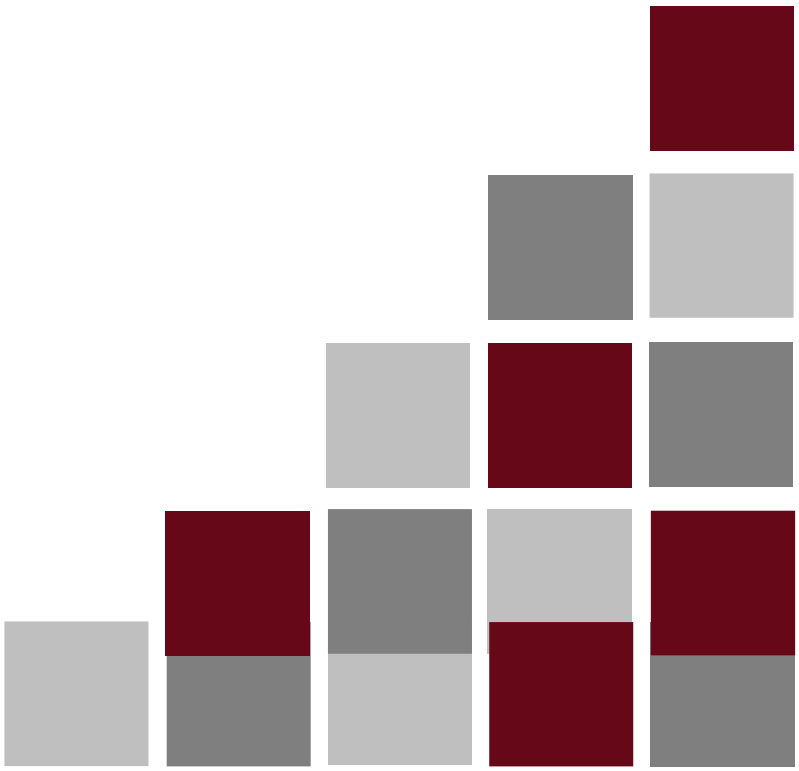
Principles by **IUCG:**

The Time is Now: AI in Drug Discovery is Here

Kush Gami



Introduction

What is Drug Discovery and Why Does it Need Change?

Drug development consists of processes associated with both identifying and developing new medications related to diseases and illnesses. The current steps are quite labor-intensive and inefficient, taking up to 6 years.[1] Moreover, most drugs that are in the development pipeline are quite unique, meaning there is not much prior scientific data to refer to. This causes companies to have to screen a high volume of compounds and their properties. With a limited compound sample size often being an issue, scientists rely on trial-and-error experimentation for development. As a result, current practices for drug development are not accurate, can take a long time, and are very expensive.[2]

Why AI?

With the usage of Artificial Intelligence (AI) and Machine Learning (ML), the hope is that companies can save both money and time while also yielding accurate results by eliminating the trial-and-error strategy. ML algorithms can process large amounts of information quickly and diagnose trends that may not be apparent to human-based analysis. Certain AI applications can also test drug-molecule interactions to see their efficacy. These are just some of the current applications of AI in drug discovery, and with a rapidly growing market, the uses are bound to increase. Let's take a closer look.[3]

---

[1] Serrano, D. R., Luciano, F. C., Anaya, B. J., Ongoren, B., Kara, A., Molina, G., Ramirez, B. I., Sánchez-Guirales, S. A., Simon, J. A., Tomietto, G., Rapti, C., Ruiz, H. K., Rawat, S., Kumar, D., & Lalatsa, A. (2024). Artificial intelligence (AI) applications in drug discovery and drug delivery: Revolutionizing personalized medicine. *Pharmaceutics*, *16*(10), 1328. https://doi.org/10.3390/pharmaceutics16101328

[2] Blanco-González, A., Cabezón, A., Seco-González, A., Conde-Torres, D., Antelo-Riveiro, P., Piñeiro, Á., & Garcia-Fandino, R. (2023). The role of AI in Drug Discovery: challenges, opportunities, and strategies. *Pharmaceuticals*, *16*(6), 891. https://doi.org/10.3390/ph16060891

[3] Blanco-González, A., Cabezón, A., Seco-González, A., Conde-Torres, D., Antelo-Riveiro, P., Piñeiro, Á., & Garcia-Fandino, R. (2023). The role of AI in Drug Discovery: challenges, opportunities, and strategies. *Pharmaceuticals*, *16*(6), 891. https://doi.org/10.3390/ph16060891

