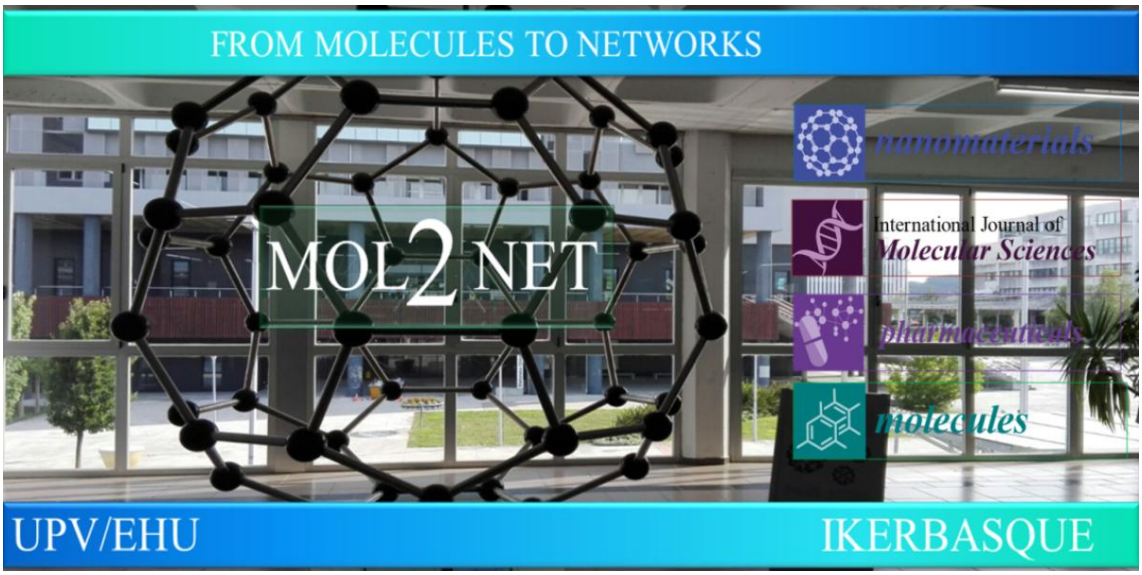

Drug discovery is a process that takes several years (Figure 1.), as it includes several different plashes, apart from being complicated, expensive, and time-consuming. Because of that, nowadays scientists and informatics are increasingly working together in the processes of drug discovery using technology based on Artificial Intelligence (AI).

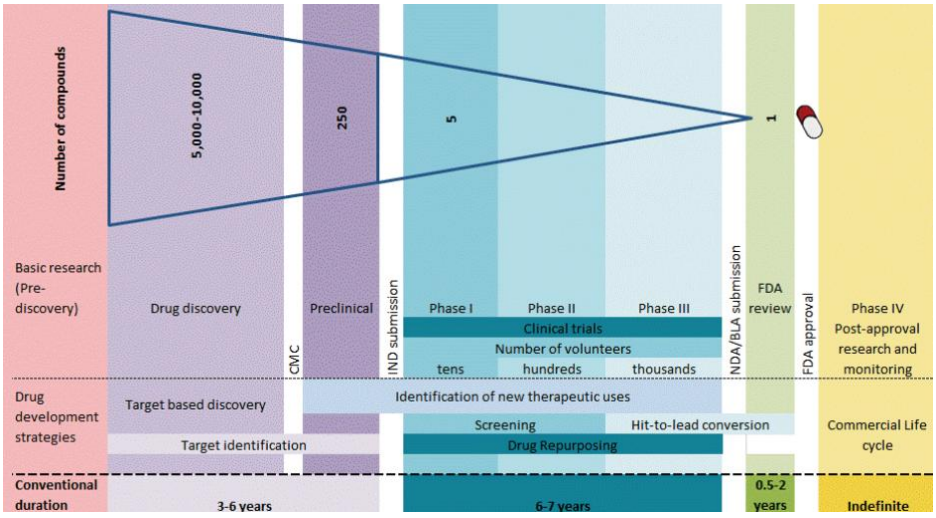

Figure 1. Drug discovery using conventional methods [1].

Computer tools were developed for being able to identify potential biological active molecules from great numbers of candidate compounds quickly and cheaply. But, when drug discovery moved into the area of AI and big data, using Machine Learning (ML) and Deep Learning (DL) was started to be possible to analyze clinically relevant massive amounts of data that guide the discovery of new potential targets, and consequently drug discovery.

As of today, several drugs were discovered using this technology. For example, the first drug created using AI was DSP-1181, which is a potent serotonin 5-HT_{1A} receptor agonist [2]. The

time that took the discovery of it was less than 12 months from initial screening to the end of preclinical testing.

In conclusion, taking into account that in science time is the key, the use of AI and big data is an option that nowadays needs to be used more and more.

[1] Hassan Farghali, Nikolina Ktinova Canová, Mahak Arora. The Potential Applications of Artificial Intelligence in Drug Discovery and Development. Physiol. Res. 70 (Supp. 4).2021.

[2] Balfour 2021, Sumitono Dainippon Pharma 2020.