

## Special Issue

# Role of Machine and Deep Learning in Drug Screening

### Message from the Guest Editors

The role of machine learning (ML) and deep learning (DL) in drug screening has emerged as a transformative force in addressing complex disease challenges. These technologies have proven especially effective in the discovery and optimization of therapeutic candidates (inhibitors) for high-priority diseases such as cancer, neurodegenerative disorders, infectious diseases, and metabolic conditions like diabetes. By leveraging large-scale biological and chemical datasets, ML and DL models are enabling precision in drug-target predictions, toxicity assessments, and virtual screening, significantly accelerating the pipeline for effective drug development. This Special Issue aims to gather state-of-the-art research and reviews that demonstrate the targeted application of ML and DL in drug screening, focusing on disease-specific use cases. It seeks to highlight advances in computational methodologies, their integration with experimental studies, and their impact on addressing unmet medical needs.

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### Deadline for manuscript submissions

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## Life

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