Growth is Expected Worldwide

Key Projections

The AI in drug discovery market encapsulates any application of AI-based tools to process biological data, identify potential candidates, predict drug safety, and streamline clinical trials. As of 2024, the market for AI in drug discovery was valued at 1.99 billion USD. However, the rising presence of chronic diseases such as diabetes, cardiovascular diseases, and cancer, is driving market size up. For example, just in the United States, 38.4 million people were affected by diabetes in 2021, making up 11.6% of the population! With an estimated global CAGR of 29.6% and the expected value of the market will be 35.42 billion USD by 2034. The United States (US) is expected to have most of the market, followed by Europe, and Asia.[4]

Trends in the United States

The US is in prime position to dominate this market. In 2023, the US had a market size of 1.9 billion USD, with that expected to jump to 19.4 billion USD by 2032. The US is expected to be leading the charge in applying AI to oncology research, as 46% of AI applications in 2023 were in the oncology therapeutic area. [5] Furthermore, the Federal Drug Administration (FDA) is also aiming to implement AI internally, showing support for what AI has to offer in the pharma space, further strengthening the US' position in the AI race.[6]

Trends in Europe

Moving onto Europe, countries like Germany and the UK are expected to contribute to significant growth in this region. Germany is expected to exceed the global CAGR at 30.3% between 2024 and 2030, showing incredible promise of growth. The UK is also on a similar trajectory with a projected CAGR of 29.9% during the same period.

---

[4] Polaris Market Research & Consulting, Inc. (2024, November 18). *AI in Drug Discovery Market Share and Forecast, 2034*. Polaris. https://www.polarismarketresearch.com/industry-analysis/ai-in-drug-discovery-market

[5] Wani, G., & Faizullabhoy, M. (2024). Artificial intelligence in drug discovery market – by component (Software, Service), technology (Machine learning {Deep, supervised}), application type (Target identification, preclinical testing), therapeutic area, end-use, Global forecast 2024 – 2032. In *Global Market Insights Inc.* https://www.gminsights.com/industry-analysis/ai-in-drug-discovery-market

[6] Reuters. (2025, May 8). *US FDA centers to deploy AI internally, following experimental run*. https://www.reuters.com/business/healthcare-pharmaceuticals/us-fda-centers-deploy-ai-internally-immediately-2025-05-08/

Europe's CAGR is slightly under the global projection at 29.4% from 2024-2030, but still quite high. Europe is also expected to focus on oncology but there is an increasing interest in infectious diseases.[7]

Trends in Asia

The fastest growth is expected in Asia by the end of 2030, with major players emerging in China and Japan. Asia is expected to grow at a CAGR of 32.4% between 2024 and 2030, which is the highest of the three major regions. That growth is primarily driven by China who has a CAGR of 34% with an increased focus on using AI to improve disease diagnosis and treatment accuracy. Japan is not far behind with a CAGR of 33.7% with the infectious disease sector expected to see the most growth over the next 5 years.[8]

Key Takeaways

The adoption of AI is and will continue to be a worldwide endeavor. As can be seen above, three key regions are all expected to grow faster than the predicted world CAGR which shows incredible promise for AI. The key areas of focus are anticipated to be oncology and infectious disease for these regions, as that is where there is the most demand for new drugs.

---

[7] *Europe Artificial Intelligence in Drug Discovery Market Size & Outlook, 2030*. (2025, May 29). https://www.grandviewresearch.com/horizon/outlook/artificial-intelligence-in-drug-discovery-market/europe

[8] *Asia Pacific Artificial Intelligence in Drug Discovery Market Size & Outlook, 2030*. (2025, May 29). https://www.grandviewresearch.com/horizon/outlook/artificial-intelligence-in-drug-discovery-market/asia-pacific

Competitive Landscape

Large Pharma "Giants" are Forced to Adapt

The pharmaceuticals industry has traditionally been dominated by well-established and long-standing companies. With the rise of AI, these large companies are scrambling to adapt to continue to remain at the forefront of innovation.

Pfizer is beginning to prioritize relationships with companies like Tempus and CytoReason[9] to integrate their technologies into drug discovery processes. Recently they utilized AI to develop Paxlovid, a COVID-19 treatment, at an accelerated rate. Reports suggested that AI allowed Pfizer to process through data and perform quality checks 50% faster during clinical trials. Moreover, on the supply chain side, they were able to reduce cycle time by 67%, allowing for 20,000 extra doses of the medicine to be produced per batch. Pfizer saw so much promise in this technology, that they are now actively attempting to utilize AI in over half of it drugs at the clinical trials phase.[10]

