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The Computational Methods for Anticancer Drug Development

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Message from the Guest Editor

Dear Colleagues,

Computational methods have become increasingly popular in anticancer drug development. The availability of data sets as well as advances in new ML technologies enable us to apply ML methods, such as for guiding the high-throughput screening and optimization as well as identifying new drug targets, predicting treatment responses, identifying new biomarkers, and repositioning approved drugs. We now still face challenges on how to interpret most DL methods due to their complex "black-boxes" nature. Since most existing methods utilize preclinical disease models, very limited solutions currently exist that can make more clinically actionable predictions using different types of data, such as clinical data. Furthermore, user-friendly toolboxes are still lacking for non-computational cancer researchers, meaning powerful computational models are unable to be used in their research. In this Special Issue, we mainly focus on novel and explainable computational methods as well as easy-to-use toolboxes to accelerate the process of developing personalized anticancer treatments.

Dr. Liye He
Guest Editor

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Message from the Editor-in-Chief

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