SCORR MARKETING

HOW ARTIFICIAL INTELLIGENCE & BLOCKCHAIN ARE CHANGING DRUG DISCOVERY

December 2021

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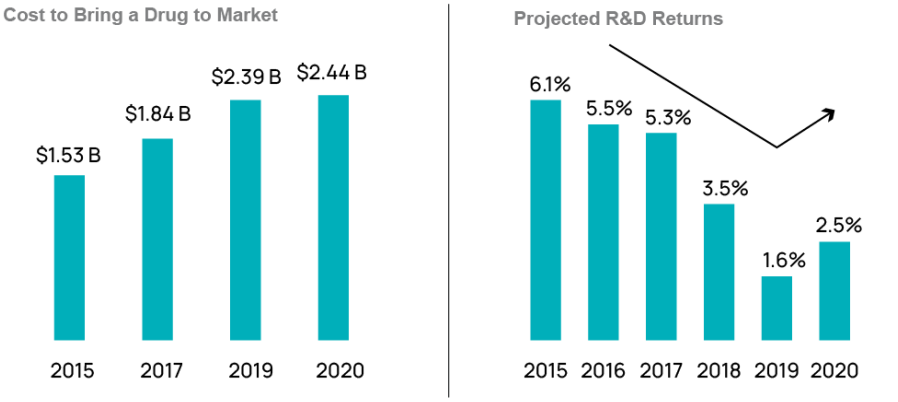
INTRODUCTION

An ongoing problem within the biopharmaceutical industry is the ever-growing cost of bringing a drug to market. From 2015 to 2020, the cost increased by almost 60%, from $1.5 billion to an estimated $2.44 billion.[1] The time required to move a new drug to commercialization has also increased. The industry is looking for solutions that will increase the efficiency of their programs while avoiding expensive failures.

The Cost and Time Needed to Bring a Drug to Market Has Continued to Increase
Data for Large Cap Biopharma



Source: GlobalData "Smart Pharma," June 2021

Artificial intelligence (AI) promises to be an exceptional tool for addressing the current issues in drug development. In a new approach, companies are developing 'machine learning' algorithms for the data intense stages of drug discovery.[2] The main hope of the pharmaceutical industry is to use AI to "minimize the hit-and-miss nature of R&D."[3] AI is an unprecedented technology with the ability to realize similarly unseen efficiency gains in the development of new therapies. Conventional techniques require human intervention and understanding; AI-based approaches can use large datasets to find new connections without the same introduction of human error. This allows AI to make stronger predictions for how to successfully drug targets than traditional methods.

Traditional vs AI-Based Drug Discovery

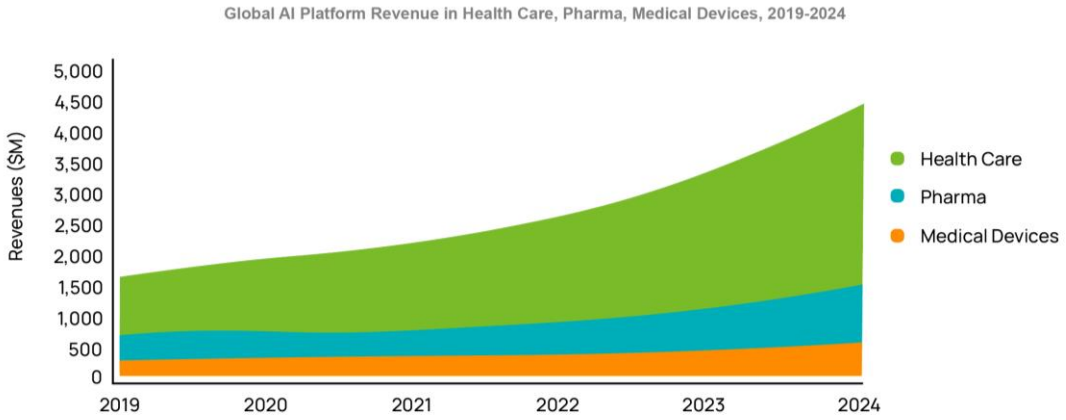
Traditional	AI-Based
› Target-Driven	› Data-Driven
› Works well for easily druggable targets that have a well-defined structure and whose interactions inside the cell are understood in detail	› Complex algorithms and machine learning can extract meaningful information from a large dataset
› Extremely limited due to the complex nature of cellular interactions & limited knowledge of intricate cellular pathways	› Identify compounds that could bind to 'undruggable targets,' i.e., proteins whose structures are not defined

