



## Cover Story

## Does artificial intelligence have the potential to transform drug formulation development?



Artificial intelligence (AI) and machine learning are some of the hottest buzz words of our time and are said to have the potential to revolutionize every industrial sector. In the past decade, interest in AI has exploded, with evidence of uptake in the pharmaceutical industry as well as drug discovery and development efforts in academia. Fig. 1, shows how the number of publications related to drug development, and encompassing some form of computational prediction or simulation element, has been growing in the last two decades. Table 1 summarizes a number of recent partnerships between ‘Big Pharma’ and AI companies. One example of Big Pharma’s embrace of AI, which has been making headlines recently, is the establishment of the Novartis AI Innovation Lab in collaboration with Microsoft Corp. [1]. Satya Nadella, CEO of Microsoft, said, “Our strategic alliance will combine Novartis’ life sciences expertise with the power of Azure and Microsoft AI. Together, we aim to address some of the biggest challenges facing the life sciences industry today and bring AI capabilities to every Novartis employee so they can unlock new insights as they work to discover new medicines and reduce patient costs” [1].

As to be expected, alongside excitement and enthusiasm, AI has brought considerable fear and anxiety. Corporations are scrambling to ensure they are not left behind, while, workers are concerned with potential job losses. This is not surprising given that AI is defined as “the ability of a digital computer or computer-controlled robot to perform tasks commonly associated with intelligent beings” [2] or “the capability of a machine to imitate intelligent human behavior” [3]. However, it’s important to recall that as a society, we have already lived through many technological advancements that have transformed

work. Examples are the invention of the personal computer and the proliferation of the internet. Do you remember using a typewriter to write-up your scientific papers or the need to graph data by hand? If you are too young to remember, then imagine life without your cell phone or personal computer and their accompanying software. These technological advancements have led to many improvements in our lives and in the way in which we conduct scientific research.

So how will AI impact us as pharmaceutical scientists? Will it and can it replace us? To date, as highlighted in Ajay Agrawal, Joshua Gans and Avi Goldfarb’s book *Prediction Machines*, the “new wave of AI does not actually bring us intelligence but instead a critical component of intelligence – prediction” [4]. At this time AI is considered “a technology of low-cost prediction and discovery” [5]. How can we tap into this? What prediction problems do we have in pharmaceutical sciences, in particular in drug delivery?

Many of us, in formulation science and drug development have considered theoretical models or computational simulations as a means to predict drug-material compatibility and to fast-track drug development efforts [6–10]. However, to this point, most often we rely on hands-on experiments to identify the most promising drug formulation candidates. Can AI change this?

In the current issue of JCR, Han et al. use machine learning techniques to develop an intelligent model to predict the physical stability of solid dispersion formulations. A challenge which can hinder the development of such formulations into effective drug products [11]. The “integrated experimental, theoretical, modeling and data-driven AI methodology” used in this study may be applicable to development of

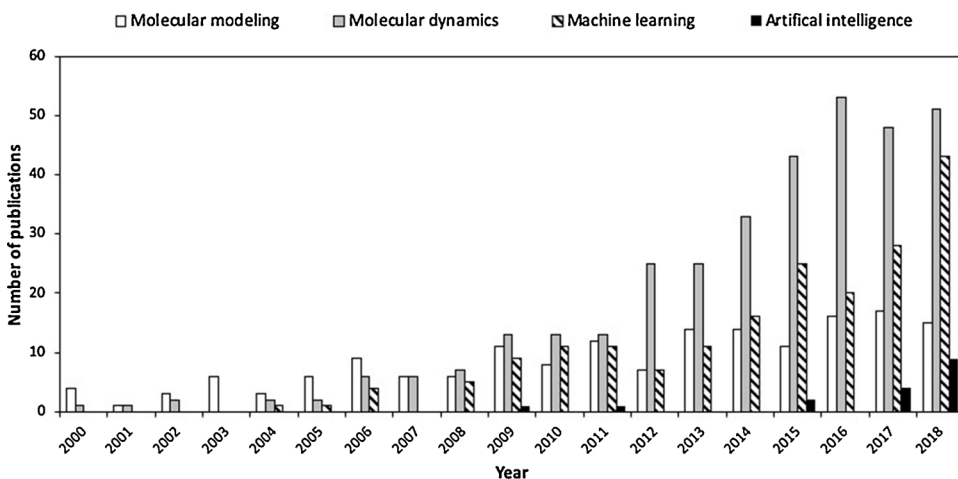


Fig. 1. Number of publications harnessing machine learning or computational tools for drug development in recent years. Source: Web of Science (Clarivate Analytics), September 30, 2019. Keywords “drug development” and “molecular modeling” or “molecular dynamics”, or “machine learning” or “artificial intelligence”.

**Table 1**  
Sample of key partnerships pursued between ‘Big Pharma’ and AI companies.

Pharmaceutical Company	AI Partnership	Project Description
AstraZeneca	Berg	To investigate therapeutic targets for treatment of neurological diseases.
	BenevolentAI	To pursue novel treatments for chronic kidney disease and idiopathic pulmonary fibrosis.
Bristol-Myers Squibb	Sirenas	To identify potential lead drug candidates for difficult therapeutic targets.
Gilead	Insitro	To identify and develop therapeutics for non-alcoholic steatohepatitis.
GSK	Exscientia	To identify lead candidates which are selective for various disease targets across a multitude of therapeutic areas.
	Insilico Medicine	To discover novel biological targets and molecules.
Novartis	Microsoft Corp.	To create new AI models and applications to tackle the next wave of challenges in medicine.
	Intel	To reduce the amount of time required for the analysis of microscopic images.
Takeda	Numerate	To develop new clinical candidates in the areas of oncology, gastroenterology and central nervous system disorders.

other dosage forms [11]. Han et al., screened eight different machine learning systems and compared their predictive power to experimental evidence. The authors found that the random forest (RF) model, originally developed by Tim Kam Ho in 1995 [12], achieved the best prediction accuracy in this study (82.5%). The predictive power of models such as these have the potential to fast-track drug development and lower the time and financial costs associated with current drug development. Perhaps predictive AI even has the potential to lessen drug attrition rates?

Will AI take over? Or the question that we all care about and may be afraid to ask: will it replace us? You may take comfort in reading ‘Prediction Machines’ as it reminds us that a “prediction is not a decision” [4]. There are many other components of a decision including data collection, judgement and action. As prediction becomes cheaper and more accessible the value of the complements including “human judgement” will increase [4].

As a community, we need to continue to embrace AI, after all it is everywhere, and we need to determine how to most effectively use it to streamline drug formulation and related drug development efforts.

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