

REVOLUTIONIZING THE FUTURE OF NEW DRUG DISCOVERY: USE OF A.I. BY INDUSTRY GIANTS AND CASE STUDY OF ABBVIE

INTRODUCTION

A.I. has emerged as a promising tool in drug discovery, revolutionizing how we identify and develop new drugs. One of the critical advantages of A.I. is its ability to analyze vast amounts of data and generate insights that would be difficult or impossible for humans to identify. Using A.I., researchers can speed up the drug discovery process and reduce the cost and risk of developing new drugs. One of the main applications of A.I. in drug discovery is target identification. A.I. can analyze large data sets and identify biological processes that may be involved in disease, helping researchers identify potential drug targets. For example, A.I. can analyze gene expression data to identify upregulated genes in diseased tissue compared to healthy tissue. This can provide researchers with potential targets for drug development. Companies like BenevolentAI and Insilico Medicine use A.I. to identify potential drug targets for diseases such as Alzheimer's, Parkinson's, and cancer. (1) Another way A.I. is used in drug discovery is drug screening. A.I. can be used to screen large libraries of compounds and identify those that have the potential to be effective drugs. By analyzing the chemical structure of compounds and predicting their biological activity, A.I. allows researchers to focus on the most promising candidates. Companies like Atomwise and Exscientia use A.I. to screen compounds and identify potential drug candidates for diseases such as cancer, COVID-19, and cystic fibrosis. (2) A.I. is also used in drug optimization. It helps researchers optimize drug candidates for maximum efficacy and minimal side effects.

By analyzing the structure of drug candidates and predicting how they will interact with biological targets, A.I. can help researchers make modifications to improve their performance. Companies like Numerate and XtalPi use A.I. to optimize drug candidates for diseases such as diabetes, hepatitis B, and cancer. (3) Moreover, A.I. can also improve

SUMMARY

A.I. has revolutionized the drug discovery process by enabling researchers to analyze vast amounts of data and generate insights that would be difficult for humans to identify. A.I. is used in various applications such as target identification, drug screening, drug optimization, and clinical trial design and execution. This has led to more effective drugs and better patient outcomes. The use of A.I. in drug discovery is expected to increase in the coming years. This paper provides an analysis of the top 27 Pharma companies giants, along with a case study of Abbvie Inc. on their use of A.I. in the pharmaceutical industry.

Keywords: A.I. in drug discovery, pharmaceutical industry, target identification, drug screening, clinical trial optimization

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the design and execution of clinical trials, making the process more efficient and effective. By helping researchers identify patients who are most likely to respond to a particular treatment, A.I. can reduce the number of patients needed for a trial and increase the likelihood of success. Companies like Berg Health and Mendel.ai are using A.I. to improve the design and execution of clinical trials for diseases such as cancer, Alzheimer's, and heart disease. A.I. is transforming drug discovery by enabling faster, more efficient, and cost-effective development of new drugs. By leveraging A.I.'s ability to analyze large amounts of data and generate insights, researchers are making significant progress in identifying new drug targets, screening compounds, optimizing drug candidates, and designing and executing clinical trials. The use of A.I. in drug discovery is expected to increase in the coming years, leading to more effective drugs and better patient outcomes.

This paper analyses top Pharma companies showing their main characteristics and Artificial intelligence use. There are selected 27 largest Pharmaceutical companies in the world out of the 100 largest pharmaceutical companies by revenue, according to the 2021 Forbes Global 2000 ranking. (4) In addition, we provide a Case study of Abbvie Inc. in which we present information on the company and its use of A.I. in the pharmaceutical industry.

INDUSTRY BACKGROUND

The pharmaceutical and biotechnology industries are frontiers in using applied artificial intelligence today. This technology was used for a significant period in predictive toxicology, biochemical modelling, bioinformatics and other applications. (5) In recent years, advances in machine learning with the combined use of knowledge in computational power and more assessable large data sets have led to a renaissance of the Artificial Intelligence. (6) When Canadian company *Deep Genomics* publicly announced in September 2019 they have used artificial intelligence to solve the problem of Wilson's disease, it was a remarkable achievement. This company has actually created a massive data set of more than 200.000 gene mutations that were implemented in training algorithms capable of cross-checking connections of human DNA. (7) This achievement not only resulted in solving this long outstanding mystery for medical experts but also trills this startup company shareholder as the company achieved value of \$575.2 million in 2019. This is

just one example of the successful application of Artificial Intelligence in the “sea of the possibilities” that artificial intelligence brings to the world of pharmacy - biomarkers ageing technology improvement, age of universal feature of every organism, cross-species search, advancement in modelling of *in silico* research - are just some of the possibilities that have already been proven as efficient by strategic use of Artificial intelligence.