Source: RoboticsBiz, "AI in Drug Discovery," April 9, 2021

MARKET OVERVIEW

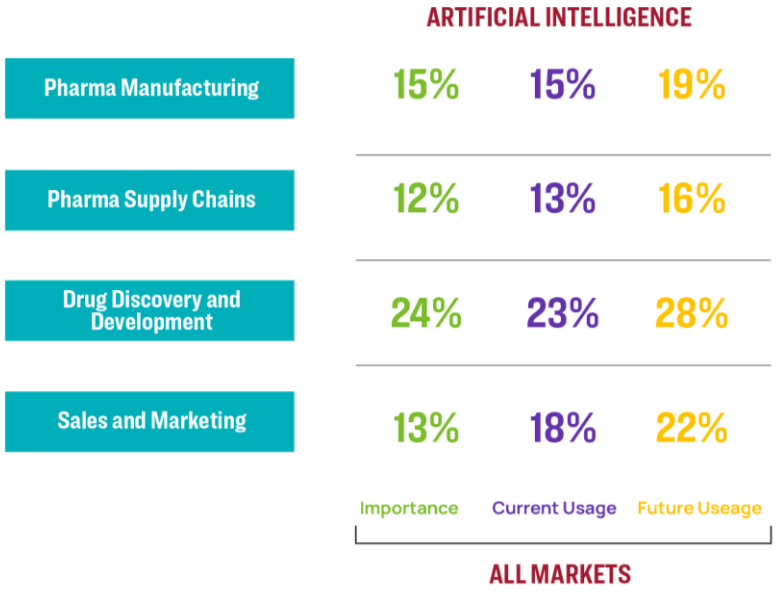
Global Revenue for AI Platforms Across Health Care Will Reach $4.3B by 2024

CAGR between 2019 and 2024 will be 24.6% in health care, 18.5% in pharma, and 20.6% in medical devices.



Source: GlobalData, "AI in Health Care," April 20, 2021

Biomedical research is not unique in its adoption of AI. However, to understand its impact within the pharmaceutical sector, it is helpful to look at AI development within this industry. According to a 2021 GlobalData analysis, AI platform revenue will exceed $4.3 billion by 2024. Notably, there is already a huge investment in this space, approaching ~$2 billion in 2021.[4]



Source: GlobalData, "Smart Pharma," June 2021

Companies in the drug discovery and development space place the highest importance on machine learning and similar breakthrough technologies. The value proposition is simple – cheaper, quicker, and more effective drugs found through algorithms.[5]

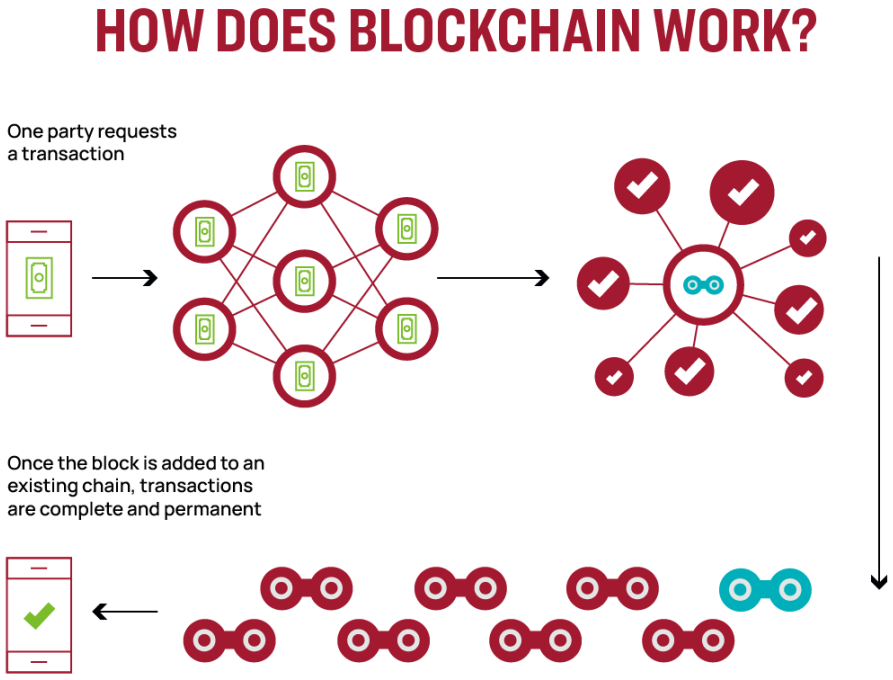
In addition, the adoption of blockchain technology offers security and a method to ensure data integrity during all steps of the development life cycle, from hit identification to commercialization.[6] This removes barriers between stakeholders involved in different aspects of the process by easing the friction generated in the traditional system, which relies on stakeholder trust when moving through the steps of development. Similarly, the blockchain empowers researchers to share authenticated data for clinical trial operations while maintaining security. However, we will focus exclusively on the use of AI and blockchain in drug discovery and consider the complexities of integrating either technology into clinical research as beyond the scope of this primer.

DEFINITIONS

Artificial intelligence (AI) is a field of computer science that uses large datasets to enable problem solving.[7] Within the field of AI are multiple disciplines, including machine learning, deep learning, and other forms of probabilistic analysis for huge datasets.

The most basic description of AI is algorithms which create predictions from an input of data.

This is an inclusive definition, which may not be used by all. Within the fields of AI and machine learning, experts still disagree whether machine learning techniques are truly AI. For the purposes of this document, machine learning is considered as a subtype of AI.



Source: cInet, "Blockchain Explained: It Builds Trust When You Need It Most," February 12, 2018

Blockchain technology is a system of public databases that continuously cross-reference each other.[8] Each block can hold a certain amount of data. Once filled, it connects to the next generated block, creating an unbroken chain of blocks throughout the system. Data cannot be changed once incorporated into the system, enforcing both security and reliability.

