



pharmaceutics



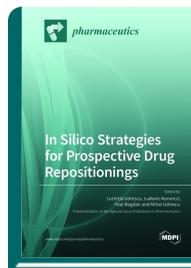
Special Issue Reprint

In Silico Strategies for Prospective Drug Repositionings

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The discovery of new drugs is one of pharmaceutical research's most exciting and challenging tasks. Unfortunately, the conventional drug discovery procedure is chronophagous and seldom successful; furthermore, new drugs are needed to address our clinical challenges (e.g., new antibiotics, new anticancer drugs, new antivirals).

Within this framework, drug repositioning—finding new pharmacodynamic properties for already approved drugs—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, drug–target and drug–drug interactions, advances in human biochemistry, and the latest molecular and cellular biology discoveries.

Following this new and exciting trend, this book is a collection of papers introducing innovative computational methods to identify potential candidates for drug repositioning. Thus, the papers in the Special Issue *In Silico Strategies for Prospective Drug Repositionings* introduce a wide array of in silico strategies such as complex network analysis, big data, machine learning, molecular docking, molecular dynamics simulation, and QSAR; these strategies target diverse diseases and medical conditions: COVID-19 and post-COVID-19



rosis, non-small lung cancer, multiple sclerosis, toxodermosis, psychiatric conditions.

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