Janssen (Johnson & Johnson) currently has over 100 projects in various stages of the drug discovery process that have been bolstered using AI. [11] Janssen is also committed to improving the accuracy of AI software, recently partnering with Abbvie, Columbia university, and Apheris, a data protection company. They are all working together to bolster an AI model dubbed OpenFold3. Janssen has provided company specific molecular information to continue to train the model to improve its accuracy.[12]

---

[9] *Artificial Intelligence in Pharmaceuticals and Biotechnology: Current Trends and Innovations*. (2025, September 1). Coherent Solutions. https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations

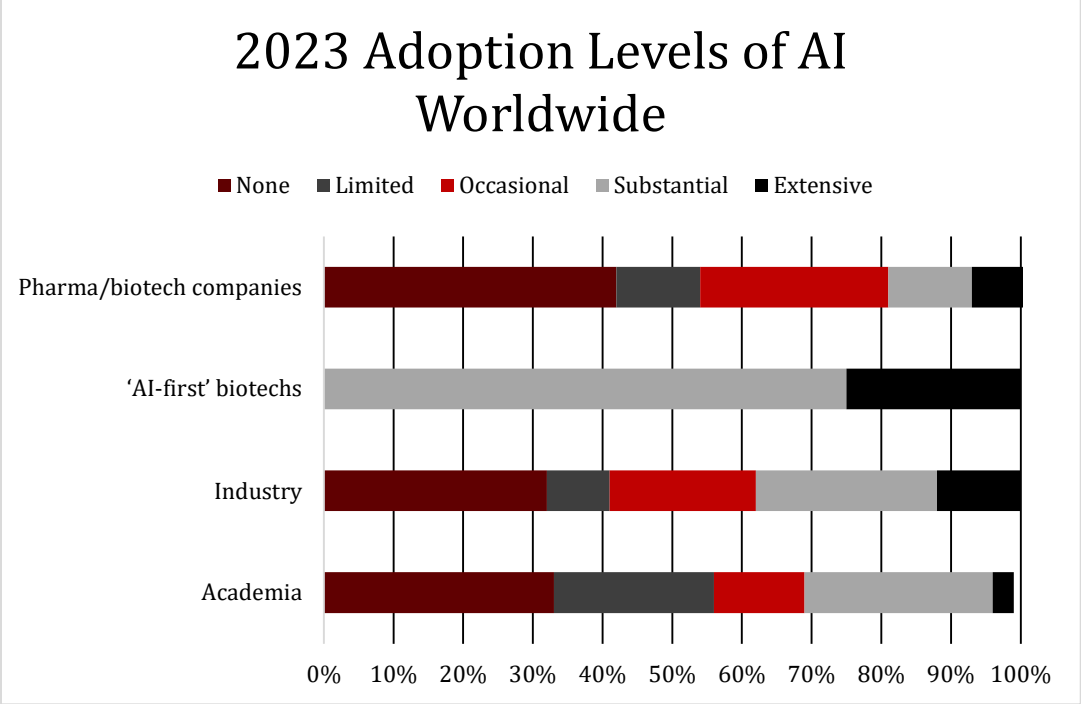
[10] *Pfizer leverages digital innovation to help deliver medicines to patients faster*. (n.d.). Pfizer 2022 Annual Report. https://www.pfizer.com/sites/default/files/investors/financial_reports/annual_reports/2022/story/data-and-ai-are-helping-to-get-medicines-to-patients-faster/

[11] *Artificial Intelligence in Pharmaceuticals and Biotechnology: Current Trends and Innovations*. (2025, September 1). Coherent Solutions. https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations

[12] Elizabeth S. Eaton. (2025, March 28). *AbbVie, J&J contribute data to fuel new molecular prediction model, OpenFold3*. FirstWord PHARMA. https://firstwordpharma.com/story/5945638

Smaller "AI-First" Companies are Closing the Gap

In an industry traditionally dominated by larger companies, smaller ones who incorporate AI as fundamental building block, have also begun to make an impact. BenevolentAI, a UK-based company for example, has been able to partner with big names like AstraZeneca and Novartis to utilize its AI software to select precise drug targets. Insilico Medicine is another company that has found success by using deep learning models with drug development and synthesis to accelerate the drug discovery process. While these companies are a lot newer, they are rapidly catching up to the overall market, with new discoveries being made frequently.



Coherent Solutions. (2025, February 12). Artificial intelligence in pharmaceuticals and biotechnology: Current trends and innovations. https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations

As can be seen from the chart above, the smaller AI biotech firms are adopting AI at a much faster pace. Specifically, this is happening 5 times faster[13] than larger pharmaceutical companies. By taking the risk on AI, it has allowed the smaller firms to catch up and level the playing field, even partnering exclusively with larger companies due to their lucrative drug development software, closing the gap between the larger and smaller companies.