Another example where the use of A.I. might be significant is the process of clinical drug development that brings new drugs to the market after approximately ten years of clinical trials and estimation of \$2.6 billion in total cost. (8) Having this in mind, we also have to underline issues with efficiency, efficacy and costly procedures that prevent innovation from reaching the market. Only 10% of drugs that enter Phase I clinical research end as marketed drugs that could be offered to the patient. Once a new drug is marketed, pharmaceutical companies have to make up that cost by charging more for medicines, which implies increasing out-of-pocket expenses for the patients.

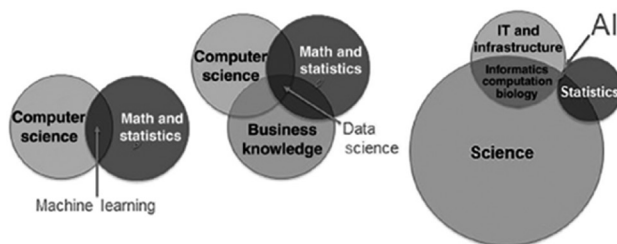


Figure 1. Machine learning development depends on Computer science, Math and statistics and business knowledge, but in the Pharma industry that is scientifically driven, it is rare to have a combination of the mentioned skills, which presents an issue for further development (6)

With the use of A.I. in the drug development process, the timeframe might be shortened, costs minimized, and the innovation process boosted. Having said this, we expect an increasing number of companies willing to adopt strategies that should lead to using artificial intelligence in the pharmaceutical industry for a broad spectrum of services. This will increase competitive stress for companies that need to adopt this technology. As time passes, competitive stress becomes more intensive and changes managerial perception. In 2019, Association DIA performed a global survey to have a snapshot of relevant aspects of the use of Artificial Intelligence in new drug production (including other applications) and the overall adoption of this concept by Pharma companies. The

study has investigated analytical platforms and innovations within companies currently using A.I. or planning to use it in future. (9)_Results of this extensive global study that analyzed 402 responses, including data from 217 unique organizations, show perceptions of technology definitions, assessment of organizational and personal A.I. expertise, and use of partnerships and perceptions about current and future use. Also, results revealed that the most significant challenges to A.I. implementation included staff skills (55%), data structure (52%), and budgets (49%).

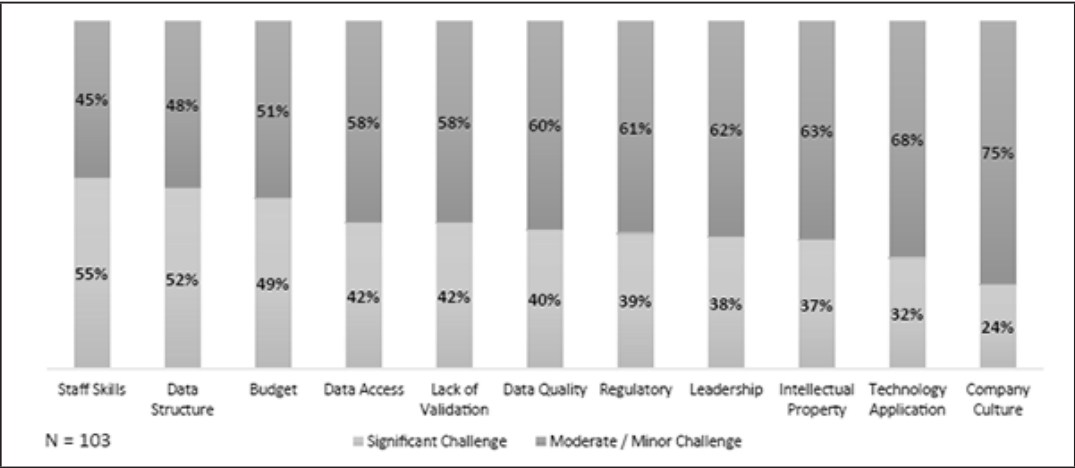


Figure 2. Artificial Intelligence Implementation Challenges (9)

The same survey also revealed that despite noted challenges, most organizations use A.I. in some capacity and show an understanding of the importance of the success of an organization's workforce. In addition, many organizations reported expectations for increasing staff as the implementation of A.I. expands. (10)

Artificial intelligence (A.I.) is revolutionizing drug discovery by providing researchers with new tools and methods for identifying potential drug targets and optimizing drug candidates and below are listed some of the ways that A.I. is used in drug discovery: (11)

1. Target Identification: A.I. can be used to identify potential drug targets by analyzing large data sets and identifying biological processes that may be involved in disease. For example, A.I. can analyze gene expression data to identify upregulated genes in diseased tissue compared to healthy tissue. This can

provide researchers with potential targets for drug development.