DNA-Encoded Libraries (DELs) is a drug discovery technology for screening many small molecules versus a drug target, numbering in the billions.[9] Each small molecule is tagged with a unique code of DNA, used as a kind of barcode, with information about its chemical makeup. This technology allows for a greater exploration of chemical space than traditional methods like High-Throughput Screening. DELs can screen billions of chemically synthesized small molecules to find a hit against a chosen drug target. Notably, this technique creates a huge output of data.

A drug target is a biological molecule within a patient, usually a protein, that is important to a disease's progression. When acted on by a drug, the patient experiences a desired therapeutic effect.[10]

High-Throughput Screening (HTS) is a method of drug discovery where investigators take a drug target and test its biological activity in response to exposure to small molecules. Much of HTS is automated, but its rate is limited by the number of molecules that can be included, numbering in the thousands to single digit millions.[11]

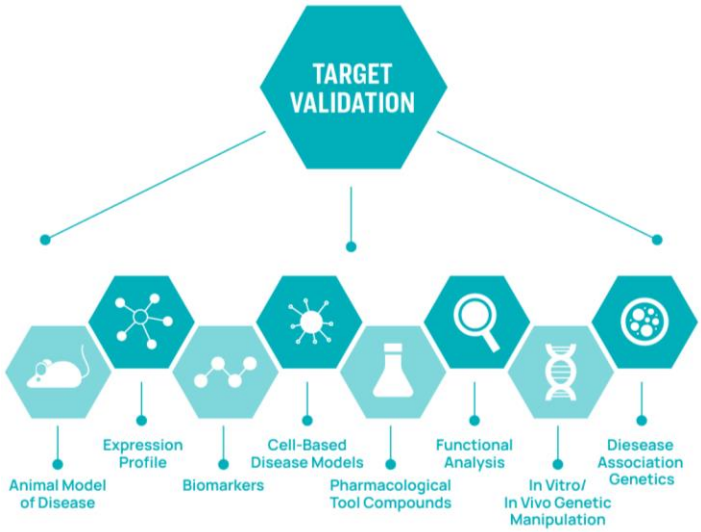
A hit is a molecular compound that shows potential for therapeutic activity when in the presence of a drug target.[12] Once a hit is found, it can be refined to better fit the target, becoming a lead.

A lead is a molecule with biopharmaceutical activity that appears to be therapeutic. However, the structure is in some way suboptimal.[13] Lead optimization is the process of modifying leads into clinical candidates with desired properties, such as better binding to the drug target.

Machine learning is an algorithmic technique modeled on the human brain.[14] Through a process of trial and error, the AI gradually improves accuracy. Famously, AlphaGo is an AI that used this "neural network" architecture to master chess. The same technology can be adapted to any high data output system.

TARGETS, HITS, & LEADS

In drug discovery, the first necessary ingredient is the drug target. Sometimes drugs are developed without any knowledge of their target, resulting in target identification. In this process, clinical pharmacologists investigate what target a small molecule acts upon to create a therapeutic effect.[15] In contrast, target discovery is the process of defining a target molecule. This may be through academic research finding that a particular molecule impacts disease or as an offshoot of separate drug discovery processes.[16]



Source: Global Data, "SmartPharma," June 2021

Both forms of target discovery lead to target validation. Before beginning the costly and time intensive process of development, researchers verify that their drug target can be altered for therapeutic benefits.[17] In addition, investigators ensure that any benefits are within an acceptable safety profile. Some promising drug targets are abandoned when scientists find off-target or high-risk effects of modifying their functions.

Hit identification is the classic method for finding a new drug. A validated drug target is screened by a system containing a diversity of small molecules, such as in High-Throughput Screening or DNA-Encoded Libraries. A "hit" is a molecule that interacts with the drug target in a desirable way.[18] Ideally, these screens are full of drug-like chemicals that have the potential to be further optimized. When some hits show promise, they are more stringently screened in a process called "hit-to-lead" or "lead optimization." Importantly, hits are narrowed into only the most promising leads. Leads are then optimized via chemical modification to compounds that have a therapeutic impact on the drug target, which can then move into preclinical animal work.[12]

"DEL samples a larger portion of the available chemical space than conventional approaches. This can be seen in the relative sizes of the chemical libraries, which number in the low millions for conventional HTS, but in the hundreds of billions for DEL. This allows DEL to address "difficult" targets that typically fail in conventional approaches. In addition, DEL can be performed faster and cheaper than older methods."

