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Beyond the hype, How AI is disrupting drug discovery and development

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Introduction Artificial Intelligence (AI), has already disrupted many industries, Herein, we investigate why the pharmaceutical industry is lagging behind in adoption & discuss the potential of non-pharma technologies

Method Based on industry-wide published surveys, peer-reviewed articles and market research on current applications of AI in drug discovery and development, this study tackles the question from two different angles: 1. The stages of drug discovery and development that machine learning has made the most progress so far & where do future potential areas lie. 2. The machine learning (ML) techniques applied in accelerating the process of development and upcoming trends.

Results Artificial Intelligence is gaining traction at several stages of development in the drug discovery process. Most tangible progress has been made in: Target selection; data mining and identification of drug-disease connection & relevant biomarkers as predictive tools for efficacy. Another approach involves processing data from diseased & healthy tissues and identifying targets through supervised learning. In lead discovery, progress has been made in studying target engagement and prediction of drug-like properties. One of the areas that machine learning could have a significant impact is synthesis-ability of small molecules. The challenge here is lack of sufficient data and more fundamentally, un-recorded data. Barrier to adoption in pharma is primarily the knowledge gap and lack of data science and technical expertise. Additionally, at research and earlier stages of development, insufficient data for statistically meaningful analysis and predictive possibilities. There is a demand for setting industry-wide best practice for data standards and pre-competitive collaboration to leverage the potential of data generated at different stages of drug discovery and development.

Conclusion AI has the potential to revolutionise drug discovery. This paper intends to raise awareness about the machine learning tools at hand. More importantly, what we can do as the drug discovery community, both in academia and in industry to leverage the potential of non-pharma technologies, streamline drug discovery process and ultimately bring benefit to patients.

References

1. Schneider G (2018). Nature Reviews Drug Discovery volume 17, 97-113.
2. Katsila T *et al (*2016) Computational and Structural Biology Journal 14, 177-184.
3. 44% of Life Science professionals Already Using or Experimenting with AI & Deep Learning, Finds Survey from the Pistoia Alliance http://www.pistoiaalliance.org/pa-ai-survey/