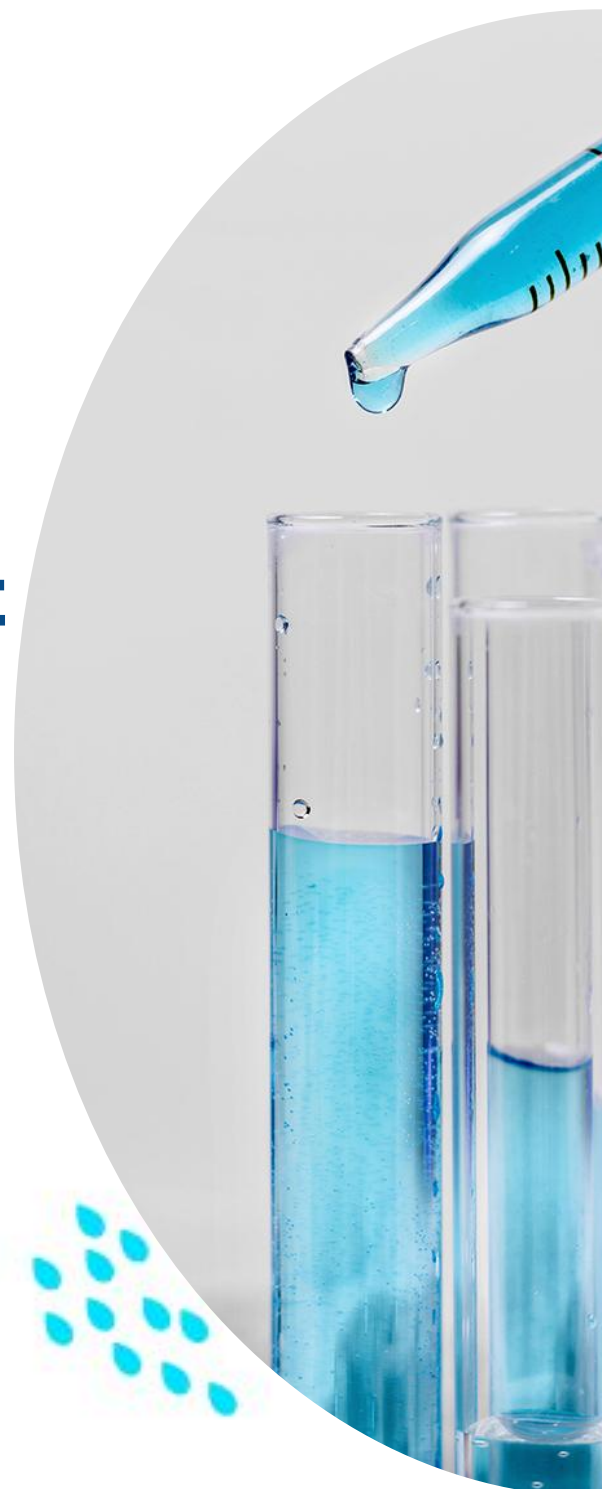





# **LARGE PHARMACEUTICAL COMPANIES USING ARTIFICIAL INTELLIGENCE**

How are top pharma companies  
using AI for next generation  
solutions to health problems?





# Contents

Looking at a few companies which have used AI to make breakthrough changes in the pharmaceutical industry





### **Opportunity**

Designing novel optimized compounds and speed identification of promising drug candidates

### **Solution and its Impact**

Almirall and Iktos, a company specialized in Artificial Intelligence for novel drug design announced a collaboration agreement in Artificial Intelligence where Iktos generative modelling technology will be used to design novel optimized compounds, to speed up the identification of promising drug candidates for Almirall's drug discovery program.

The company's AI technology, based on deep generative models, helps bring speed and efficiency to the drug discovery process, by automatically designing virtual novel molecules that have all desirable characteristics of a novel drug candidate. This tackles one of the key challenges in drug design: rapid and iterative identification of molecules which simultaneously validate multiple bioactive attributes and drug-like criteria for clinical testing.



### **Opportunity**

Predicting the pharmacological activity and properties of compounds

### **Solution and its Impact**

Astellas initiated a collaboration with Elix, a research-oriented technology company specializing in deep learning and machine learning with the objective of developing algorithms that use artificial intelligence for predicting compound activity, generating compound structures, and conducting retrosynthetic analysis. This collaborative research aims to use AI for predicting the pharmacological activity and properties of compounds (e.g., absorption, distribution, metabolism, and excretion; physical properties; and toxicity), generating compound structures and conducting retrosynthetic analysis.

