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Novel *in silico* nano-drug design and delivery systems employing the density functional theory: a review

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Abstract

Nanoinformatics is a next-generation method for designing and simulating nanodrug candidates. It involves combining bioinformatics and quantum tools to predict and evaluate drugs. This approach addresses scientific problems in cheminformatics, configuration optimization, drug development, and administration. The integration of bioinformatics and quantum tools is crucial for the understanding of these advancements.

KEYWORDS

nanoinformatics, *in silico*, density functional theory, bioinformatics, nano-drugs

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1. INTRODUCTION

These methods help with the design and improvement of drug delivery systems in addition to providing important insights on drug behavior. The progress in computational drug design and genomic analysis has resulted in the rise of nanoinformatics as a cutting-edge tool for drug design and the undertaking of simulation studies for nanodrug candidates. Through computational tools, nanoparticle libraries, different modeling techniques, and simulation approaches, nanoinformatics plays an important role in enhancing the development of anticancer nanomedicines. The development of tailored nanomedicines in anticancer research might be accelerated by nanoinformatics, which is unquestionably important at this point. In addition, when compared to other *ab initio* methods that are currently in use, computational techniques like the density functional theory (DFT) offer very high levels of accuracy within a comparable computation timeframe, and are more economical in terms of processing resources [1-3].

2. NANOINFORMATICS IN DRUG DESIGN AND DELIVERY SYSTEMS

Nanotechnology enhances drug delivery, but challenges like tissue penetration and safety persist. Computational models aid in understanding biological processes and selecting effective anticancer

treatments. Professionals in nanoinformatics evaluate biotechnological data, predict nanoparticle structure, and manage biomedical data [3-5]. Some tools (like AutoDock Vina) can predict the binding affinities and orientations of ligands, are fast, accurate, and easy to use, but may not be as accurate for complex systems. While AutoDock and GOLD are used for ligand binding affinities and the prediction of orientations, particularly for flexible ligands, they require a license and can be expensive. Another tool is Glide, which can predict the binding affinities and orientations of ligands with accuracy, and can be integrated with other Schrödinger tools; however, the latter requires the Schrödinger suite, which can be expensive. Both LigandFit and SwissDock may not be as accurate for complex systems, but they are easy to use, accessible online, and integrated with other Schrödinger tools; these platforms are usually used for predicting the binding affinities and orientations of ligands (Table 1) [3-8].

DFT has significantly transformed drug delivery system design and development, particularly for biodegradable and bioabsorbable polymers. DFT simulations can accurately predict properties and structural characteristics, thereby providing insights into medication pharmacokinetics and metabolism parameters. As computing power increases, the emergence of multidisciplinary initiatives for nanomedicine from an atomic viewpoint, at a low cost, and with accurate quantum mechanics calculations are expected [3,7].

Table 1. List of companies using artificial intelligence (AI) and machine learning technologies in pharmaceutical research.

Domain	Technology and Outcome	Industry and Collaborations
Drug design	Innovative medicinal antibodies	Exscientia
Molecular drug discovery	Computing platform for structure-based drug creation powered by deep learning and AtomNet	AtomWise
Gene mutation related disease	Recursion operating system for biological and chemical datasets based on machine learning	Recursion
Drug design	*De novo* drug design using ligands and structures, particularly in multiparametric optimization	Iktos
Drug discovery	AI technology for generative modeling	Iktos and Galapagos
Drug development	Suitable candidates for preclinical research	Iktos and Ono Pharma
Drug design	Quick drug creation with “Makya” software	Iktos and Sygnature Discovery
Drug discovery and development	Pharma.AI, PandaMics, ALS.AI	Insilico Medicine
Drug target	Drug target selection for idiopathic pulmonary fibrosis and chronic kidney disease	BenevolentAI and AstraZeneca, GlaxoSmithKline, Pfizer
Clinical trials	AI in clinical trials	Pfizer and Vysioneer

3. ADAPTING PROFESSIONAL SKILLS FOR ANALYZING NANOBIOTECHNOLOGICAL DATA

Nanoinformatics is a rapidly evolving field that uses computational chemistry and bioinformatics to analyse data on nanobiotechnology. It plays a crucial role in drug design, advancing research in nanodrug delivery systems and regenerative medicine. Despite challenges like ethical considerations and computational modeling risks, successful case studies demonstrate the significant impact on the pharmaceutical industry, leading to efficient nanomedicines for better cures [6,7].

4. POTENTIAL BENEFITS AND IMPLICATIONS

The integration of nanoinformatics with computational methods like DFT and machine learning offers numerous benefits, including optimization, standardization, and understanding of the nanomaterials’ synthesis, characterization, and biological effects. This integration has potential to transform the pharmaceutical sector and improve patient outcomes [5].

5. THEORETICAL AND COMPUTATIONAL MODELING IN NANOINFORMATICS

Nanoinformatics and nanomodeling are crucial for computational nanodrug design and delivery systems. Theoretical and computational modeling can help solve problems in configuration, medication creation, and administration optimization. Combining traditional bioinformatics with chemical tools allows for accurate medication prediction and assessment. DNA computing information and artificial intelligence (AI) algorithms enable nanomedicine and regenerative medicine advancements. Computational modeling tools have shown promise in addressing empirical models and advancing nanomedicine by addressing shortcomings in existing models [3,5-7].

6. CONFIGURATION, MEDICATION CREATION, AND ADMINISTRATION OPTIMIZATION

Nanoinformatics and nanomodeling are crucial in computational nanodrug design and delivery systems. AI models can accurately forecast drug delivery systems by analysing physicochemical parameters and molecular features. They can also predict medication release and absorption characteristics, dissolution rates, and formulation properties. These features can advance computational nanodrug design and delivery systems by improving nanoparticle design, by predicting medication release and absorption, and by optimizing drug formulations [8].

7. POTENTIAL RISKS AND UNCERTAINTIES

Computational modeling in nanoinformatics for drug design and delivery systems has risks and uncertainties, including over-reliance on predictions without experimental confirmation, as well as challenges in representing molecular flexibility in biological molecules. Ethical considerations, patient privacy, and data security are crucial [3,4].

8. CASE STUDIES

Nanoinformatics can revolutionize drug design and delivery systems, optimizing site-specific drug delivery through deep learning and AI algorithms. This has already led to successful drug design, efficient interaction prediction, and personalized treatment regimens [1-9].

9. CONCLUSION AND FUTURE DIRECTIONS

The integration of data and information science has significantly impacted nanomedicine, thereby optimizing and standardizing nanomaterial synthesis and accelerating drug design. Traditional bioinformatics and computational chemistry tools have been adapted for data storage, analysis, and visualization. Nanoinformatics can enable personalized nanomedicines for cancer treatment.

The future of nanoinformatics and computational nanodrug design will involve quantum computing, AI integration, biomedical data standardization, and sustainability metrics. Future research should focus on flexible informatics systems and collaboration between computational scientists and pharmaceutical industry professionals.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

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