– Matthew A. Clark, Ph.D., Chief Executive Officer, X-Chem

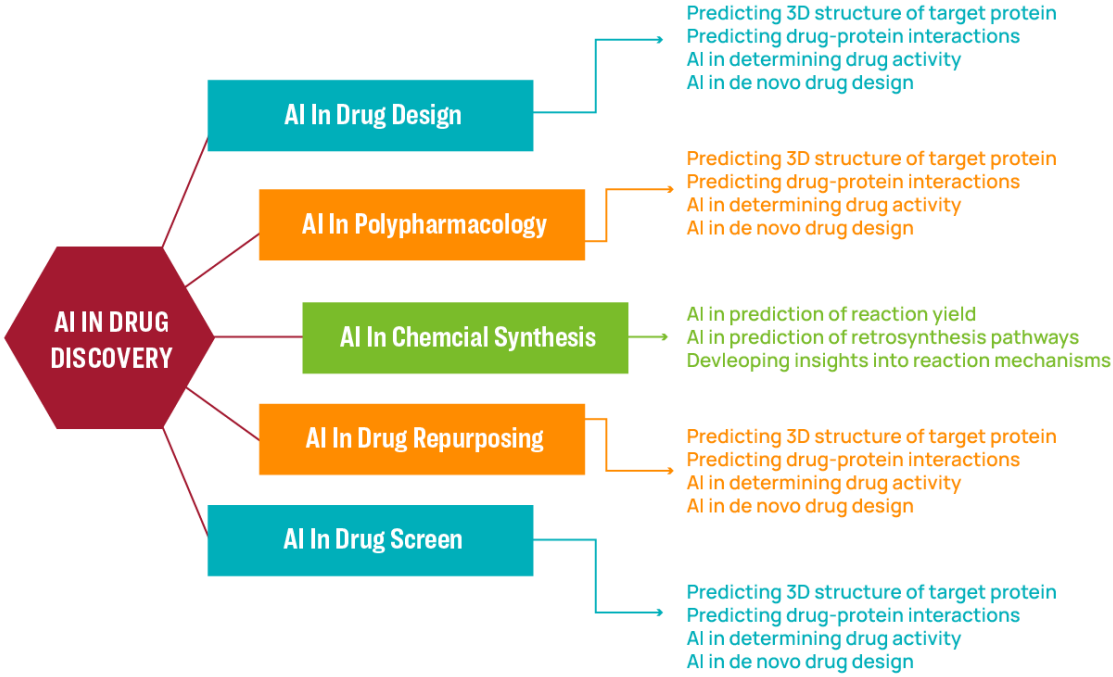
To give the best chance of finding a promising hit series, the size of HTS is ever-increasing. Unfortunately, this has greatly increased timelines and costs for drug discovery screens. In fact, screening campaigns now regularly cost in the hundreds of thousands of dollars, with no guarantee of finding a viable hit.[19] Alternatives like DEL technology innately explore a greater chemical space than HTS systems.[9] As such, DEL has found multiple novel inhibitors of drug targets that were invisible to traditional screening methods. Both systems now need to grapple with massive datasets produced by every individual screen.

Blockchain

Early in the drug discovery process, companies produce data during target identification and validation. Transferring this proprietary data is a vulnerability. However, blockchain technology promises to facilitate better data sharing. The blockchain can maintain data confidentiality while moving results between stakeholders. In this way, blockchain prevents duplication of work by collaborators and accelerates drug development.[6]

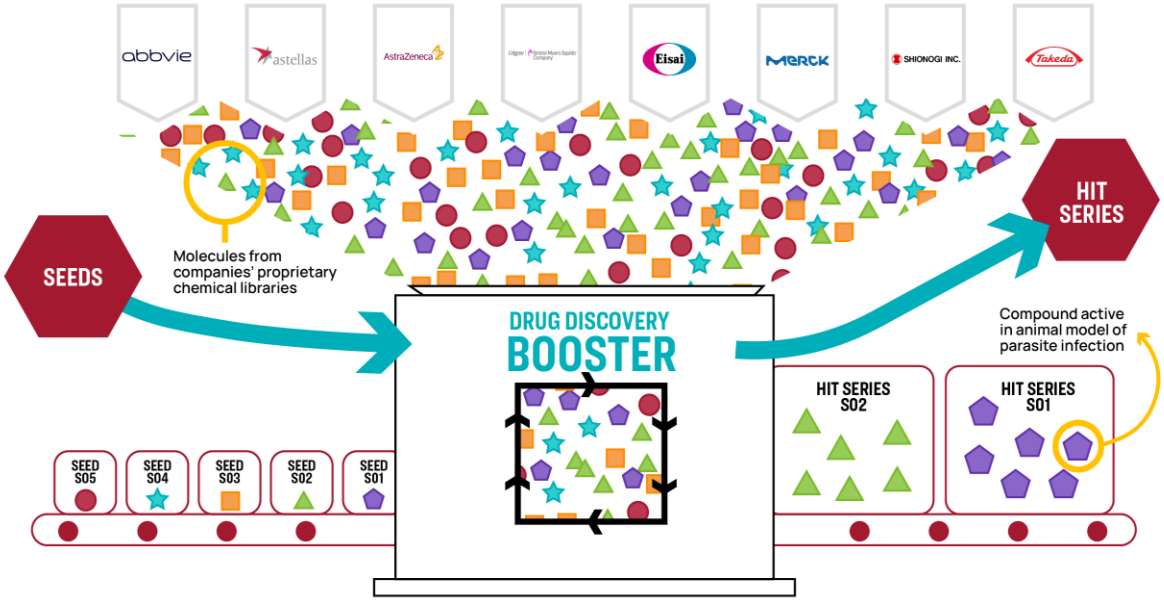
Artificial Intelligence (AI)

Given the data rich environment of drug discovery, drug developers are implementing automated systems. This automation can be broken down into two major categories: predictive and process.