[13] *Artificial Intelligence in Pharmaceuticals and Biotechnology: Current Trends and Innovations*. (2025, September 1). Coherent Solutions. https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations

AI in Drug Discovery

Initial Research

AI can aid companies from the very beginning of the drug discovery process, the initial research phase. Traditionally, the initial research phase took lots of time given that data had to be manually processed and understood. Often, the manual analyzation would also lead to a lack of comprehensiveness. Newer AI tools can process and understand large amounts of data and scientific information, increasing initial manual assessments by 30%. Researchers can easily pose questions to AI to deepen their understanding and seamlessly add more evidence for the model to process, making the whole process much easier.

Compound Screening

Using the initial manual assessments, AI can also help with initial compound screening. Using its own chemical modeling capabilities, it can screen known chemical compounds to make predictions about atom interactions to estimate what compounds can be used as leads to continue further testing on. Through repeated iterations, the model can be further trained to offer even more precise predictions and insights, improving performance by 250%. The screening process can now be up to 4 times faster, allowing what once took months to be completed in just weeks.

Trial Design

The help doesn't stop there; AI can be used for further testing and trial development as well. AI can help with finding the appropriate patients that can be tested, a longstanding problem in oncology-based research. It can also help with fundamental operational optimizations, causing up to a 20% reduction in cost and an accelerated approval by 2 years. [14] And during the trials, AI can actively look for hidden biomarkers or visual signatures that can lead to a better understanding of disease activity or breakthroughs for new treatments.

---

[14] Bhavik Shah, Chaitanya Adabala Viswa, Delphine Zurkiya, Eoin Leydon, and Joachim Bleys. (2024, January 9). *Generative AI in the pharmaceutical industry: Moving from hype to reality*. McKinsey & Company. https://www.mckinsey.com/industries/life-sciences/our-insights/generative-ai-in-the-pharmaceutical-industry-moving-from-hype-to-reality

Current Risks and Challenges

AI Continuously Needs Data

While there is immense potential in what AI has to offer, there are still some aspects that need continued improvement. With AI algorithms relying on large amounts of data to generate recommendations, there often isn't enough of it for the algorithm to produce effective results. With a lack of sample size, AI has shown to produce variable and sometimes inaccurate results which can be a problem in the context of the pharmaceutical field. One current method companies use to solve data sparseness is data augmentation. Data augmentation allows synthetic data to be generated to supplement the existing data to continue to increase both data quantity, diversity, and ultimately quality.[15]

AI Harbors Sensitive Information

Secondly, AI poses many ethical concerns that impact the willingness for companies to adopt the technology, given that millions of patients will be impacted worldwide. There are unfortunately not enough laws in place in healthcare to protect consumer data, hacking into databases for information can occur. That data can then be sold or used with malicious intent which can cause concern for both the business and consumers. [16] Currently one of the best solutions companies can use is partnering with a data security company, like how Janssen is partnering with Apheris. This way sensitive data related to the organization and potential patients involved can be effectively encrypted and secured.

---

[15] Blanco-González, A., Cabezón, A., Seco-González, A., Conde-Torres, D., Antelo-Riveiro, P., Piñeiro, Á., & Garcia-Fandino, R. (2023). The Role of AI in Drug Discovery: Challenges, Opportunities, and Strategies. *Pharmaceuticals*, *16*(6), 891. https://doi.org/10.3390/ph16060891

[16] Farhud, D. D., & Zokaei, S. (2021). Ethical issues of artificial intelligence in medicine and healthcare. *Iranian Journal of Public Health*. https://doi.org/10.18502/ijph.v50i11.7600

Recommendations

The Time is Now.

As of 2023, the adoption of AI has been skyrocketing, and the smaller competitors are beginning to close the gap. Nevertheless, the route forward is quite simple; all companies need to do *everything* in their power to adopt AI, or they will fall behind. This especially applies to large pharma companies, as their current adoption levels are low. Experts like Garrett Goodwin believe that "companies that will succeed [in the near future] will embrace this endeavor". Goodwin is currently leading the AI revolution charge at Pfizer, urging higher-ups to further prioritize AI.

Choosing Where to Start

The first key is companies need to choose a focus area to begin AI implementation, especially if they have not made much progress initially. Choosing from initial research, compound screening, or initial clinical trial development is a great start. Starting small is a good way to begin because of how the industry operates. Goodwin mentioned that the industry is very data driven and likes to have the most information possible when making a decision. Starting with one focus area can be a way for companies to see for themselves the benefit AI can have, giving them the data they require for them to feel comfortable incorporating AI companywide.

