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ARTIFICIAL INTELLIGENCE EMPOWERS THE DEVELOPMENT OF MATERIALS IN NEW PHARMACEUTICAL ENGINEERING: SCREENING AND APPLICATION OF POLYMER NANOPARTICLES

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With the rapid development of the nanomedicine field, polymer nanoparticles, as a key component of drug delivery systems, have shown great potential in improving drug bioavailability, enhancing targeting ability, and optimizing therapeutic efficacy. This type of carrier can effectively package hydrophobic drugs, improve drug stability, achieve controllable release, and play a significant role in multiple cutting-edge medical directions such as tumor treatment, gene delivery, and immune regulation. However, the traditional research and development model of polymer nanoparticles mainly relies on experimental experience and trial-and-error strategies. From material screening, formula optimization to process scale-up, the entire process is not only time-consuming but also costly. These bottlenecks severely restrict the clinical transformation and application expansion of polymer nanoparticles. In recent years, the rapid development of artificial intelligence (AI) technology has brought a brand-new path to break through the above-mentioned predicament. AI methods represented by deep learning, active learning, and reinforcement learning are gradually reshaping the design concepts and development processes of polymer nanoparticles. This paper systematically reviews the latest research progress of artificial intelligence in the structural design, performance prediction, formulation screening and practical application of polymer nanoparticles. It focuses on analyzing how AI integrates high-throughput experimental data and multi-source theoretical descriptors to construct a mapping model among materials, formulations and performance. This enables precise prediction of key attributes such as the particle size, Zeta potential, drug loading capacity and release behavior of nanoparticles. In addition, the combination of AI and computational simulation methods (such as molecular dynamics, dissipative particle dynamics, etc.) can further reveal the delivery mechanism of nanoparticles in complex biological environments and their interactions with cells, providing theoretical support for the rational design of targeted systems. The article also explores the key challenges currently faced by AI-driven nanomedicine development platforms, including interdisciplinary studies, data, and talent cultivation. Finally, this paper looks forward to the future development direction of artificial intelligence in pharmaceutical engineering, providing theoretical references for the in-depth application of artificial intelligence in pharmaceutical engineering.