Tentative Outline

Special Thematic Issue for the Journal: Drug Delivery Letters

Title of thematic Issue: New Age of Deep Learning in Drug Discovery: Research to Practice

Guest Editor: Dr. Wali Khan Mashwani

Scope of the Thematic Issue:

Deep Learning is a kind of machine learning established on artificial neural systems in which numerous levels of the process are employed to gradually extract superior features from informational data. Deep Learning ensures pharmaceutical discovery, comprising progressive image study, the prognosis of molecular form and process, and automatic creation of creative chemical substance commodities with custom effects. Deep Learning has reformed most dimensions of science and technique, containing drug discovery.

Drug Discovery is included in sites that can benefit from this success of Deep Learning. Drug Discovery is a very time-consuming and expensive task, and Deep Learning can make this process faster and cheaper. Over the past several years, there has been a remarkable enlargement in the amount of available combination training and biomedical data owing to the appearance of distinctive practical approaches such as HTS, and parallel synthesis, among others. In large-scale alchemy, data evolves into a critical problem for drug discovery. Deep Learning enormously expedites the Drug Discovery approach and provides global measures to prevent the dissemination of transmissible diseases. Furthermore, improving the productivity of straining antimicrobial combinations in opposition to a wide range of pathogens, Deep Learning has even the prospect of effectively and dependably recognizing drug contenders against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Therefore, Deep Learning has successfully identified several potential drugs against SARS-CoV-2. AI incorporated with Deep Learning furnishes more additional effects on drug discovery. Deep Learning accesses a future in this area to create new drug innovations to control, handle, alleviate or heal diseases. More progressive technology guides the immediate vision and develops quicker. It is even a complicated method, expensive, and takes a lot of time. It is high-priced due to elaborate data standards, and it needs additional informational data to execute a task. This applied science is extending quicker from day one today. Current improvements in AI and the development and evolution of more complicated machine learning approaches have created a massive consequence on the pharmaceutical outcome process. AI applied science can handle several major challenges, mainly decreasing cost, duration, and function demands throughout earlier drug discovery, by manipulating silico techniques, amalgamation prediction, and bioactivity forecast. An expansion method from machine learning is Deep Learning.

The specialization of supervised drug structure and molecular treatment is positioned to increase proportionally, assisted significantly by inroads created in omics research, preciseness medicine, big data capture and computation, Deep Learning, and artificial intelligence. Based on the above, in the present Special Issue, we invite researchers to contribute original research articles and review papers that will approach that it is not challenging to envision that one day individually patients will satisfy with the benefit of smart developer drugs customized to that specific individual.

Keywords:

- Parallel Synthesis
- SARS-CoV-2
- Pharmaceutical Discovery
- Silico Techniques
- Big Data Capture and Computation
- Omics Research
- Bioactivity Forecast

Sub-topics:

- Deep Learning ineffective screening of Potential Drug Candidates for Specific diseases
- Deep Learning algorithms in the formulation of drug delivery device
- Deep Learning and its potential benefits include increased safety, reduced development time, and improved patient outcomes.
- Deep Learning and its application in detecting and recording the location of the drug particle and its delivery to the target site
- DL algorithms for enhancing the Bioavailability of Drugs to the targeted site of action
- DL-driven automated Strategy for the preparation of paclitaxel nanoparticles
- Deep Neural Networks and their role in drug discovery, especially for predicting the therapeutic potential of new chemical entities
- Deep Learning in early-stage drug-lead molecule identification
- Integrated DL algorithms for a better understanding of molecular interactions among proteins
- Deep Learning-based Neural Networks for simulating Pharmacodynamic and Pharmacokinetic studies
- DL for analyzing the Drug Physicochemical parameters
- DL in Evaluating the toxic parameters of the developed drug molecule

Tentative titles of the articles:

- Deep Learning-based Drug Screening: Traditional to Modern Research Practices
- DL and Drug formulation: A insilico-based Approach
- Enhancing the Bioavailability of Drugs through Deep Learning Approaches
- DL for Evaluating Drug Physico-chemical parameters: A Computational Approach
- DL for screening Drug toxic parameters: From Research to Reality
- DL for Effective understanding of Molecular mechanisms in cells
- Deep Learning-based Neural Networks for simulating Pharmacodynamic and Pharmacokinetic studies
- DL-driven automated Strategy for the preparation of paclitaxel nanoparticles
- Deep Learning and its application in detecting and recording the location of the drug particle and its delivery to the target site
- Deep Neural Networks and their role in drug discovery, for predicting the therapeutic potential of new chemical entities

Schedule:

- ✧ Article Submission Deadline: Oct 1st 2022
- ✧ Authors Notification Date: Nov 1st 2022
- ✧ Revised Papers Due Date: Dec 1st2022
- ✧ Final notification Date: Mar 1st 2023

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