This research also would improve AI-assisted prediction of properties and compounds structure generation, its core mission will be to drive forward AI-assisted retrosynthetic analysis. This will not only enable AI to generate compounds, but ensure those compounds are





Atomwise is revolutionizing how drugs are discovered with AI. They invented the use of deep learning for structure-based drug discovery, today developing a pipeline of small-molecule drug candidates advancing into preclinical studies.

Their portfolio of joint ventures and partnerships with leading pharmaceutical, agrochemical, and emerging biotechnology companies represents a collective deal value approaching \$7 billion.

To date, Atomwise has raised over \$174 million from leading venture capital firms to advance their mission to make better medicines, faster.

### **Opportunity**

Artificial Intelligence used for Drug Discovery

### **Solution and its impact**

Created conventional neural networks, the subset of machine learning that looks to the human brain for inspiration, for drug discovery. The company's AtomNet is a deep learning neural network used for binding affinity prediction for small molecules, a key part of the drug discovery process.

The company claims this technology has improved hit rates by up to 10,000 times, delivering results 100 times faster than conventional screening. AtomNet itself is capable of screening over 100 million compounds per day.



### **Opportunity**

Coming up with an artificial intelligence software that aims to support clinical decision making of chronic thromboembolic pulmonary hypertension (CTEPH)

### **Solution and its Impact**

Bayer and Merck & Co were granted the Breakthrough Device Designation from the FDA for artificial intelligence software. The aim of the software is to help radiologists detect certain patterns faster, who are often on the frontline for identifying CTEPH patients. The AI would analyze image findings from cardiac, lung perfusion, and pulmonary vessels in combination with a patient's clinical history and then pass the insights to the radiologists leveraging this technology. This tool will eventually be able to assist in diagnosing patients earlier and more reliably, leading to earlier treatment and better patient outcomes.



# Benevolent<sup>AI</sup>

## **Opportunity**

End-to-end drug discovery

## **Solution and its Impact**

BenevolentAI has developed an AI platform that can identify new drug target candidates for any therapeutic area. The company has its own pharmaceutical team to investigate potential leads and develop their own products.

Seamless drug target identification and development of drugs. The company is working on its own drug candidates



## **Opportunity**

Identifying New Therapeutic Targets to Treat Neurological Disorders such as Parkinson's Disease

## **Solution and its Impact**

Research collaboration with AstraZeneca to identify and evaluate novel targets and therapeutics to treat neurological disorders such as Parkinson's disease. AstraZeneca will initially provide BERG with its curated library of central nervous system (CNS) optimized fragments. BERG will employ AstraZeneca's fragment library to assist in discovering drug candidates for therapeutic development.

Parkinson's disease is a devastating progressive disorder. Through this research collaboration, drug discovery can be approached in an innovative new way and identification of new therapeutic targets that can potentially benefit patients with neurological disorders, an area of significant unmet medical need







## **Opportunity** Drug Discovery

### **Solution and its Impact**

Boehringer Ingelheim entered into a drug discovery collaboration agreement with UK-based AI tech company Bactevo to identify novel small molecule lead compounds. This collaboration leverages Bactevo's revolutionary TIME (Totally Integrated Medicines Engine) platform, incorporating its ground-breaking synthetic chemistry technology, designed specifically to combine medically-relevant 'tagless' chemical diversity with ultra-fast phenotypic or molecular target screening in human samples, to further enhance speed, efficiency and quality in identifying novel in vivo enabled leads.

Combining cutting-edge TIME drug discovery platform with the powerful therapeutic drug development and commercialization experience at Boehringer Ingelheim would create much needed new medicines in areas outside of the current therapeutic focus



## **Opportunity**

### Drug target identification

### **Solution and its Impact**

Cyclica is currently using Excelra's GOSTAR Database to develop AI & ML based deep learning algorithm for drug target identification. GOSTAR is the largest online structure activity relationship database comprising of over 5.5 million small molecules and their associated chemical, biological and pharmacological properties.

This collaboration would ultimately equip researchers with insights to generate novel ideas in drug design in the early as well as optimization stages of drug discovery. This collaboration will have a direct impact on the development of more precise and efficacious medicines for patients in need.

The company is working on developing precise, exclusive and efficacious medicines for patients in need.



## **Opportunity**

Using AI to learn and cure Wilson's disease.

