Special Issue

Computational Intelligence (CI) Tools in Drug Discovery and Design

Message from the Guest Editors

The demand of new drugs has increased in the last decades. Therefore, the discovery and development of new drugs and their pharmaceutical forms need to be fast and efficient, while maintaining a high quality. This may require the use of computational intelligence (CI) tools. CI usually refers to a program which is able to solve complex problems without prior knowledge of a phenomenon, by learning from data or experimental observations. Computers currently surpass the human brain in terms of data processing, and, if properly designed, computer programs could significantly accelerate the development of new drugs. Moreover, CI tools could help to discover complex and sometimes unobvious interactions between drugs and biological targets. The purpose of this Special Issue is to gather novel and interesting scientific research regarding the applications of computational intelligence tools in drug discovery and development. The focus will be on research articles and reviews on drug dosage forms and novel substances whose development was motivated by CI tools. Studies on other technological and pharmaceutical aspects of computer-aided drug design will also be welcome.

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