2. **Drug Screening:** A.I. can be used to screen large libraries of compounds to identify those potentially effective drugs. A.I. can analyze the chemical structure of compounds and predict their biological activity, allowing researchers to focus on the most promising candidates.
3. **Drug Optimization:** Once potential drug candidates have been identified, A.I. can be used to optimize them for maximum efficacy and minimal side effects. A.I. can analyze the structure of the drug candidate and predict how it will interact with biological targets, allowing researchers to make modifications that will improve its performance.
4. **Clinical Trials:** A.I. can be used to improve the design and execution of clinical trials, making the process more efficient and effective. For example, A.I. can help researchers identify patients most likely to respond to a particular treatment, reducing the number of patients needed for a trial and increasing the likelihood of success.

Based on the analysis of top Pharma companies selected by the revenue size, we are summarising here the use of A.I. per company in the area of drug discovery:

Table 1. Top Pharma Companies using A.I. - selected characteristics(12)

Company Name	Stock Exchange	Date Joined	AI Services Used	Number of Employees	Country of Origin
AbbVie	New York Stock Exchange (NYSE)	2013	Natural Language Processing, Machine Learning, AI	47,000	USA
Almirall	Madrid Stock Exchange (BME)	2007	Image Analysis, Predictive Analytics, Machine Learning	1,800	Spain
Amgen	NASDAQ	1983	Drug Discovery and Development	24,000	USA
Astellas	Tokyo Stock Exchange (TSE)	2005	Predictive Analytics, Natural Language Processing	16,500	Japan
AstraZeneca	London Stock Exchange (LSE)	1993	Predictive Analytics, Machine Learning, AI	76,000	UK
BASF	Frankfurt Stock Exchange (FSE)	1952	Predictive Maintenance, Supply Chain Optimization	110,000	Germany
Bayer	Frankfurt Stock Exchange (FSE)	1953	Predictive Maintenance, Supply Chain Optimization	99,000	Germany
Boehringer Ingelheim	Private	N/A	Predictive Analytics, Natural Language Processing	50,000	Germany
Bristol-Myers Squibb	New York Stock Exchange (NYSE)	1934	Drug Discovery and Development	30,000	USA

CJ Healthcare	Korea Exchange (KRX)	2011	Machine Learning, Predictive Analytics	5,000	South Korea
Celgene	NASDAQ (acquired by BMS in 2019)	1987	Predictive Analytics, Machine Learning, AI	7,000	USA
Daewoong Pharmaceutical	Korea Exchange (KRX)	2002	Machine Learning, Natural Language Processing	1,800	South Korea
Eisai	Tokyo Stock Exchange (TSE)	1949	Predictive Analytics, Machine Learning, AI	10,000	Japan
Eli Lilly	New York Stock Exchange (NYSE)	1926	Machine Learning, Predictive Analytics	38,000	USA
Evotec	Frankfurt Stock Exchange (FSE)	1999	Drug Discovery and Development	3,000	Germany
GSK	London Stock Exchange (LSE)	2000	Machine Learning, Predictive Analytics	97,000	UK
Genentech	Subsidiary of Roche	N/A	Drug Discovery and Development	12,000	USA

Table 2, Use of A.I. in drug development for selected companies (12)

Company Name	Use of AI in drug discovery
Atomwise	Uses AI to identify potential drug candidates by analyzing the structure of molecules and predicting their biological activity.
BenevolentAI	Uses AI to analyze large data sets and identify potential drug targets.
Berg Health	Uses AI to analyze patient data and identify potential drug targets for cancer and other diseases.
Cyclica	Uses AI to analyze the structure of compounds and predict their biological activity.
Insitro	Uses AI to design and optimize drug candidates by analyzing large data sets and identifying the most promising drug candidates for further development.
Recursion Pharma	Uses AI to identify potential drug targets by analyzing images of cells and tissues.
Schrödinger	Uses AI to design and optimize drug candidates by predicting their biological activity and optimizing their chemical structure.
Insilico Medicine	Uses AI to identify potential drug targets and design new compounds by analyzing large data sets and predicting the biological activity of compounds.
Verge Genomics	Uses AI to identify potential drug targets for neurological diseases by analyzing genomic data and identifying potential targets for drug development.
Nuritas	Uses AI to identify potential drug targets by analyzing genomic and proteomic data for the treatment of inflammation and other conditions.

