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HIGHLIGHT

Advancing cancer nanomedicine with machine learning

KEY WORDS

Machine learning;
Artificial intelligence;
Nanomedicine;
Drug design;
Cancer treatment

Nanomedicine, a captivating and highly promising field in biomedicine, is driving the transformation of medical technologies and treatments, catalyzing revolutionary advancements in areas such as cancer therapy, drug delivery, diagnostics, and imaging[1-3]. With the notable progress in nanomedicine to tackle the complexities of various diseases, the biomedical sector is presented with abundant opportunities for innovation and progression. In this process, machine learning (ML) and artificial intelligence (AI) emerge as pivotal themes in the realm of science and technology[4]. They are reshaping our lifestyles and workplaces with unparalleled rapidity and magnitude, while also providing fresh possibilities and potentials for the evolution of nanomedicine[5,6].

ML is a technique within the realm of AI that uncovers patterns from data and facilitates predictions or decisions by enabling computer systems to autonomously learn and enhance through experience[7]. In contrast to conventional rule-based programming, ML operates on a data-centric approach by training models to execute specific tasks like classification, clustering, prediction, or optimization. Throughout the training phase, ML algorithms scrutinize extensive datasets to discern patterns and trends, enabling them to make precise predictions or decisions when confronted with new data in the future. In the exploration, design, and optimization process of drugs, ML demonstrates its outstanding advantages. Currently, more and more research is dedicated to integrating ML into various stages of drug discovery and development[8,9]. With the help of ML algorithms and software, researchers can identify new targets, predict and optimize new compounds based on database patterns, and predict the results of their actual applications. This is also of significant importance for the clinical translation of nanomedicine.

Rapidly advancing ML has paved the way for fresh avenues in the design and development of nanoparticles (NPs) for the efficacious treatment of cancer. Recent research aiming at gaining insights into the design patterns of inorganic nanoparticles through data mining and ML techniques can be considered a breakthrough in cancer nanomedicine by integrating ML and data mining into inorganic nanoparticle design (Fig. 1)[10]. Drawing insights from datasets derived from preclinical investigations of cancer nanomedicine, the team has leveraged this information to shape standardized nanoparticle design and manufacturing processes, culminating in the establishment of a comprehensive database encompassing inorganic NPs. Nonetheless, as highlighted in this study, the adoption of ML in nanomedicine is hindered by the limited scale of datasets. It is imperative, therefore, to cultivate and enhance large-scale datasets to maximize the utilization of ML techniques and expedite the progress of nanomedicines. This study serves as a pivotal starting point for forthcoming research in nanomedicine by showcasing that through data mining and ML methodologies, it is viable to delve deeper into the design patterns of inorganic NPs and furnish insightful information on therapeutic effects. Moreover, the findings of this study not only supply valuable perspectives into the realm of nanomedicine but also underscore that in data-centric scientific research, the quality and volume of the dataset are fundamental to the efficacy of ML algorithms. By establishing and disseminating databases comprising copious amounts of experimental data, researchers can gain an enhanced understanding of the attributes, applications, diagnostic approaches, and administration methodologies of inorganic NPs, offering robust backing for future therapeutic possibilities. Furthermore, this endeavor advocates for heightened data sharing and standardization in the domain of nanomedicine to propel advancements in the field and mitigate research uncertainties.

