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Artificial Intelligence and Machine Learning in Drug Development

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Deadline for manuscript submissions:
closed (30 April 2022)

Message from the Guest Editor

Human biological complexity and genomic variability lead to different responses to therapeutic approaches at both the individual and population levels. Molecular profiling is now able to stratify diseases into their distinct molecular subtypes for matching with appropriate drugs, thus beginning to shape a translational systems medicine for better tailored predictive and pharmacotherapeutic guidance. This new research paradigm, powered by state-of-the-art artificial intelligence (AI)/machine learning (ML)-based prediction algorithms, presents great challenges and opportunities for researchers in the field.

This Special Issue welcomes original research, short communications, and review papers. Potential topics include, but are not limited to, the application of AI/ML to: target identification and characterization; protein networks/pathways prediction; mechanism of disease; drug–target complex formation and characterization; drug identification; drug repurposing; generation of novel drug candidates; drug efficacy metrics; and toxicology, biopharmaceutical properties prediction, etc. Wet-lab and clinical-data-based submissions with biomolecular experiments are welcomed.

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Message from the Editor-in-Chief

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