



# editorial



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## The Art of Virtualizing Pharma R&D

In the last two decades, virtual research and development (R&D) in the pharma sector was characterized by decentralized R&D structures, open innovation models, out- and in-licensing, and new forms of research collaborations. Today, virtualizing pharma R&D is increasingly related with data analytics and artificial intelligence (AI), technologies that have been developed by software companies outside the healthcare sector. The process of virtualizing pharma R&D is closely related to the technological advancements that result in the generation of large data sets ranging from genomics, proteomics, metabolomics, medical imaging, IoT wearables and large clinical trials, making it necessary for pharma companies to find new ways to store and ultimately analyze information. As a consequence, pharma companies are experimenting with AI in R&D ranging from *in-silico* drug design to clinical trial participants identification or dosage error reduction. They expect to benefit from

new drug targets, improved lead compounds, fundamentally new understandings of biological mechanisms or the predictions of market behaviors. An example demonstrating the effectiveness of AI in drug discovery is Alphabet's (Google's) subsidiary DeepMind whose AI system AlphaFold won the Critical Assessment of Structure Prediction experiment, an international protein 3D-structures simulation contest [1]. The relevance of AI is indicated by a projected pharma market potential of USD 10 billion by 2024, a foreseen 10–25% clinical trials costs reduction or an expected annual growth rate of healthcare data of 48% [2,3,4].

### Who are the new players in the AI-pharma sector?

The pharma-related AI market is strongly growing. It consists of about 1.000 healthcare-related AI companies globally. Most of them are start-ups that were founded in the past 10 years [5]. The market leaders are tech giants such as Google, Amazon, Microsoft and IBM, which have already successfully entered the healthcare sector, acquired AI companies to strengthen their technology leadership position in a global growth market and have used this next generation technology to access the pharma business. In addition to these new entrants, further new competitors for pharma companies arise through partnerships of service providers and AI-specialists. For example, Atomwise, an AI company that uses deep learning algorithms for compound screening, recently signed a potentially USD 2.4 billion strategic alliance with Charles River Laboratories to provide end-to-end drug discovery solutions [6].

The AI technologists come from less regulated industries. They make easy use of the given opportunities and provide their technological competencies to pharma companies which strengths and expertise are in developing safe and efficacious drugs. The lack of R&D efficiency and the productivity gap of the pharma industry coupled with the yet to be developed AI-competency of drug makers provide great opportunities for AI companies to shape and maybe disrupt the pharma sector.

Today's situation reminds us in many aspects of the late 1990s when there was a "gold rush" regarding new technologies in drug discovery. Meanwhile, the value of deciphering the human genome or of HTS has been put into a more realistic perspective [7].

## What are the hurdles pharma companies face to leverage AI?

An AI-driven R&D strategy is not easy to implement, and pharma companies are cautious with AI-related major investments. As of now, none of the top pharma firms has made a deal of the size of Alphabet's USD 600 million acquisition of DeepMind. The reasons are manifold:

The number of AI experts on the market is limited and pharma companies need to compete with banks, carmakers and IT companies to get the best brains. AI talents are not attracted to the highly regulated pharma industry. The lack of willingness to share proprietary data, the worries about data quality and the use of AI in decision-making ("garbage-in, garbage-out") are further hurdles. The fear to lose ground when collaborating closer with the insatiable tech giants, unclear business cases, the lack of regulatory rules for AI or financial claims of AI-providers are additional challenges they face. A sometimes too conservative perspective towards new technologies, a risk-aversion of pharma executives to make investments outside the core business, and unprofitable investments for formerly new technologies are further barriers for an AI-driven strategy. Lastly but importantly, AI has not yet fully materialized in the pharma business.

## How do pharma companies make AI part of their strategy?

In our perspective, smaller and medium-sized pharma companies have neither the financial power nor the absorptive capacities required to be successful in the AI market. They may have the opportunity to collaborate with specialized AI companies in niches in order to start the AI learning process.

The level of activity of the big pharma players is diverse today and they seek different strategies to leverage AI. Some companies are focused on ongoing business challenges such as blockbuster patent expiration or post-acquisition integration efforts, which make AI for them a second priority at this stage. The consequences are not predictable, but there are examples from other industries, such as Kodak, that illustrate what can happen to former market leaders if they miss fundamental breakthrough innovations. In contrast, Novartis, AstraZeneca or GlaxoSmithKline are very serious about leveraging the potential of AI. For example, Novartis has developed an AI-driven strategy that aims to systematically use AI in marketing, sales and R&D, made the digital and AI-technologies to an executive board priority, and recently created the position of a Chief Digital Officer. Vas Narasimhan, CEO of Novartis, said, that "*we need to become a focused medicines company that's powered by data science and digital technologies*" [8]. The recent deal with Oxford's Big Data Institute illustrates that in particular, R&D is a focus area for a digital Novartis. Two therapeutic areas, neuroscience and immunology, have been chosen to leverage the power of AI [9]. For this purpose, Jay Bradner, President of the Novartis Institutes of BioMedical Research, explained that his company has identified about 12 areas where AI could make drug development faster and better. Suitable opportunities range from drug repurposing, patients stratification and a collaboration with Apple in clinical trial management [3].

## Outlook

Although no pharma company has yet made a major strategic investment and AI may still be years away from its final breakthrough in the pharmaceutical sector, the strategic decisions to benefit from AI are made today. In this context, we foresee four future archetypes that will develop in the coming years:

- (1) *Conservative Pharma Players* are the traditional research-based pharma companies that will lose speed in innovation by not using AI strategically on a larger scale.
- (2) *Selective AI-Explorers* use AI for project-specific challenges. They do not develop core competencies in AI and rely mainly on external data-based AI-partners. This can be a successful niche strategy if partnering capabilities on both sides are developed.
- (3) *New Analytic Entrants* are tech companies such as Alphabet (Google) that are more rooted in data analytics than in healthcare. They may take large portions of the healthcare sector starting in health prevention or with life style applications and wearables. They may enter the market of chronic diseases, such as Alzheimer, diabetes or oncology, with longitudinal data-analytics and digital interventions. This is a classical disruption from the low end, mostly underestimated by the current industry actors.
- (4) *Digital Pharma Players* consist of pharma companies that build up AI competencies and digital literacy in all fields of their business. They combine AI-based analytics along the entire pharma R&D value chain - from drug discovery to clinical development. Machine learning and deep neural networks will become core elements of an integrated innovation process. They will not have separate IT-departments but data analytics in all functions - from research, over clinical development to medical affairs.

The use of AI will require a major change in the mindset of big pharma to behave more like agile biotech companies. "Think big, start small, fail cheap and move fast" might become the new imperative for these companies. Today, the question is who can develop and implement an AI-driven R&D strategy fastest and to the greatest effect. Independent of which model companies will choose, early entrants will materialize from AI, build market barriers and pace out competitors that miss the trend of AI. Pharma companies need to develop more digital competencies, especially an excellent understanding of deep neural networks, if they do not want to lose ground in the race for better, safer and affordable drugs.

The exponential improvement of information processing capabilities, the future availability of low priced AI-applications in combination with faster and cheaper hardware will boost the trend of digitalization. The immense need to increase R&D efficiency will do its part for the success of AI in pharma R&D. The AI sector will become an integral part of pharma R&D and, in a few decades, AI may dominate pharma and healthcare innovation overall.

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