Recent Advances on Small Molecule Medicinal Chemistry to Treat Human Diseases

Medicinal Chemistry, in particular the small molecules-based drug discovery, is a challenging, strategic, and scientific key for augmenting the chemical facets of drug discovery. It helps us to understand how the chemical structure of bioactive molecules determines their pharmacodynamic/pharmacokinetic, as well as the physico-chemical properties and, hence, their therapeutic potential. Considering the quality/purity as well as the cost-effective nature of drug-like molecules, the present thematic issue discusses assistsances, trials, case studies, and industrial views for improving drug discovery programs. In this regard, drug discovery focuses on the design, synthesis, chemical characterization, and biological evaluation of novel compounds against biological targets of therapeutic, diagnostic, or theranostic interest, and/or the assessment of their physicochemical and pharmacokinetic properties.

In this thematic issue, several research and review articles contributed by the scientist in the area of Biological Science including current developments in rational drug design, medicinal chemistry, natural products, synthetic chemistry, biochemistry, new emerging multi-drug targets were collected. This issue begins with a research article on “Detection of natural inhibitors against human liver cancer cell line through QSAR, Molecular Docking, ADMET and System Pharmacology studies” by Khan and his group, reporting liver cancer QSAR model for Phytomolecule. This QSAR model showed a high activity descriptors relationship accuracy of 91%, referred by regression coefficient ($r^2 = 0.91$), and a high activity prediction accuracy of 89%. The external predicted (pred $r^2$) ability of the model was 90%. These results may be of great help for optimizing a new class of cancer lead from a very common, inexpensive, and non-toxic natural product [1].

The next article of this issue is a review article on the “Role of Extracellular Vesicles in Glioma Progression: Deciphering cellular biological processes to clinical applications” by Rana et al and focus on current diagnostic methods are limited in their data acquisition and interpretation, markedly affecting treatment modalities and patient outcomes. Circulating extracellular vesicles (EVs) or “magic bullets” contain bioactive signature molecules such as DNA, RNA, proteins, lipids, and metabolites. These secretory “smart probes” participate in myriad cellular activities, including glioma progression. EVs are released by all cell populations and may serve as novel diagnostic biomarkers and efficient nano-vehicles in the targeted delivery of encapsulated therapeutics. They describe the potential of EV-based biomarkers for glioma management [2].

Recently, many efforts have been made by various medicinal chemists around the world for the development of antifungal drugs with high efficacy with least toxicity and maximum selectivity in the area of antifungal chemotherapy. The role of various natural product inspired benzo-fused N-/O-containing bioactive heterocycles in medicinal chemistry in which significant advancements and developments in the area of 1,4-benzoxazine-3-ones, 1,4-benzoxazin-2-ones, spiropyrrolidine-/spiropyrrolizine-based fused heterocycles, benzopyran-fused coumarins and 2H-indazoles class of bio-heterocycles has been discussed in details. The third article of this issue is a review on the “Organic Antifungal Drugs and Targets of Their Action” by Maksimov at all. The study revealed that the methods of bioinformatics, genomics, and proteomics were extensively investigated for the development of new antimycotics. This review article incorporates some of the most significant studies covering the basic structures and approaches for the synthesis of antifungal drugs and the directions for their further development [3].

The fourth article of this issue is a review on “Coumarin-1,2,3-triazole Hybrid Molecules: An Emerging Scaffold for Combating Drug Resistance” by Upadhyay H. The study focus on overcome this problem either multidrug therapy or single drug acting on multiple targets may be used. The later are called ‘hybrid molecules’ which are formed by clubbing two biologically active pharmacophores together with or without an appropriate linker. Coumarins (benzopyran-2-one) are one of the earliest reported plant secondary metabolites having clinically proven diverse range of pharmacological properties to biomolecular targets. In this review we discuss recent advances in Coumarin-1,2,3-triazole hybrids as potential antibacterial agents aiming to provide a useful platform for the exploration of new leads with broader spectrum, more effectiveness, less toxicity with multiple modes of action for the development of cost-effective and safer drugs in the future [4].
The last article of this issue is a review on “MicroRNA-based therapeutic approach in Th2-mediated immune disorders” by kumar et al. The review focused on the role of miRNAs associated with Th2-disorders and strategies for therapeutic development and current clinical trials [5].

REFERENCES


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