Source: Drug Discovery Today, "Artificial Intelligence in Drug Discovery and Development," October 21, 2020

Predictive AI are meant to replace or complement physical screening of drug targets. By using huge databases of small molecules and their characteristics, these predictive AI identify likely hits and leads. Some even provide structure optimization assistance and suggestions.[20] For example, Exscientia's 'Centaur Chemist' AI design platform was able to compare millions of virtual small molecules likely to impact the A2 receptor, then suggest 10-20 to synthesize and test.[21] The program successfully identified an A2 receptor antagonist that helps T cells attack solid tumors within 8 months. In comparison, the researchers estimated the traditional paradigm of drug discovery would have taken 4-5 years to reach a similar result. Similarly, X-Chem's DEL platform has been combined with machine learning to generate a higher effective hit finding rate than running the screen alone.[22]

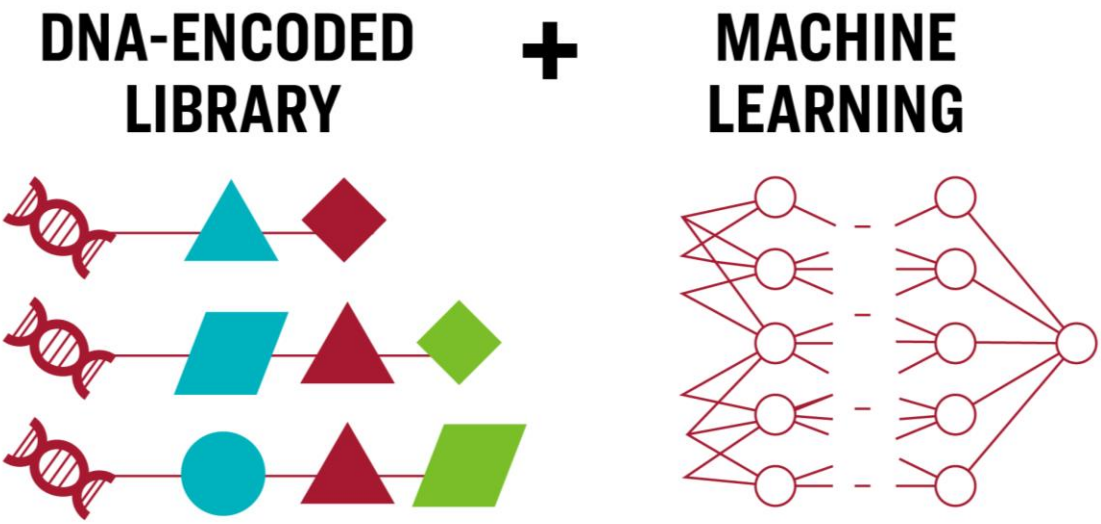


Source: Drugs for Neglected Diseases Initiative (DNDi) "NTD Drug Discovery Booster Hit-to-Lead," June 1, 2021

Process AI are a more traditional incorporation of automated systems into pre-existing workflows, similar to how machines have been added into traditional manufacturing. Because much of the drug discovery process is systematic, execution can also be physically automated. According to Science Advances, "[a]utomating the molecular design-make-test-analyze cycle accelerates hit and lead finding for drug discovery."[23] Ultimately, AI will increase the efficiency of the entire industry.

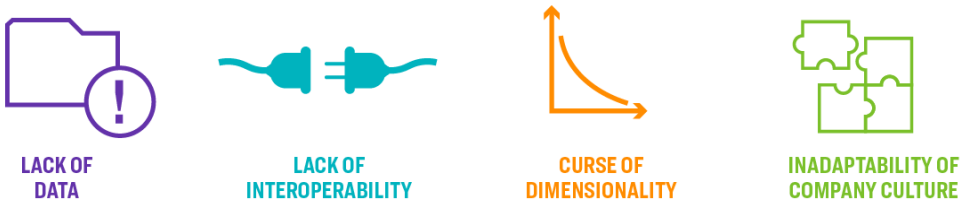
"AI is already poised to be universally adopted. It's impact, however, will be determined by the scope and quality of the data it is provided."

– Matthew A. Clark, Ph.D., Chief Executive Officer, X-Chem



Source: Journal of Medicinal Chemistry "Machine Learning on DNA-Encoded Libraries," June 11, 2020

CHALLENGES & LIMITATIONS



Blockchain

The blockchain offers data security and integrity with the additional benefit of easy transference between stakeholders. However, the blockchain is new technology and is associated with cryptocurrencies, creating a social challenge to adoption, especially as many consider mentions of Bitcoin as synonymous with speculative investments. Physicians, scientists, and other stakeholders remain skeptical of blockchain technologies in their areas.[24]

However, the challenge in adopting blockchain technology is more deeply rooted in the pharmaceutical industry. Competition is a hallmark of pharma, but blockchain relies on coordination between institutions. This is a paradigm shift that many stakeholders have been reticent to accept, which has prevented industry buy-in, at least until the technology matures.[25]

AI

Similarly, AI is a promising technology when applied to drug discovery and is disruptive to the industry's status quo.

