Special Issue

Nitrogen-Containing Heterocyclic Compounds in Drug Design: Synthesis, Characterization, and Biological Activity

Message from the Guest Editors

Nitrogen-containing heterocyclic compounds are central to modern medicinal chemistry due to their structural versatility, reactivity, and roles in biological processes. They are the basis of nucleic acids, with purine and pyrimidine rings found in essential nitrogenous bases—adenine, guanine, cytosine, thymine, and uracil. Nitrogen heterocycles also appear in various biomolecules such as vitamins, coenzymes, hormones, antibiotics, and alkaloids. They are key components in many drugs, including antimicrobial agents, antidepressants, antihypertensive medications, and anticancer drugs. These structures enhance a drug's interaction with biological targets like enzymes, receptors, or nucleic acids, improving therapeutic efficacy and selectivity. Medicinal chemists also use nitrogen-based heterocycles to optimize pharmacokinetic properties like solubility and metabolic stability. This Special Issue aims to present recent advances in the synthesis, characterization, and biological properties of nitrogen-containing heterocyclic compounds. We welcome submissions of original research and review articles, as well as computational studies supporting drug candidate development.

Guest Editors

Dr. Anita Kornicka

Department of Chemical Technology of Drugs, Faculty of Pharmacy, Medical University of Gdansk, Gen. J. Hallera Av. 107, 80-416 Gdansk, Poland

Dr. Łukasz Balewski

Department of Chemical Technology of Drugs, Faculty of Pharmacy, Medical University of Gdansk, Gen. J. Hallera Av. 107, 80-416 Gdansk, Poland

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Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

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As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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