Artificial intelligence (A.I.) is transforming the healthcare industry, especially drug discovery and development. One of the critical areas where A.I. is used is identifying drug targets, which is the first step in the drug discovery process. A.I. can analyze vast amounts of data, including genomics and proteomics data, to identify potential targets for drug development. This approach can save time and resources and increase the chances of success in drug development.

CASE STUDY: ABBVIE'S USE OF A.I. TO DRIVE DRUG DISCOVERY

Abbvie is a global biopharmaceutical company focusing on researching, developing, and commercialising innovative therapies to address some of the most complex and severe diseases. The company was founded in 2013 as a spinoff from Abbott Laboratories and is headquartered in North Chicago, Illinois, USA. Abbvie primarily focuses on developing and producing pharmaceutical drugs to treat various medical conditions. Abbvie's corporate structure comprises four central business units: Immunology, Oncology, Virology, and Neuroscience. The Immunology division produces drugs for treating autoimmune diseases such as rheumatoid arthritis, psoriasis, and Crohn's. The Oncology division focuses on developing treatments for various types of cancer, including lymphoma, leukaemia, and breast cancer. The Virology division produces antiviral drugs for treating HIV and hepatitis C. In contrast, the Neuroscience division concentrates on drugs for treating conditions such as Parkinson's disease and multiple sclerosis. (13)

Abbvie's most successful drug, Humira,, treats various autoimmune diseases such as rheumatoid arthritis, psoriasis, and Crohn's disease. In 2020, Humira generated approximately \$20 billion in revenue, making it the highest-grossing drug in the world.

Abbvie offers its customers a wide range of pharmaceutical drugs and healthcare services. The company has over 47,000 employees worldwide and had a revenue of approximately \$45 billion in 2020. Abbvie's portfolio of drugs includes some of the most widely used treatments in the world, such as Humira, Imbruvica, and Skyrizi. Humira, Abbvie's most successful drug, treats various autoimmune diseases such as rheumatoid arthritis, psoriasis, and Crohn's disease. In 2020, Humira generated approximately \$20 billion in revenue for Abbvie, making it the highest-grossing drug in the world. Imbruvica, another successful drug produced by Abbvie, is used to treat certain types of cancer and generated over \$4 billion in revenue in 2020. (14)

Abbvie's financial performance has been impressive in recent years. The company's net income increased from \$5.7 billion in 2019 to \$10.1 billion in 2020, primarily due to the continued success of Humira and other drugs in its portfolio. Abbvie's revenue has steadily increased since its inception in 2013, with a revenue of \$18.8 billion in 2014 and reaching \$45.8 billion in 2020. In addition, the company's net income has also been steadily increasing, with a net income of \$3.3 billion in 2014 and reaching \$5.5 billion in 2020. (15)

Abbvie has used A.I. in various projects to drive drug discovery and development. One of the significant A.I.

projects is the use of A.I. in identifying drug targets, a critical step in drug discovery. Abbvie also uses A.I. to analyze large amounts of data generated in clinical trials to optimize trial design and identify patients who will benefit most from the therapy. Abbvie has been investing in A.I. to improve the efficiency of drug discovery and development. The company's AI-powered drug discovery platform uses machine learning algorithms to predict the most promising drug targets and molecules to target those targets. The platform analyzes vast amounts of data from multiple sources, including genetic data, clinical data, and scientific literature, to identify novel drug targets and develop new therapies. In addition, Abbvie is using A.I. in clinical trials to analyze large amounts of data generated during the trial and optimize the trial design. The company also uses A.I. to identify patient subgroups most likely to benefit from a particular therapy, which can help develop personalized medicines. Abbvie's investment in A.I. has been driving drug discovery and development, which is crucial in bringing new therapies to patients. The company's use of A.I. in identifying drug targets and optimizing clinical trial design has the potential to improve the efficiency of the drug development process significantly. While the revenue figures related to their A.I. projects are not publicly available, the steady growth in revenue and net income indicates that their investment in A.I. has been a smart move for the company. Abbvie has invested in new technologies such as artificial intelligence and machine learning to improve drug discovery and development. They have also invested in genomics and personalized Medicine. (16)

