Role of the Computational Intelligence in Drugs Discovery and Design: Introduction, Techniques and Software

Abstract

Drugs discovery & design is an intense, lengthy and consecutive process that starts with the lead & target discovery followed by lead optimization and pre-clinical in vitro & in vivo studies. This paper throws light on different computational techniques that play a vital role in the drugs discovery & design process. Earlier, computational techniques are use in the field of computer science, electrical engineering and electronics & communication engineering to solve the problems. But, now day's use of these techniques has changed the scenario in drugs discovery. & design from the last two decades. This paper present brief description of different computational techniques such as Particle Swarm Optimization, Ant Colony Optimization, Artificial Neural Network, Fuzzy logic, Genetic Algorithm, Genetic Programming, Evolutionary Programming, Evolutionary Strategy and also provide a tabular comparison of these techniques as well as a list of computational tools/ software.

References
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- James Cunha Werner and Terence C. Fogarty, "Genetic programming applied to pharmaceutical drugs design", The Seventh ACM SIGKDD International Conference on Knowledge discovery and data mining, USA/ San Francisco, August 26-29, 2001.


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