Artificial Intelligence in Drug Discovery - From Model to Process, From Academic Publication to Decision Making

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The amount of chemical and biological data available has increased in the public as well as the private domain, and both on the algorithmic and hardware side progress has been tremendous in machine learning. Press releases describe the design of functional proteins and antibodies from scratch, and several 'first AI-designed drugs' have already entered clinical phases.

However, all is not well when it comes to the marriage of algorithms with drug discovery, in particular when it comes to the *in vivo* relevance of what we are able to do with chemical and biological data at this point in time. Reasons for this are that the field is still stuck in reductionist thinking, in combination with a lack of relevant data and our ability to handle it computationally to support decision making. Likewise, chemical space behaves very different from biological information, which has a distinct impact on our ability to use predictive models in decision making processes.

This contribution will review the current status of the field, as well as provide case studies where data and computational methods have been able to select compounds with the desired effects on a biological system, and explain what currently still hampers further progress.

Further Reading:

Bender A, Cortés-Ciriano I. Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 1: Ways to make an impact, and why we are not there yet. Drug Discov Today. 2021 Feb;26(2):511-524. doi: 10.1016/j.drudis.2020.12.009. (open access)

Bender A, Cortes-Ciriano I. Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 2: a discussion of chemical and biological data. Drug Discov Today. 2021 Apr;26(4):1040-1052. doi: 10.1016/j.drudis.2020.11.037. (open access)