LAKIC Aleksandra

L0

Source: Google Scholars

Big Data and AI Modeling for Drug Discovery

KEYWORDS: Drug research and discovery, Artificial Intelligence, deep learning, Big Data, cloud computation, GPUs, missing pieces of information, biased results, machine learning, Rational Nanomaterials Design, Convolutional Neural Networks (CNNs), Personalized Medicine.

Drug research and development has turned out to be a very complexed process that tackles many challenges, especially in clinical studies due to high churn rate. With the evolution of use of **Artificial Intelligence**, in particular of **deep learning** in this case, a certain improvement was noticed in regard to advancements in rational drug discovery.

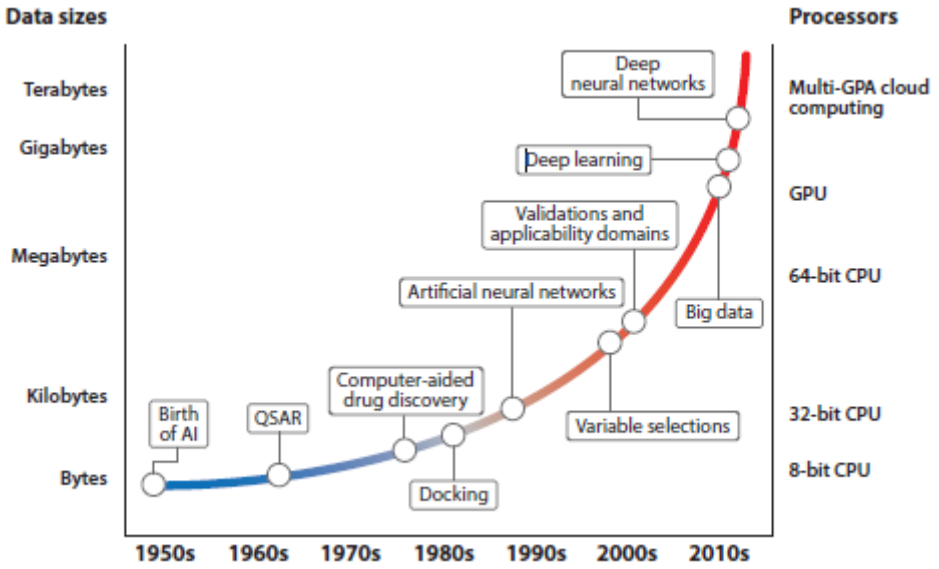
Even though revolutionizing of drug discovery was backed by the use of **Big Data**, the managing of vast data on compounds, targets, mechanisms, interactions and toxicity, that is generated by notable databases, such as **PubChem**, **ChEMBL**, **DrugBank**, **DrugMatrix**, and **BindingDB**, has arisen many difficulties. However, the adoption of cutting-edge hardware techniques as **cloud computation** and **GPUs** was imposed as solution to processing and analyzing these enormous data.

Among other issues generated by using big data for drug discoveries the fact that there are oftentimes **missing pieces of information**, which can cause **biased results** and therefore a disproportion of **active** and **inactive responses**[1]. For example, well-known drugs like acetaminophen and aspirin show different numbers of effective and ineffective outcomes. In the past, in order to tackle the missing data issue, a singular solution was proposed for each test. Nonetheless, for handling such complex data, **advanced methods** are necessary, such

[1] **active** and **inactive responses** indicates that the tested drug or compound has demonstrated a desired (for active) and non-desired (for inactive) effect or activity.

as **machine learning** before-mentioned, particularly the recent advancements in **deep learning**, which helps to adjust the data to balance positive and negative results.

The following photo shows the **historical progression of artificial intelligence (AI) in drug discovery**, from early machine learning techniques to the emergence of deep learning in the 2010s.



There are other areas of computational modeling that use AI for drug discovery, such as **Rational Nanomaterials Design** that involves nanotechnology for drug delivery and the use of AI in modeling nanoparticle interactions. In terms of **Convolutional Neural Networks (CNNs)**, AI is used in clinical diagnoses and drug discovery, by recognizing molecular features and predicting cancer outcomes. Moreover, in the domain of **Personalized Medicine**, there is a significant importance of computational modeling's role in drug-target predictions and supporting precision medicine initiatives.