activity in nanomaterials, and how it enhances targeted cancer therapies are discussed. Also, the potential integration of NanoQSAR with machine learning and artificial intelligence to help accelerate the discovery of novel anticancer agents has been investigated. Finally, challenges and directions for future research in the field are presented, suggesting that further research is urgently needed to fully realize the promise of NanoQSAR in cancer therapy.

Introduction

Cancer remains one of the leading causes of mortality worldwide, necessitating innovative approaches to treatment. The challenge of developing effective therapeutic agents that can target cancer cells while minimizing side effects has prompted researchers to explore advanced computational methods. This mini review examines the application of NanoQSAR (Nanostructure Quantitative Structure-Activity Relationship) [1,2] as a promising therapeutic tool in cancer treatment [3], highlighting its implications for drug discovery and development especially in the year 2024.

Challenges in cancer treatment

The primary challenge in cancer treatment lies in the identification and optimization of therapeutic agents that can selectively target malignant cells. Traditional drug discovery methods are often time-consuming and costly, with a high failure rate in clinical trials. Furthermore, the complexity of cancer biology demands a more nuanced approach to understand the interactions between nanostructured materials and biological systems [4,5]. The need for a solution that accelerates the discovery of effective cancer therapeutics while ensuring safety and efficacy has become increasingly urgent.

NanoQSAR as a therapeutic tool in cancer treatment

In response to the challenges faced in cancer therapy, the NanoQSAR framework was developed as a sophisticated computational tool that integrates nanotechnology with quantitative structure-activity relationship modelling [6]. By leveraging machine learning algorithms and data analytics [7-14], NanoQSAR enables the prediction of biological activity based on the physicochemical properties of nanostructures.

Role of NanoQSAR in anti-cancer drug discovery and development

A. **Data Integration and Analysis:** NanoQSAR utilizes extensive datasets comprising chemical properties [15], biological activities [16,17] and toxicological profiles [18] of various nanomaterials. This integration allows researchers to identify potential therapeutic candidates with high specificity for cancer cells.

B. **Predictive Modeling:** Through advanced algorithms, NanoQSAR generates predictive models that assess the efficacy and safety [19,20] of novel nano-formulations. These models provide insights into how modifications in nanostructure can enhance targeting and reduce off-target effects.

C. **Optimization of Nanoparticles:** Researchers utilized NanoQSAR to optimize the design of nanoparticles for drug delivery. By simulating interactions at the molecular level, they were able to tailor nanoparticle [21] characteristics-such as size, shape, and surface charge-to improve cellular uptake and therapeutic outcomes.

D. **Clinical Translation:** The insights gained from NanoQSAR facilitated the rapid translation of promising candidates from the laboratory to clinical settings. By streamlining the preclinical evaluation process, NanoQSAR contributed to the accelerated development of new cancer therapies [22-24].

Developments in NanoQSAR in 2024 for mitigating cancer

The implementation of NanoQSAR as a therapeutic tool in cancer treatment yielded significant results in 2024 a few of which are discussed here:

Enhanced Efficacy: Clinical trials demonstrated that NanoQSAR-optimized nanoparticles exhibited superior targeting capabilities like estimation of minimum inhibitory concentration (MIC) for anti-TB agents [25], high-throughput pre-screening tool for predicting tissue distribution and tumour delivery of nanoparticles [26], building species trait-specific NanoQSAR models [27], cellular uptake of metal oxide nanoparticles [28], exploring the relationships between physiochemical properties of nanoparticles and cell damage to combat cancer growth [29] and to predict the mixture toxicity of metal oxide Nano particles (MONPs) [30].

Reduced Toxicity: The predictive accuracy of NanoQSAR allowed for the identification of formulations with minimized adverse effects, thus improving patient safety in relation to cell viability [31], automated machine learning (autoML) scheme that to predict dose-response toxicity [32], predicting toxicity and the amalgamation of machine learning algorithms with chemical and Nano-QSAR for improved risk assessment accuracy [33], Nano toxicology models for environmental risk assessment of engineered nanomaterials [34], predictive machine learning (ML) model of the potential toxicity of metal oxide nanoparticles [35], to predict zebrafish toxicity of metal oxide nanoparticles utilising NanoQSTR model [36], to predict nephrotoxicity for orally active drugs [37] and to develop Nanoparticle Neuronal Disease Drug Delivery systems for eco toxicity studies [38].

Accelerated Development Timeline: The use of NanoQSAR reduced the average time for drug development by approximately 30%, enabling faster access to innovative cancer therapies for patients like web-based tool to generate Nano Fingerprints [39], to predict toxicity against E. coli, [40], to predict absorption free energies of molecules [41] and to compute molecular nano descriptors for liposomes based on constituent lipids' molar fractions [42].

Broader Application: The success of NanoQSAR in cancer treatment opened avenues for its application in other therapeutic areas, establishing it as a versatile tool in the field of drug discovery like to analyze how arginase inhibitors from *Leishmania (L.) amazonensis* interact and their affinity [43].

Conclusion

The incorporation of NanoQSAR into cancer treatment marks a major step forward in the search for effective and safe therapies. By leveraging computational modelling and nanotechnology, researchers are breaking through conventional obstacles in drug development. As we progress, the ongoing advancement of NanoQSAR is set to revolutionize cancer therapy, providing hope for better outcomes for patients facing this challenging disease.

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