UNIVERSITÀ DI TRENTO
Dipartimento di Fisica

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Artificial Intelligence in Drug Discovery: from Predictive to Generative Models

Abstract

Drug Discovery (DD) is a resource-intensive and time-consuming process that requires significant financial investments. The pharmaceutical industry is prioritizing the acceleration of the DD pipeline, and computational tools are playing an increasingly important role in minimizing the number of candidates that must undergo expensive pre-clinical and clinical testing. Recent advancements in artificial intelligence, particularly in the field of deep learning, have led to the emergence of new in-silico approaches that have been successfully applied, revolutionizing the pharma industry. Two representative case studies will be presented:

- A structure-based investigation enabling the building of predictive models for in-silico cardiac safety assessment of drug candidates.[1] This goal was achieved by using a machine learning algorithm that enabled the integration of docking scores and protein-ligand interaction fingerprints (i.e., LASSO regularized support vector machines).
- A deep learning generative algorithm called DeLA-Drug,[2,3] which was developed for denovo design of similar-to-bioactive compounds. This algorithm is based on a recurrent neural network model and is intended to automate the generation of new drug-like compounds. DeLADrug, available as a free web platform (http://www.ba.ic.cnr.it/softwareic/deladrug/), will be presented as an attractive tool for medicinal chemists interested in generating focused libraries for further virtual screening procedures.

[1] T.M. Creanza, P. Delre, N. Ancona, G. Lentini, M. Saviano, G.F. Mangiatordi Journal of Chemical Information and Modeling 2021, 61 (9), 4758-4770.
[2] T.M. Creanza, G. Lamanna, P. Delre, M. Contino, N. Corriero, M. Saviano, G.F. Mangiatordi, N. Ancona Journal of Chemical Information and Modeling 2022, 62 (6), 1411-1424.
[3] G. Lamanna, P. Delre, G. Marcou, M. Saviano, A. Varnek, D. Horvath, G.F: Mangiatordi, Journal of Chemical Information and Modeling 2023, 63 (16), 5107-5119

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