

Drug discovery driven by artificial intelligence

M Jean-Philippe RAMEAU (Molecular Design Science France, Paris)

Abstract

Drug discovery is a complex problem: finding a synthetic chemical that fulfills all the requirements to become a drug is a challenge. Over the years the process of discovery has evolved from observation and serendipity to more data-driven and then rationally data driven. Even if we claim from decade that the rational drug design is a core activity of drug discovery, the evolution of computing capabilities and the development of new algorithms especially in the field of Artificial Intelligence (AI) have given a boost to this domain. Today AI is under the spotlight in drug discovery and some recent developments in machine learning especially neural networks brought interesting opportunities for the chemical space exploration.

I will present some examples of Machine-learning capabilities, from the single point exploration of chemical space to the optimized exploration of the chemical space provided by the de-novo design by reinforcement learning (GenAI). Machine learning can also be used on top of other traditional physics-based technologies to increase the capability and access to numbers not usually accessible i.e., Virtual-Screening or combined with Free-Energy Perturbation. Combination of machine learning and first principal technologies gives access to a powerful mixed technology pushing the boundaries of research. A lot is expected from these technologies to explore the "druggability" of some difficult biological systems.

These algorithms are used daily to support our research portfolio but still the most important operation remains the decision-making process. Although assisted by machine especially using multi-parametric optimization, the human remains at the center. In this respect AI provides a real improvement of our "In-silico toolbox" but on a project perspective the intelligence lies into the team. Today we refer to "Augmented Medchem" or "Augmented Intelligence" when speaking of this shift of ways of working. But still drug discovery remains a complex problem...