## **Solution and its Impact**

The company identified a genetic mutation that causes the disease, the chemical properties needed in a molecule to target the mutation, and a compound that warrants further investigation. They also nominated the first-ever AI-discovered therapeutic candidate DG12P1. It has been designed to help the body remove the excess copper. The discovery of DG12P1 occurred following a long-term scan from Deep Genomics' AI system.

The company is eager to move it rapidly into the clinic for the potential benefit of patients with this breakthrough. The discovery is unprecedented and opens the door to a smarter, faster, and vastly more efficient means of identifying viable drug candidates for a host of diseases.

Deep Genomics would be collaborating with BioMarin on advancing programs identified using Artificial Intelligence.



## **Opportunity**

Developing new medicines

## **Solution and its Impact**

Exscientia uses a suite of AI technologies called Centaur Chemist to develop new medicines. It uses a set of predetermined computer algorithms to design brand new drugs, from scratch, far more quickly than any human ever could.

Exscientia also has several other AI-developed drugs in the pipeline, awaiting approval for human trials, which the company says took a fraction of the time it would ordinarily take to go from an idea to the preclinical stage.



# Genentech

*A Member of the Roche Group*

## **Opportunity**

Finding potential drug candidates for a variety of diseases.

## **Solution and its Impact**

Collaboration between Roche group's member, Genentech and Genesis Therapeutics leverages Genesis' graph machine learning and drug discovery expertise to identify innovative drug candidates for therapeutic targets in multiple disease areas. This partnership also enables the small company to leverage their AI technology platform with Genentech's unmatched capabilities in molecular innovation and structural biology. The companies have accelerated their innovation in AI and developed next generation algorithms, thus pioneering the intersection of protein motion -- a key element of drug binding -- with neural networks to develop fast and accurate technology for predicting the potency, selectivity, and ADME properties of drug-like molecules.

AI can help unlock the next generation of innovative therapies for patients in need of additional options. Using both the companies technologies and innovative techniques discovering medicines currently out of reach using conventional methods would be an easy task.





## **Opportunity** Clinical Development

### **Solution and its Impact**

Gilead Sciences and Glympse Bio, entered into a collaboration in nonalcoholic steatohepatitis (NASH) clinical development. Glympse Bio's AI powered synthetic biomarkers – bioengineered to identify stage and progression of disease as well as early detection of treatment response – will be used to determine clinical trial participants' stage of disease at initial screening and to determine responses to study treatment in Gilead's NASH clinical program. By utilizing this innovative technology, the company aims to better characterize this complex disease and improve their understanding of how compounds impact disease progression.



GNS HEALTHCARE

## **Opportunity**

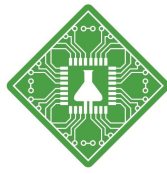
Drug development in the era of precision medicine

## **Solution and its Impact**

GNS Healthcare, a precision medicine company leveraging artificial intelligence to model individual patients' response to drug treatment, have unveiled the first in silico multiple myeloma patient. Called Gemini, the in silico multiple myeloma patient is a computer model of disease progression and drug response at the individual patient level.

Gemini has multiple applications for precision medicine including discovering markers of response and nonresponse for clinical trial design, predicting optimal combination therapies, and running head-to-head in silico trials. Clinical applications could include providing information to switch patients to more effective treatments and optimizing treatment sequencing.

To support the future formation of in silico patients, GNS recently convened an in silico patient advisory board to guide development and commercialization strategy. The in silico patient for multiple myeloma represents the first of several poised to expand the world's understanding of causal response to therapeutics across a range of diseases within oncology, immunology, and neurology.



**Insilico  
Medicine**

## **Opportunity Drug Discovery**

### **Solution and its Impact**

Insilico and Taisho Pharmaceutical Co., Ltd. entered into a research collaboration to identify novel therapeutics against aging. Insilico Medicine will utilize both the target discovery and generative chemistry parts of its Pharma.AI platform in this collaboration. It will use its proprietary Pandemics Discovery Platform to identify novel targets for senolytic drugs and Chemistry42 platform for a molecular generation.

This collaboration brings together Insilico's state-of-art artificial intelligence (AI) technologies in drug discovery with Taisho's expertise in drug development, aimed to extend the human healthspan.

Through this collaboration, Insilico is trying to adopt their AI-powered drug discovery suites together with Taisho's validation platform to explore the new space of anti-aging solutions



## **Opportunity**

Drug discovery and development

## **Solution and its Impact**

Insitro will leverage the Haystack's DNA encoded libraries technology to collect massive small molecule data sets that inform the construction of machine learning models able to predict drug activity from molecular structure. This acquisition of Haystack Sciences will lead to more efficient drug discovery.

