In Silico Strategies for Prospective Drug Repositionings

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Message from the Guest Editors

Dear Colleagues,

The conventional drug discovery procedure is chronophagous and seldom successful; furthermore, new drugs are needed to address the clinical challenges we face. Within this framework, drug repositioning becomes a worthy drug discovery strategy.

Recent drug discovery techniques combine traditional tools with in silico strategies to identify previously unaccounted properties for drugs already in use. Indeed, big data exploration techniques capitalize on the ever-growing knowledge of drugs' structural and physicochemical properties, the drug–target and drug–drug interactions, and the latest discoveries in molecular and cellular biology.

We welcome papers presenting innovative methods that connect traditional drug discovery techniques with computer-based tools to deliver robust drug repurposing hints. We do not necessarily require in vitro or in vivo validation of such hints; however, the authors need to perform cross-validation with existing knowledge or other state-of-the-art drug repurposing pipelines.

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Special Issue

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Message from the Editor-in-Chief

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