EDITORIAL

Current Advances in Computational and Experimental Approaches for Nanoparticle-Drug Conjugates

Xubo Lin

Drug development is always one of the main missions in *Medicinal Chemistry*. In the past several decades, nanoscience and nanotechnology have made great progress in facilitating drug development. Especially, nanoparticle-drug conjugates, which integrate both the advantages of nanoparticles and drugs, have shown great potential in treating a series of diseases including cancers. In this thematic issue, we focus on the current advances in computational and experimental approaches in nanoparticle-drug conjugates.

In the first paper, Cheng *et al*. [1] gave a comprehensive review on the lipid nanoparticles using as drug and gene delivery carrier. Especially, they emphasized the importance of the rational combination of experiments and computations in the development of efficient, robust and safe lipid nanoparticles to treat diverse diseases. Interdisciplinary integration of chemistry, biophysics or soft matter physics, computer simulations and so on will help establish the relationships between the structural and the functional properties of lipid nanoparticles, which are essential for the optimization of the complex of lipid nanoparticles and drugs/genes.

In the second paper, Bhatia *et al*. [2] focused on the nanoparticle-based drug delivery systems for treating glaucoma. Ocular drug delivery to the target area is difficult. Through the detailed review, the authors discussed the applications of various inorganic and organic nanoparticles in delivering the antiglaucoma drugs to the specific target of the eye, and pointed out that *in silico* approaches play key roles in facilitating the experimental approaches for the effective design of novel ocular drug delivery systems.

In the third paper, Zhang *et al*. [3] discussed in detail about biomedical researches and applications of one attractive biopolymer (hyaluronan, HA), which is a natural linear polysaccharide with excellent hydrophilicity, biocompatibility, biodegradability, and low immunogenicity. HA has the intrinsic affinity for CD44, a receptor highly expressed in a variety of cancer cells. Besides, HA has several functional sites to conjugate many drug molecules or ultra-small imaging nanoparticles. Hence, HA serves as a potent case for nanoparticle-drug conjugates to achieve the effective synergistic combination therapy and promote the integration of therapy and diagnostics. Besides, potential challenges for translational applications of HA-based therapeutics were also discussed in this paper.

In the fourth paper, Kandasamy *et al*. [4] provided a case study, which used nanotechnology to enhance the solubility of methotrexate (MTX) and its efficacy to treating small cell lung carcinoma. The authors synthesized MTX loaded nanodispersions (MTXND) using solvent evaporation technique. The obtained MTXND was found to have longer residence time and thus high concentration in the target cancer tissue, which showed better anti-tumor effects.

In the last paper, Duan *et al*. [5] performed a comprehensive review on the Alzheimer's Disease (AD), which is a devastating neurodegenerative disease and still open to the development of effective therapeutic methods. The authors discussed in detail about the toxicity of amyloid β protein (Aβ) dimer and oligomers as well as their interactions with cell membrane based on both experimental and computational research progresses. Based on the knowledge of the pathogenesis and atomic-level structural information, the authors further explored the applications of potential therapeutic molecules and nanoparticles in binding onto Aβ proteins and thus inhibiting their abnormal aggregation process.

REFERENCES

[1] Chan, C.; Du, S.; Dong, Y.; Cheng, X. Computational and experimental approaches to investigate lipid nanoparticles as drug and gene delivery systems. *Curr. Top. Med. Chem.*, **2021**, *21*(2), 92-114.

[2] Sharma, S.; Bhatia, V. Nanoscale drug delivery systems for glaucoma: experimental and *in silico* advances. *Curr. Top. Med. Chem.*, **2021**, *21*(2), 115-125.

1568-0266/21

[3] Gao, M.; Deng, H.; Zhang, W. Hyaluronan-based multifunctional nano-carriers for combination cancer therapy. *Curr. Top. Med. Chem.*, **2021**, *21*(2), 126-139.
[4] Rajalingam, K.; Krishnaswami, V.; Alagarsamy, S.; Kandasamy, R. Solubility enhancement of methotrexate by solid nanodispersion approach for the improved treatment of small cell lung carcinoma. *Curr. Top. Med. Chem.*, **2021**, *21*(2), 140-150.
[5] Wang, K.; Na, L.; Duan, M. The pathogenesis mechanism, structure properties, potential drugs and therapeutic nanoparticles against the small oligomers of amyloid-β. *Curr. Top. Med. Chem.*, **2021**, *21*(2), 151-167.

Prof. Xubo Lin
(Guest Editor)
Current Topics in Medicinal Chemistry
Beijing Advanced Innovation Center for Biomedical Engineering
Beihang University
Beijing 100191
China
Tel.: +8615510029836
E-mail: linxbseu@buaa.edu.cn
Website: http://shi.buaa.edu.cn/linxubo