Special Issue

Computational Tools for Drug Discovery in Veterinary and Biomedical Sciences

Message from the Guest Editor

Advances in computational technologies are transforming drug discovery across veterinary and biomedical sciences. This Special Issue explores how *in silico* tools accelerate the identification and optimization of novel therapeutics targeting infectious diseases, antimicrobial resistance, parasitic infections, and zoonoses. From molecular docking and pharmacophore modeling to molecular dynamics simulations and AI-driven virtual screening, these approaches enable cost-effective and efficient exploration of the chemical space. This Special Issue will highlight innovative studies applying computational pipelines to veterinary pathogens and neglected diseases, illustrating how digital tools can bridge the gap between laboratory research and clinical application. Contributions should also address challenges such as model validation, data quality, and the need for robust experimental confirmation. By showcasing interdisciplinary applications, this Special Issue aims to inspire the broader adoption of computational drug discovery in veterinary medicine and underscore its pivotal role in developing next-generation therapeutics that safeguard both animal and human health.

Guest Editor

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As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal *Applied Sciences* has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

Editor-in-Chief

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