Developing the Technology

Once companies decide what they want AI to do for them, they need to determine how they are going to develop the technology. There are two ways, either developing an algorithm in-house, or utilizing the technology of other companies through partnerships and/or acquisitions. This will also require the company to set aside time to develop training materials for employees to become familiar with the new protocols associated with the new technology.

Protecting Data

Finally, companies in this space should prioritize data security. First, is deciding what software they want to use to encrypt and secure company-specific data. This can be done internally or by hiring an external company to help with the process. Secondly, along with training employees on how to use AI technology, creating robust training courses on data management and security will also assist with good data management practices.

Those three steps will put any company in a good position to reap all the benefits of what AI has to offer. AI is here to stay, and the industry must adapt to incorporate it as much as possible.

References

1. *Artificial Intelligence in Pharmaceuticals and Biotechnology: Current Trends and Innovations*. (2025, September 1). Coherent Solutions. https://www.coherentsolutions.com/insights/artificial-intelligence-in-pharmaceuticals-and-biotechnology-current-trends-and-innovations

2. *Asia Pacific Artificial Intelligence in Drug Discovery Market Size & Outlook, 2030*. (2025, May 29). https://www.grandviewresearch.com/horizon/outlook/artificial-intelligence-in-drug-discovery-market/asia-pacific

3. Bhavik Shah, Chaitanya Adabala Viswa, Delphine Zurkiya, Eoin Leydon, and Joachim Bleys. (2024, January 9). *Generative AI in the pharmaceutical industry: Moving from hype to reality*. McKinsey & Company. https://www.mckinsey.com/industries/life-sciences/our-insights/generative-ai-in-the-pharmaceutical-industry-moving-from-hype-to-reality

4. Blanco-González, A., Cabezón, A., Seco-González, A., Conde-Torres, D., Antelo-Riveiro, P., Piñeiro, Á., & Garcia-Fandino, R. (2023). The role of AI in Drug Discovery: challenges, opportunities, and strategies. *Pharmaceuticals*, *16*(6), 891. https://doi.org/10.3390/ph16060891

5. Elizabeth S. Eaton. (2025, March 28). *AbbVie, J&J contribute data to fuel new molecular prediction model, OpenFold3*. FirstWord PHARMA. https://firstwordpharma.com/story/5945638

6. *Europe Artificial Intelligence in Drug Discovery Market Size & Outlook, 2030*. (2025, May 29). https://www.grandviewresearch.com/horizon/outlook/artificial-intelligence-in-drug-discovery-market/europe

7. Farhud, D. D., & Zokaei, S. (2021). Ethical issues of artificial intelligence in medicine and healthcare. *Iranian Journal of Public Health*. https://doi.org/10.18502/ijph.v50i11.7600

8. *Pfizer leverages digital innovation to help deliver medicines to patients faster*. (n.d.). Pfizer 2022 Annual Report. https://www.pfizer.com/sites/default/files/investors/financial_reports/annual_reports/2022/story/data-and-ai-are-helping-to-get-medicines-to-patients-faster/

9. Polaris Market Research & Consulting, Inc. (2024, November 18). *AI in Drug Discovery Market Share and Forecast, 2034*. Polaris. https://www.polarismarketresearch.com/industry-analysis/ai-in-drug-discovery-market

10. Reuters. (2025, May 8). *US FDA centers to deploy AI internally, following experimental run*. https://www.reuters.com/business/healthcare-pharmaceuticals/us-fda-centers-deploy-ai-internally-immediately-2025-05-08/

11. Serrano, D. R., Luciano, F. C., Anaya, B. J., Ongoren, B., Kara, A., Molina, G., Ramirez, B. I., Sánchez-Guirales, S. A., Simon, J. A., Tomietto, G., Rapti, C., Ruiz, H. K., Rawat, S., Kumar, D., & Lalatsa, A. (2024). Artificial intelligence (AI) applications in drug discovery and drug delivery: Revolutionizing personalized medicine. *Pharmaceutics*, *16*(10), 1328. https://doi.org/10.3390/pharmaceutics16101328

12. Wani, G., & Faizullabhoy, M. (2024). Artificial intelligence in drug discovery market – by component (Software, Service), technology (Machine learning {Deep, supervised}), application type (Target identification, preclinical testing),

therapeutic area, end-use, Global forecast 2024 – 2032. In *Global Market Insights Inc.* https://www.gminsights.com/industry-analysis/ai-in-drug-discovery-market