Privileged Scaffold for Drug Design and Activity Improvement - Part III

Scaffolds have become increasingly important as privileged structures in the design and discovery of drugs. For rational drug design, some of the scaffolds, such as imidazole, have gained wide acceptability due to their drug-like properties. The review entitled “Imidazole Scaffold based Compounds in the Development of Therapeutic Drugs” focused on the recent developments of imidazole derivatives as well as their different pharmacological activities [1]. The imidazole scaffold interacted with different targets via hydrogen bonds, coordination, ion-dipole, cation-π, hydrophobic effects, etc. Two other aromatic heterocycles, thiadiazole and thiazolidinedione, had attracted Han and Sun’s attention [2], respectively. Thiadiazole and its unique chemical properties and biological characteristics showed strong anticancer, antibacterial, antifungal, anti-tuberculosis, anti-inflammatory, antiviral, anti-leishmanial, and other functions. Considering the important role of thiazolidinedione for anticancer drug discovery, its derivatives with different positions of the substituents had been clarified, showing involvement in anticancer development strategies, cancer progression, and metastasis. Except for the heterocycle scaffold, the review entitled “γ-AApeptides as a New Class of Peptidomimetics: Design, Synthesis, and Applications” focused on linear scaffolds [3]. γ-AApeptides possessed prominent advantages such as resistance to proteolytic degradation, enhanced chemodiversity, good selectivity, and outstanding bioactivity. Different intriguing structures and applications of γ-AApeptides had been developed by different approaches such as structure-based design, combinatorial library screening, and peptides self-assembly and folding with the potency of activities such as anticancer, anti-T2DM (Type 2 diabetes mellitus), anti-HIV (human immunodeficiency virus), and anti-Alzheimer’s disease. Interestingly, Qiu and her co-authors discussed the progress of artificial intelligence and cheminformatics-guided modern privileged scaffold [4]. Some representative cases with an emphasis on distinct research aspects are presented, including an update of the knowledge on privileged scaffolds, proof-of-concept tools, and workflows to identify privileged scaffolds. Beyond all question, this special issue covers a broad spectrum. I am hopeful that these papers will entertain readers.

REFERENCES