The company aims at combining the power of machine learning with high quality DEL (DNA Encoded Libraries) datasets to address two difficult protein-protein interface targets





### **Opportunity**

New surgical methods, Drug development, Next generation solutions to health problems

### **Solutions and its Impact**

Robotizing surgeries (robot-assisted surgery)

Baby Intelligence using AI to monitor, quantify and analyze breathing habits and sleeping patterns of babies, to personalize healthcare for individual babies

AI for Alzheimer's: speech-based AI platform to analyze collection of speech data acquired from ongoing clinical trials.

Artificial intelligence is giving J&J the ability to discover new treatments and techniques faster than they would've thought possible just a decade ago. Companies like Johnson & Johnson are combining their scientific expertise with the power of AI and machine learning to create next generation solutions.

The company is finding new ways to apply this technology to the healthcare field. They think that no one can predict the future—but we can make it healthier by incorporating these techniques and technologies.





## **Opportunity**

Discovery and development of treatments for psychiatric and neurological disorders

## **Solution and its Impact**

Lundbeck is tapping into IBM Watson Health's cognitive and knowledge-based health data analytics platform to speed the discovery and development of treatments for psychiatric and neurological disorders, including schizophrenia and Parkinson's disease. The collaboration aims to combine Lundbeck's knowhow in the field of neurological and psychiatric disease therapy with the IBM Watson platform to derive information from clinical data through the Watson Health Cloud.

The company strives to develop treatments that affect the underlying biological mechanisms of psychiatric and neurological disorders rather than treating only symptoms. By combining their expertise in brain research with IBM's cognitive computer technology, Lundbeck expects to improve the foundation for this work, so they can develop new and improved treatments for the 425 million people who suffer from the psychiatric and neurological disorders which the



## **Opportunity**

Developing Deubiquitinase (DUB) inhibitors in the fight against Parkinson's and Alzheimer's

## **Solution and its Impact**

Mission Therapeutics and AbbVie, a pharmaceutical business known for its strong neurodegenerative disease research, have partnered to develop Deubiquitinase (DUB) inhibitors. Both Alzheimer's and Parkinson's patients have an abnormal accumulation of misfolded, toxic proteins, resulting in impaired brain functionality and the death of nerve cells. This is where DUBs come in. They regulate the degradation of these proteins to maintain their health and stability.

By modulating specific DUBs within the brain, Mission Therapeutics is aiming to find potential treatments which will enable the degradation of these toxic proteins and prevent their accumulation.



### **Opportunity**

Novartis uses innovative science and digital technologies to create transformative treatments in areas of medical need.

### **Solution and its Impact**

Novartis and Microsoft announced a multiyear partnership that will leverage data and Artificial Intelligence to transform how medicines are discovered, developed, and commercialized. Starting with generative chemistry, image segmentation and analysis for smart and personalized deliveries of therapies, and optimization of cell and gene therapies at scale. By bringing together Novartis's datasets with Microsoft's AI technology, the AI Empowerment lab aims at creating AI models and applications that will assist Novartis's associates in overcoming the next generation of challenges in medicine.

Novartis aims to address some of the biggest challenges facing the pharmaceutical industry today, by bringing AI expertise to every employee so they can work to discover new medicines at scale and reduce costs.



### **Opportunity**

Developing a data and analytics platform to change the way medicines are manufactured and delivered, and changing the way they approach the supply chain processes

### **Solution and its Impact**

Collaboration with Amazon Web Services to accelerate digital transformation of its business operations, and modernize various aspects of manufacturing and supply chain. A lot of challenges faced by the companies requires manufacturers to make their upstream supply chains, manufacturing processes, and downstream distribution more visible, predictable, efficient, and adaptable. Novartis and AWS collaboration aims at fulfilling these requirements. Novartis is trying to bring innovative medicines to patients faster.



## **Opportunity**

### Artificial Intelligence solutions in Ophthalmology

## **Solution and its Impact**

Collaboration between Novartis and RetinAI to study patients with neovascular age-related macular degeneration. The study is designed to investigate the influence of optical coherence tomography (OCT) image solutions using Artificial Intelligence (AI) on the assessment of disease activity. this collaboration would make lots of things easy for the company, to navigate imaging data, compute imaging biomarkers and track changes over time for some of the most common forms of eye diseases are some of them. This research and collaboration would also support diagnostic analyses and clinical workflows as well as patient monitoring & adherence to treatment.

