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Design, Synthesis, and Evaluation of Multi-Target Ligands

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Message from the Guest Editor

Designing entirely new multi-target drug, although it seems very easy in concept, is in fact a complex task. The development of various strategies based on ligands or structures, experimental techniques, in silico, and artificial intelligence methods, increase the chances of success in this field. Computer-aided drug design based on modern techniques such as molecular docking, which accelerates screening, and molecular dynamics simulations, which add a "degree of flexibility" to structures, provide insight into the mechanism of ligand-target binding. In silico and artificial intelligence methods predict the physicochemical profiles of ligands and reveal structure-activity relationships. Both of these classes of methods significantly facilitate ligand modelling, analogue design and optimisation of leading compounds.

In this Special Issue, we welcome submissions on recent advances in the design, synthesis, evaluation and applications of multi-target drugs.

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Message from the Editor-in-Chief

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