Contribution ID: **22** Type: **not specified**

DeLA-Drug: A Deep Learning Algorithm for Automated Design of Drug-like Analogues

Wednesday, 21 June 2023 16:10 (15 minutes)

We present DeLA-Drug,(1) a recurrent neural network (RNN) model composed of two Long Short-Term Memory (LSTM) layers and conceived for data-driven generation of drug-like compounds. DeLA-Drug captures the syntax of SMILES strings of more than 1 million molecules belonging to the ChEMBL28 database and generates analogues starting from a single user-defined query compound by employing a new strategy called Sampling With Substitutions (SWS). The generative model preserves drug-likeness and synthetic accessibility of the known bioactive compounds belonging to the ChEMBL28 repository. The absence of any time-demanding fine-tuning procedure enables DeLA-Drug to perform a fast generation of focused libraries for further high-throughput screening and makes it a suitable tool for performing de-novo design even in low-data regimes. DeLA-Drug, available as a free web platform (http://www.ba.ic.cnr.it/softwareic/deladrugportal/), can help medicinal chemists interested in generating analogues of compounds already available in their laboratories and, for this reason, good candidates for an easy and low-cost synthesis.

See the attached picture: Main steps of the DeLA-Drug workflow.

[1] Creanza, T. M.; Lamanna, G.; Delre, P.; Contino, M.; Corriero, N.; Saviano, M.; Mangiatordi, G. F.; Ancona, N. DeLA-Drug: A Deep Learning Algorithm for Automated Design of Druglike Analogues. J. Chem. Inf. Model. 2022, 62 (6), 1411–1424. https://doi.org/10.1021/acs.jcim.2c00205.

Presenter: Dr LAMANNA, Giuseppe (IC-CNR)

Session Classification: Session