Both of these companies together are working on end-to-end solutions to generate swift and comprehensive disease insights to better treat patients and improve patient outcomes





## **Solution**

Creating new and improved treatments and find ways to get people access to treatment quickly.

## **Solution and its Impact**

Novartis is currently using machine learning to classify digital images of cells, each treated with different experimental compounds. The machine learning algorithms collect and group compounds that have similar effects together, before passing on the clean data to researchers who can decide how to leverage these insights in their work. To speed up the screening process, Novartis research teams use images from machine learning algorithms to predict which untested compounds might be worth exploring in more details.

As computers are far quicker compared to traditional human analysis and laboratory experiments in uncovering new data sets, new and effective drugs can be made available sooner, while also reducing the operational costs associated with the manual investigation of each compound.



## **Opportunity**

### Studying pathology slides

### **Solution and its Impact**

Novartis researchers are collaborating with tech startup PathAI to search for hidden information in pathology slides. The company is training an AI system developed by PathAI to learn to see the same patterns pathologists see and then building on that to determine if the system can detect hidden but informative patterns too subtle or complex for pathologists to discern. The effort is part of a larger effort at Novartis to leverage data and digital technologies in ways that could help drug developers get the right drugs to the right patients faster.

Novartis aims to create a platform that enables the field of pathology to support the accelerating pace of drug development



## Drug Discovery

Pfizer is using IBM's AI technology on its immuno-oncology research, a strategy of using a body's immune system to help fight cancer. Watson's deep pool of information can enable it to make non-obvious connections that could lead to combination medicines for cancer.

With the help of IBM's Watson, which has been trained with historical data, Pfizer is trying to predict the winning combination for medicines and treatments.



## Automating medical literature review.

Sanofi recognized that utilizing an AI software reduced the review time from 13 minutes per paper to about one second per paper. The AI document processing solution is using natural language processing (NLP) to read and review scientific articles, summarize them, and determine to which departments they are most relevant. Furthermore, the platform is able to categorize scientific papers at a high level, determining, for example, whether the paper is an observational study or an experimental study.

Reviewing scientific information is easier due to AI which is making it much faster, far simpler, and much more accurate. The company is currently working in the field of development, manufacturing, and marketing of pharmaceutical drugs. Sanofi covers seven major therapeutic areas like cardiovascular, central nervous system, diabetes, oncology, internal medicine, thrombosis, and vaccines.



## Identifying new drug candidates for glaucoma.

Santen, a speciality ophthalmology company headquartered in Osaka, Japan, and twoXAR, an artificial intelligence-driven biopharmaceutical company have entered a partnership to focus on identifying new drug candidates for glaucoma.

twoXAR will use its proprietary computational drug discovery platform to discover, screen, and prioritise novel drug candidates with potential application in ocular indications.

These efforts will see the discovery of new therapeutic candidates to treat this particular disease, leading to the discovery of more effective treatments for those suffering from glaucoma.





## Drug discovery

Servier and Iktos, a company specialized in artificial intelligence technologies applied to chemistry, announced their intention to pursue their collaboration in the coming months, in line with Servier's strategy to invest strongly in AI technologies for new drug discovery. The technology developed by Iktos, which is based on deep generative models, feeds on the data already generated in a research project to perform the design and optimization of new molecules meeting all project specifications in silico.

This technology addresses one of the major issues encountered in early-stage pharmaceutical R&D: multi-parameter optimization, i.e., identification of molecules that simultaneously meet all in vitro criteria required for a preclinical drug candidate. This technology also led to the acceleration of the discovery of promising new compounds in a real-life drug discovery project.



## Artificial intelligence to better understand cancer tumors

What Turbine does is to use tumor-specific DNA and RNA data to then create “Simulated Cells” which are simulations that mimic the behavior of actual cancer cells. These simulated cells are nothing but a high definition virtual tumor cell. Through this technological advancement, the company was able to take a patient’s cancer cells, create a computational model of the tumour. They are currently figuring out what drugs the tumor will respond to.

Turbine is applying a technology that helps clarify the underlying biology of diseases and develop more effective, personalised therapies and rationalising drug discovery.



## **Bringing AI Expertise To Your Life Sciences Initiatives**

**For more information, visit our website.  
[www.iReadRx.ai](http://www.iReadRx.ai)**