Machine learning models for predicting drug properties

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Technology

There is a huge unmet medical need in the biopharma to accelerate drug discovery and development, reduce costs, increase safety and lower the risk for faliures. While hundreds of start-ups are using artificial intelligence (AI) tools in drug discovery, the progress is far too slow, to specific and the need still remind high for novel AI-based-solutions. Here, the researchers generated models which are based on supervised multimodal machine learning (ML) to resolve this problems. Their unique approach is combining fusion of multiple drug modalities from over 200 drug-related databases and literature review, applying recommender systems methos for modelling graph interactions, active learning with doamine expert in the loop and most importantly focus on the activity rather than specific targets. The *in silico* models are optimized, evaluated and validated using *in vitro* and *in vivo* research done by medicinal chemists and pharmacologists. The researchers developed drug properties predicting tools to drug-drug interaction, drug safety, drug recall and drug synergy. More than that they generated model to predict activity of drugs. At first, in order to developed the model this was done on known drugs (repurposing). The model was trained with several enriching drug features. The result was that combining two features, drug-drug interaction and drug-target interaction, demonstrated superior performance. Based on this model and domain expert opinion, 3 coumpounds with anti-cancer activity were chosen and examined *in vitro* and *in vivo*. Currently, the reseachers develop predication models for generation and optimization of new chemical entity (NCE).

Application

Ml tools to be applied during all stages of drug discovery and drug development to shorten process, reduce risk, increase profit. The tools pave the way for discovery of NCE.

Advantages

- ML approach that allowes identifying new properties for known and unknown drugs
- The tools are being optimzated and validated with researchers expert in the field of medicinal chemistry and pharmacology
- The models are based on information available already at early stages discovery. Contrary, current methods used for drug safety prediction are largely using data available in advanced stages of drug development, or even after the drug is released on to the market
- Can be used for drugs from discovery stage till market

Patent

Patents covering the following inventions were filed by BGN technology