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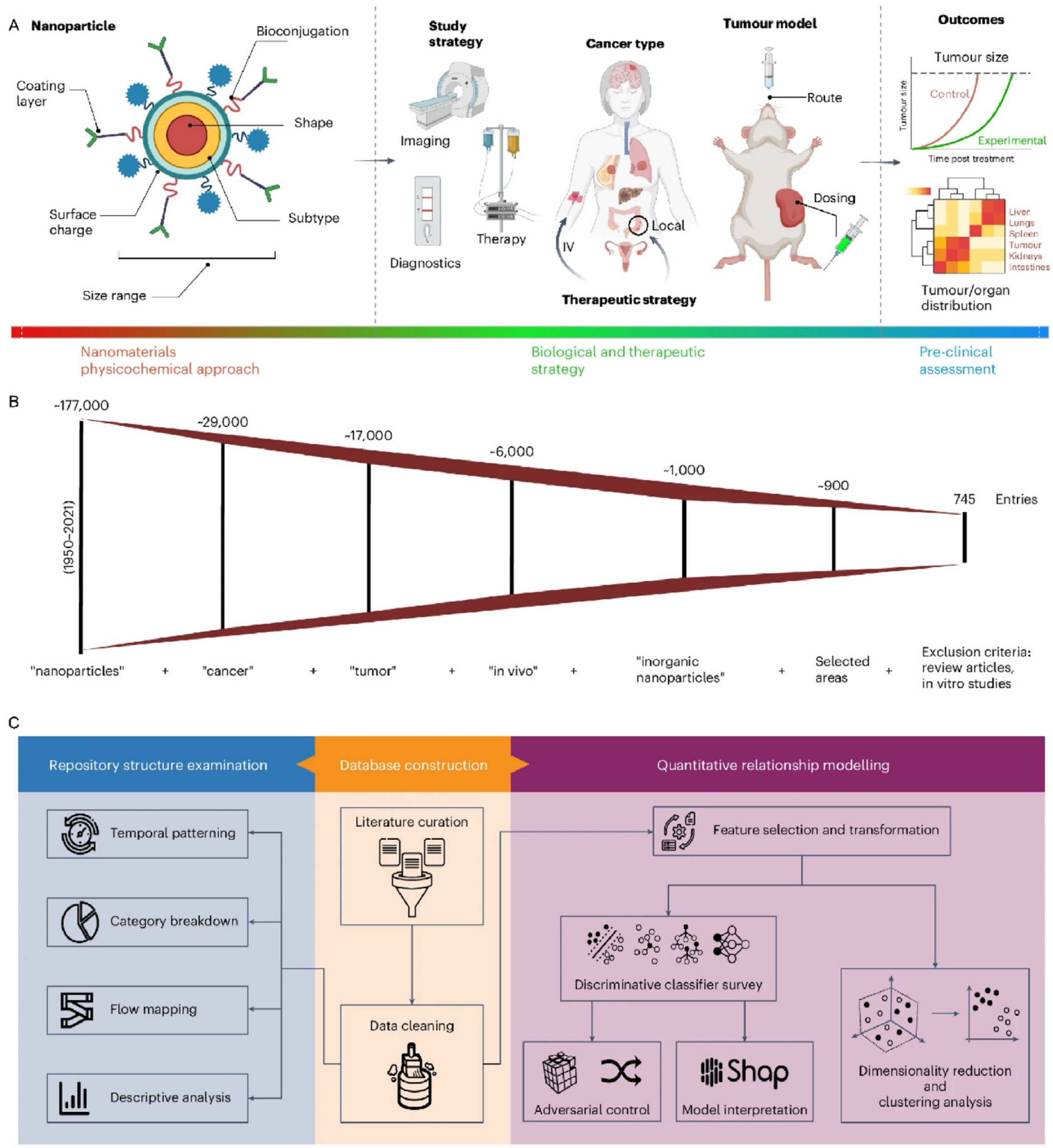

Figure 1 Study design, meta-analysis and artificial intelligence modelling of the workflow. (A) Schematic representation of the design of NP and its further biomedical applications. (B) Procedure used for database curation using several search terms. (C) Workflow of the analysis, including data curation and preparation, statistical analysis and machine learning-driven modelling. Reprinted with the permission from Ref. 10. Copyright © 2024 Springer Nature.

Therefore, this ML-based drug design pattern can achieve efficient and precise prediction of NP structures, aiming to provide important references for the design of highly versatile NPs in cancer treatment.

With the continuous progression of ML technology and the deepening exploration of nanomedicine, we eagerly anticipate the future utilization of ML to expedite innovation in the realm of cancer nanomedicine. It is noteworthy that the synergy of ML and AI still necessitates the development of models that prioritize interpretability, explainability, and dependability as well. Additionally, human-AI collaboration is pivotal, whose essence resides in the mutual leveraging of their respective strengths to compensate for each other's weaknesses, thereby collaboratively unraveling the intricacies of cancer therapy. This amalgamation not only facilitates the rapid identification of therapeutic modalities but also underscores the role of AI as a facilitator and augmenter, rather than a substitute, for the nuanced insights of human investigators. Concurrently, the advent of ethical AI, or human-centered AI centered around principles of equity and responsibility, is critical to ensuring that progress in nanomedicine is equitable and adheres to the strictest benchmarks of patient care. By amalgamating the intricate therapeutic methodologies of nanomedicine with the intelligent analytical capabilities of ML, we can achieve enhanced disease diagnosis accuracy, personalized treatment strategies, and drug design precision, introducing a potent driving force towards enhancing human health and medical care. This symbiotic interdisciplinary synergy and cross-pollination will further propel the advancement of nanomedicine and unveil broader horizons for augmenting human health and quality of life. Moving forward, we anticipate witnessing more akin initiatives dedicated to constructing more encompassing and accessible data repositories, advocating the widespread integration of ML in nanomedicine, and heralding novel breakthroughs and progressions in cancer treatment and clinical practice.

Author contributions

Xifeng Qin: Writing − original draft, Writing − review & editing. Tun Lu: Writing − original draft, Writing − review & editing. Zhiqing Pang: Writing − original draft, Writing − review & editing.

Conflicts of interest

The authors have no conflicts of interest to declare.

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