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Abstract

Artificial Intelligence in Drug Discovery

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Abstract:
Artificial Intelligence (AI) takes up anessentialaction in drug discovery. Specifically, artificial neuralnetworksystems such as deep neural network systems or recurrentnetworksystems drive this zone.The productivity of pharmaceutical industries is on the decay. Disappointment rates of clinical trials surpass90% after treatments are tested in model organisms, and the expenseto developanother medication surpassesbillions of dollars. Current advances in AI may assistwith switching this pattern and quicken and improve pharmaceutical R&D. While the term AI and the idea of profoundlearning are not new, current advances in superior computing, the accessibilityof huge annotated data sets required for training, and new frameworks for implementing deep neural network systems (DNN) brought about an extraordinaryacceleration of the field. Since 2014, it has been found that the DNN have outperformedhuman accuracy duringvoice,image, and text recognition, independent driving, and numerous differenttasks.Greatness of the rapiddevelpoment of the computing ability and the fastadvancementof the computational biologyandchemistry, the computer-aided drug design techniques have been effectively appliedin pretty much every phaseof the drug discovery and advancementpipeline to acceleratethe procedure of research and diminishthe expense and hazard identified withclinical and preclinical trials. In 2017, numerouspharmaceutical industries started joining with AI startups and academics or initiated internal R&D programs. From training DNN on transcriptional repercussioninformation for forecasting the pharmacological actions of small molecules and biomarker improvement, to the creation of novel chemistry, profoundlearning procedures quickly engendered into numerous zonesof biomedical research.Inferable from the improvementof AI hypothesisand the collection of pharmacological information, the AI innovation, as a super strong data mining tool, has cut a figure in differentfields of the drug design, for example,action scoring, virtual screening, quantitative structure-activity relationship (QSAR) experiment, de novo

drug design, and lastly the in silico evaluation of absorption, distribution, metabolism, excretion and toxicity (ADME/T) characteristics.In spite of the fact that it is as yet testing to give a physical clarificationof the AI-based models, it indeed has been acting as anextraordinary capacity to help controlling the drug discovery through versatile framework. Currently, because ofthe strong generalization capability and strong feature extraction capacity, profoundlearning strategieshave been usedin foreseeingthe molecular properties just as creating the desired molecules, which will additionallypromote the utilizationof AI innovationsin the field of drug design.

Biography:
Sagorika Rai have done 2 month training in CSIR-SRTP during June to August in 2020. In these training, I work on Project Title: Interdisciplinary approach for sustainable use of resources.

Publication of speakers:

- Gao, X. W.; Qian, Y. Prediction of Multidrug-Resistant TB from CT Pulmonary Images Based on Deep Learning Techniques. Mol. Pharmaceutics 2018.
- Russo, D.; Zorn, K.; Clark, A.; Zhu, H.; Ekins, S. Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. Mol. Pharmaceutics 2018

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