Abbvie has been actively involved in developing and using artificial intelligence (A.I.) and machine learning (ML) technologies in recent years. The company has partnered with several tech firms and startups to leverage A.I. and ML in its operations, including drug discovery, clinical trials, and patient care. One of Abbvie's most significant partnerships in this area is with a startup called Insilico Medicine. Insilico Medicine is a company that specializes in applying A.I. and ML in drug discovery and development. Abbvie has collaborated with Insilico Medicine to develop novel drugs for treating age-related diseases such as Alzheimer's and Parkinson's. The partnership aims to use Insilico Medicine's A.I. platform to identify new drug targets and accelerate drug discovery timelines. Abbvie has also partnered with several other companies in the A.I. and ML space, such as Biocorpora and Cyclica, to improve its drug discovery and

The company's AI-powered drug discovery platform uses machine learning algorithms to predict the most promising drug targets and molecules to target those targets.

development processes. The company is also using A.I. and ML to optimize its clinical trials and improve patient outcomes. (17)

Abbvie is a pharmaceutical company that has established itself as a leader in the healthcare industry. The company's success can be attributed to its focus on innovation, research, and developing novel drugs to treat various medical conditions. In addition, Abbvie's use of A.I. and ML technologies is expected to continue to drive its growth and success in the years to come.

CONCLUSION

A.I. is a promising tool in drug discovery that has revolutionized the identification and development of new drugs. A.I.'s ability to analyze vast amounts of data enables researchers to speed up the drug discovery process, reduce the cost and risk associated with drug development, and generate insights that are difficult or impossible for humans to identify. A.I. is used in several ways in drug discovery, including target identification, drug screening, drug optimization, and improving the design and execution of clinical trials. Pharmaceutical and biotechnology industries are frontiers in the use of applied artificial intelligence. The use of A.I. is expected to increase in the coming years, leading to the development of more effective drugs and better outcomes for patients. There have been significant achievements in using A.I. in drug discovery, including the successful use of A.I. by the Canadian company Deep Genomics to solve the problem of Wilson's disease. However, issues with efficiency, effectiveness and costly procedures prevent innovation from reaching the market. Companies like Abbvie are investing in A.I. to improve the efficiency of drug discovery and development, with the potential to improve the drug development process's efficiency significantly.

Another area where A.I. is showing promise in drug discovery is in the prediction of drug toxicity. Traditional methods of predicting drug toxicity involve animal testing, which is costly and time-consuming and may not accurately predict toxicity in humans. By using A.I., researchers can analyze large amounts of data on compounds' molecular structure and biological activity and predict their potential toxicity, reducing the need for animal testing. As a result, companies like Insilico Medicine and BioSymetrics are using A.I. to predict drug toxicity and improve the safety of new drugs.

However, the use of A.I. in drug discovery is challenging. One of the main challenges is the quality and availability of data. To train A.I. models, researchers need large amounts of high-quality data. Unfortunately, in drug discovery, data is often proprietary and subject to intellectual property restrictions, making it difficult for researchers to access the data they need. In addition, the need for more standardization in data collection and storage can make comparing data from different sources difficult. Another challenge is the interpretability of A.I. models. While A.I. can generate insights that are difficult for humans to identify, it can be challenging to understand how the A.I. arrived at its conclusions. This lack of interpretability can make it difficult for researchers to trust the results and limit the adoption of A.I. in drug discovery. Overall, while the use of A.I. in drug discovery presents significant opportunities, addressing these challenges will be critical to realizing its full potential.



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REVOLUCIJA U BUDUĆNOSTI KOD OTKRIĆA NOVIH LEKOVA: UPOTREBA VEŠTAČKE INTELIGENCIJE OD STRANE INDUSTRIJSKIH DIVOVA I STUDIJA SLUČAJA KOMPANIJE ABBVIE

REZIME

Veštačka inteligencija (AI) je revolucionarno uticala na proces otkrivanja lekova omogućavajući istraživačima da analiziraju ogromne količine podataka i generišu uvide koje bi ljudima bilo teško da identifikuju. AI se koristi u različitim aplikacijama kao što su identifikacija cilja, skrining lekova, optimizacija lekova i dizajn i izvođenje kliničkih ispitivanja. To je dovelo do razvoja efikasnijih lekova i boljih ishoda za pacijente. Očekuje se da će se upotreba veštačke inteligencije u otkrivanju lekova povećati u narednim godinama. U ovom radu je data analiza 27 farmaceutskih giganta, zajedno sa studijom slučaja kompanije Abbvie Inc. o njihovoj upotrebi veštačke inteligencije u farmaceutskoj industriji.

Ključne reči: veštačka inteligencija u otkrivanju lekova, farmaceutska industrija, identifikacija mete u veštačkoj inteligenciji, skrining lekova, optimizacija kliničkih ispitivanja