There is a shortage of high-quality data in drug discovery, meaning there is a dearth of data to train machine learning algorithms.[26] Currently, researchers throughout the industry are attempting to address common but suboptimal "noisy" datasets — data with errors in bookkeeping, such as duplicate entries or those with incomplete values. Similarly, small sample size and the complexities of real-world datasets often prevent the collection of ideal training data for machine learning.[27]

In addition, the datasets are not standardized between companies, which again stymies machine learning approaches.[27] Other problems, such as the millions of compounds included in the screens, create massive datasets that are not interoperable.[28] Finally, the industry has significant barriers to sharing data, including costs, legality, and lack of incentives for cooperation.[26,30]

"The industry needs to adopt a mind-set that the primary purpose of laboratory experimentation is to provide data to AI, rather than providing a data deliverable to end-users. With AI in mind, the industry will focus more rigorously on the standardization, curation, and cleaning of data."

– Matthew A. Clark, Ph.D., Chief Executive Officer, X-Chem

AI is important to the advancement of precision medicine, meaning it is included in the "curse of dimensionality."[31] So many variables are being included in precision medicine that there are not enough samples or patients to produce the data needed to effectively train the AI. There are more possible observations than empirical data, creating an environment for the generation of false positives – patterns that look promising but are due to random chance.

So far, combining AI with patient data has been difficult. The initial AI offerings did not allow interoperability between Electronic Health Records (EHRs) nor existing electronic infrastructures.[27] This initial failure has long-ranging consequences.

Some business leaders in the biomedical space are now distrusting of AI. By nature, AI integration will be deeply disruptive to the status quo across the pharmaceutical industry and in health care delivery.[32] Given the history of failed enactments, AI developers need to show experts and business leaders their technology's value proposition and clearly explain why it will help rather than hinder business goals. AI implementation requires a strategy that is satisfactory to experts, business leaders, and coders before initiating the process.[32] Otherwise, at least one stakeholder party is likely to prevent successful integration of the AI systems.

No individual challenge to blockchain or AI implementation is insurmountable, but in total, they have prevented universal adoption. As each major challenge is overcome, a gradual increase in AI implementation will follow, as opposed to a single breakthrough causing wide-spread deployments.

DRUG DISCOVERY SERVICE PROVIDERS THAT USE AI

Drug developers are investigating the use of AI to compete in the global biopharmaceutical market, including by attracting expertise and talent from top drug makers. AI adoption is another point of differentiation for these drug discovery service providers within the competitive research and development industry.[33]

All sponsors – pharmaceutical or biotech – are drug discovery companies. Below are some research organizations who offer drug discovery services. Each one addresses or shows how AI is used while presenting their drug discovery service offerings.

Drug Development Service Provider	How They Address Drug Discovery
ALTASCIENCES	Artificial Intelligence Application in Early Drug Development (blog post)
BIODURO-SUNDIA 保诺-桑迪亚	Discovery
charles river	Artificial Intelligence for Drug Discovery
ICON	The Power of AI to Transform Clinical Trials (blog post)
IMMUNOCORE	Computational Chemistry Services - AI - Drug Discovery
IQVIA™	AI & Machine Learning with a Healthcare IQ

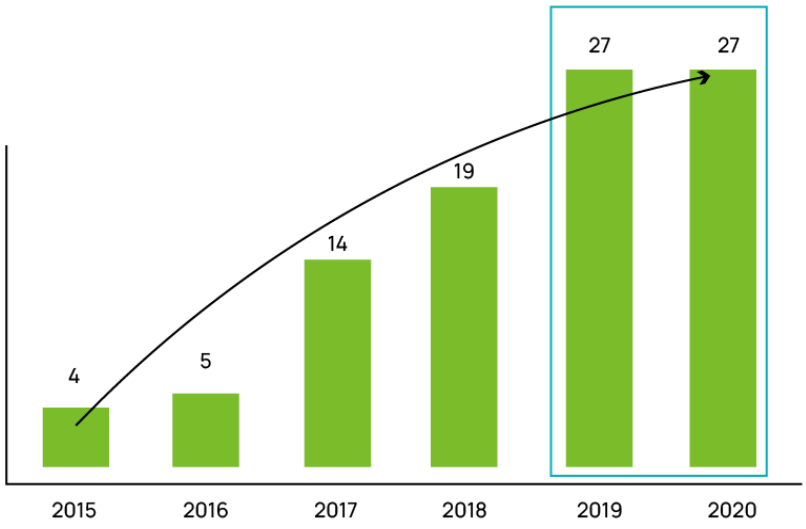
labcorp Drug Development	Artificial Intelligence in Clinical Trials and Disease Prediction (event presentation)
WuXi Biologics Global Solution Provider	Integration of Validated AI Tools in Chemistry Workflow
X-CHEM TAKE THE LEAD. DRIVE DISCOVERY.	Machine Learning Needs Big Data to Revolutionize Drug Discovery (article)

AI-BASED DRUG DISCOVERY PARTNERSHIPS

AI implementation requires large scale cooperation within the biopharmaceutical industry, especially for data sharing to train machine learning algorithms.[34] Young start-up companies in the AI-drug discovery space compete for access to the large databases of information held by larger companies, especially multi-omics or specific disease area information.[35]

