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Special Issue Reprint

Heterocyclic Compounds in Medicinal Chemistry

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Although current medicinal chemistry landscapes seem to have changed thanks to the great advent of modern biological drugs, small molecules remain of crucial prominence in the identification of new drugs. Indeed, small molecules exert therapeutically favorable advantages, such as oral administration, tailored distribution, cell membrane crossing, accessible synthesis, and standardization. As a result, heterocycle-based small-molecule drugs represent the majority fraction of drugs currently marketed or in development. On the other side, the pharmacokinetic and pharmacodynamic properties, such as potency, selectivity, lipophilicity, polarity and water solubility can be modulated through the strategic inclusion of heterocycles in the molecule. Furthermore, heterocycles provide a fertile ground for the optimization of drug candidates due to their adaptable ability to hydrogen bond with target proteins, and the high prevalence of rings containing oxygen, sulfur, and nitrogen derives from their widespread presence in a wide range of natural products, whose structural motifs have always been emulated by the efforts of medicinal chemistry.

Taking all these aspects into account, this Special Issue has collected new studies and new perspectives on the topic, further emphasizing the challenges that are still open and possible in the field of medicinal chemistry.



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