Special Issue

Design, Synthesis and Biological Evaluation of Novel Heterocyclic Antitumor Compounds

Message from the Guest Editor

Heterocyclic compounds, monocyclic and fused ring systems, represent the largest and most diverse family of organic compounds with biological active properties, namely antitumor and/or antiangiogenic activities. The ability to bind via hydrogen bonding or hydrophobic interactions seems to be an important factor in the development of target-based molecular designs using docking studies. Pharmacokinetics (absorption, distribution, metabolism, excretion, toxicity or ADMET) may also be predicted by in silico studies and confirmed afterwards. The synthesis of novel heterocyclic compounds with antitumor and/or antiangiogenic properties using different methodologies, including those that are more sustainable (green), continues to interest many researchers around the world. The evaluation of their antitumor/antiangiogenic properties and toxicity remains essential in the search for compounds with better efficacy and fewer side effects than the ones currently in use to treat different types of cancer.

Guest Editor

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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