Pharmaceutical giants are creating alliances through AI, especially in drug discovery. The number of partnerships is ballooning in number, along with large-scale financing efforts. The promise of AI is too alluring – powerful tools that could revolutionize drug research and development.[21]

Number of AI Drug Discovery Partnerships with Big Pharma
As of June 16, 2021



Source: GlobalData "Smart Pharma," June 2021

PHARMACEUTICAL ORGANIZATION	AI ORGANIZATION	COLLABORATIVE WORK
Roche	OWKIN	Drug discovery and development, clinical trials based on ML networks
Pfizer	XtalPi	Use of quantum mechanics and ML algorithms with cloud computing architecture to predict the 2D structure of molecules, depicting their mechanical and chemical properties, and how they bind with protein receptors
Pfizer, Novartis	IBM Watson	Use of ML, natural language processing, and cognitive reasoning technologies in immuno-oncology to find new drug targets, combination therapies, and patient selection strategies
Novartis	Microsoft	Improved health outcomes for patients with breast cancer
		Research on cell and gene-based therapies, generative chemistry, image segmentation and analysis for smart and personalized delivery of therapies, and optimization of cell and gene therapies at scale.
MATEON THERAPEUTICS	PointR DATA	Treatment of late-stage melanoma, gliomas, and pancreatic cancer
Bayer	Sensyne Health	Clinical development of new treatments for cardiovascular disease using Sensyne Health's proprietary clinical AI technology platform
Bayer, Sanofi	Exscientia	Exscientia uses its Centaur Chemist™ AI drug discovery platform to optimize novel lead structures for potential drug candidates for treatment of cardiovascular and oncological diseases
Sanofi	Exscientia	To discover and develop bispecific small molecules for diabetes and its comorbidities
Boehringer Ingelheim	healx	Healnet, an AI-based platform, is used to find therapies for rare neurological diseases.
Takeda, Servier	Numerate	To find drug molecules for oncology, gastroenterology, and central nervous system disorders
Takeda, Servier	Numerate	Design of small-molecule modulators of ryanodine receptor 2 (RyR2), a target identified in cardiovascular diseases using proprietary algorithm-driven discovery platform
Lilly	Atomwise	Develop drugs on novel protein targets
Janssen, AstraZeneca	BenevolentAI	BenevolentAI assumes exclusive right to develop, manufacture, and commercialize Jannssen's novel clinical-stage drug candidates; already used to provide clinical data in Phase IIb trials of bavisant in patients with Parkinson's disease and excessive daytime sleepiness
Janssen, AstraZeneca	BenevolentAI	Neural network-based platforms for discovery and development of new treatments for chronic kidney disease and idopathic pulmonary fibrosis

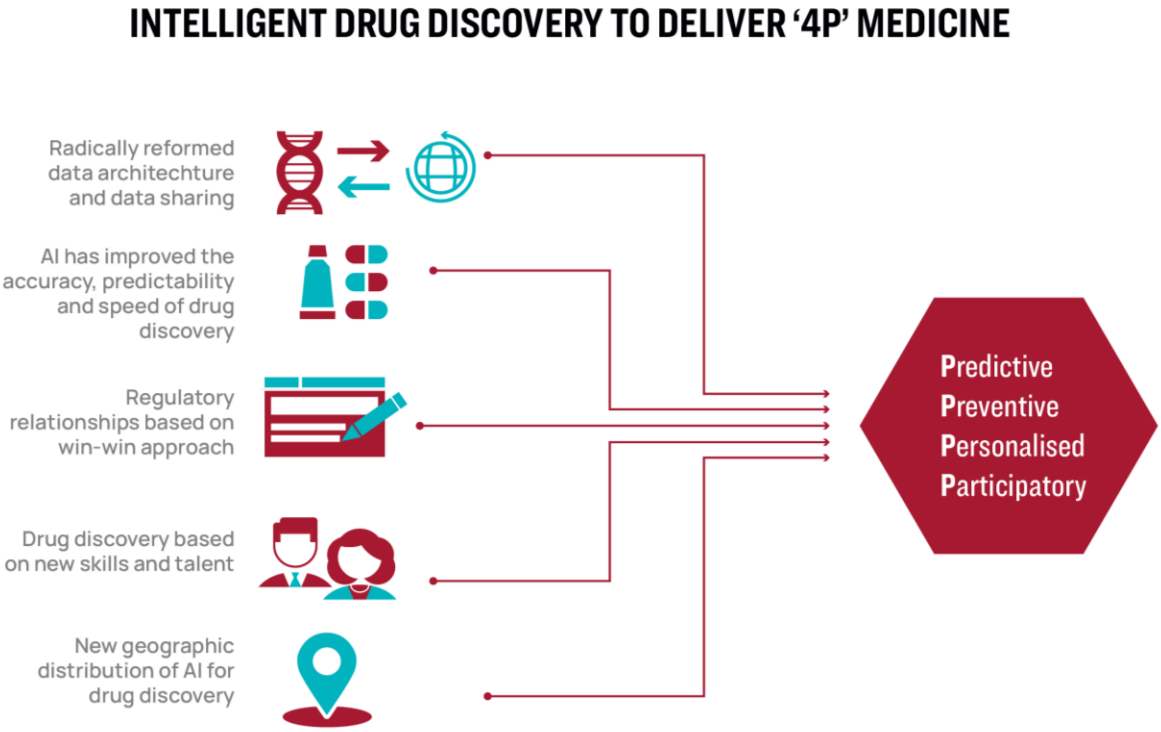
FUTURE IMPLICATIONS

AI and blockchain will disrupt the status quo in medicine and drug discovery, though the exact nature of the coming changes is still unclear.

Precision Medicine

Precision medicine appears to be the primary beneficiary of advancing technology. Ultimately, health care delivery should be more efficient and effective. We have previously written extensively on the near-term future of precision medicine.

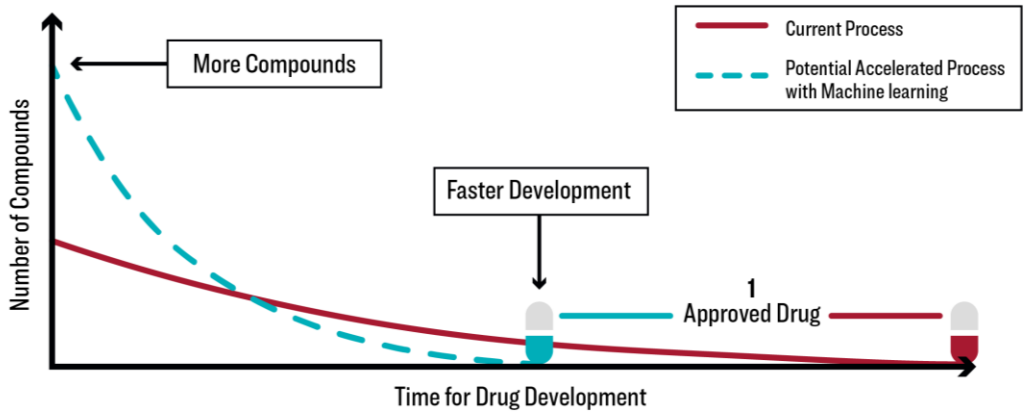
Large data sets will produce more precise and targeted treatments, pushing health care to the "4Ps" model – personalized, predictive, preventative, and participatory.[35]



Source: Deloitte, "Intelligent Drug Discovery," November 7, 2020

Drug Discovery

AI is already changing drug discovery programs, ushering in a paradigm shift in development, especially through machine learning.[26] By taking large datasets into predictive models that test virtual versions of compounds, fewer physical compounds need to be synthesized and tested.[36] Currently, AI is predicted to save an estimated $70 billion in drug discovery processes by 2028. In addition, timelines are already being accelerated by machine learning AI.[25] Together they promise to bring about a new "era of drug development that is faster, cost-effective, and more successful."[37]



Source: US GAO, "Artificial Intelligence in Health Care," January 21, 2020

SUMMARY

The incredible cost of bringing a drug to market has pushed biopharmaceutical companies to pursue more efficient and effective drug discovery. AI machine learning algorithms are just beginning to meet this need. In addition, blockchain technology promises to facilitate data security, integrity, and transference between stakeholders.

Market Overview

Current investment in AI for drug discovery is estimated to be around $2 billion, which is expected to more than double by 2024, indicating a large financial interest.

Targets, Hits, and Leads

There is a common cycle of drug discovery: target discovery -> target validation -> hit identification -> lead identification -> lead optimization. Target discovery identifies the drug target. Target validation verifies that a molecule can likely be drugged safely. Hit identification through lead optimization is the major work of most drug discovery companies seeking viable drug candidates by screenings, such as HTS or DEL. AI promises to increase the efficiency of each stage of drug discovery through both predictive and process improvements. Similarly, blockchain promises to increase process efficiency by facilitating data sharing and maintain data integrity.

Challenges and Limitations

Blockchain is considered an unproven and immature technology by many companies, slowing its adoption. AI requires a standardization of data between companies that does not currently exist. In addition, too many 'dimensions' can be included in training data, without enough empirical data from real world samples. Both technologies require a much greater degree of collaboration within the traditionally competitive biopharmaceutical industry before they will be universally embraced.

CROs That Use AI for Drug Discovery

CROs and biotech with drug discovery programs are now featuring their use of AI, representing the first stage of adoption and general usage.

AI-Based Drug Discovery Partnerships
Large pharmaceutical corporations are creating alliances to create better AI systems in the drug discovery space. Smaller startups attempt to enter these partnerships for access to highly valuable datasets that only large corporations can generate.

Future Implications
AI and blockchain will facilitate better, more efficient drug discovery. Both technologies save costs and shorten timelines, which are desperately needed as the industry has trended upwards in each category for decades. The allure of accelerating drug discovery and development timelines is pushing innovation of both technologies.

ABOUT THE AUTHOR

Alex Generous, Ph.D., a scientific writer at SCORR Marketing, earned his Ph.D. in biomedical sciences from Mayo Clinic and B.A. in biochemistry, cell and molecular biology from Drake University. He served as a science writer for Mayo Clinic's Research Communications and subsequently as associate director of science communication for the National Cattlemen's Beef Association. He is currently a member in good standing of the National Association of Science Writers.

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