Pharmaceutical Artificial Intelligence in 2020: The Sector is Heating Up For Investments

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Introduction

Artificial Intelligence (AI) has been a top trend in many industries lately, attracting massive media attention and investments. Over the last decade, this complex area of research has rapidly progressed from being a “resurrected cool technology from the past” to a full-blown driver of nothing less than a new industrial revolution -- a digital one. As of today, AI is widely commercialized in such applications as manufacturing robots, smart assistants (e.g. Siri), automated financial investing systems, virtual travel booking agents, social media monitoring tools, conversational bots, surveillance systems, online security systems, language translators, self-driving cars, and much more.

In some industries, AI (including its many technologies and sub-disciplines, such as deep learning, recommender systems, and natural language processing), is becoming a standardized component rather

than a cutting-edge innovation it once was.

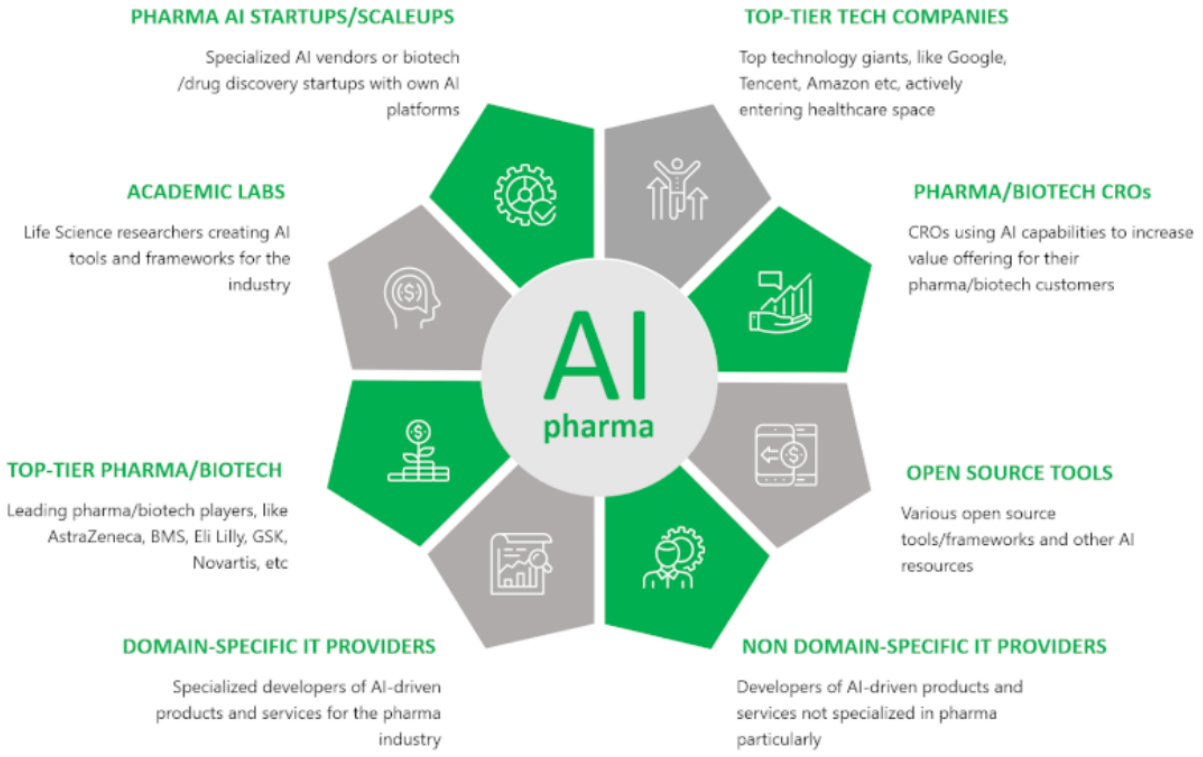
This rapid progress in AI adoption is also seen in the pharmaceutical industry -- not without caveats, however. Unlike “mainstream” use cases, like image recognition or spam email filtering, drug discovery research appears to be a much harder case for several reasons.

First, the amount of data, suitable for training, is way smaller in biology and biomedical research, than in languages, everyday images, or videos.

Second, training itself is less straightforward. One can immediately assess a photography prediction by the AI system, and flag results with the “right” or “wrong” label to make the system learn. In the case of AI identifying patterns in complex omics data, or creates a hypothesis from the research literature, let’s say, it takes time and experimentation to be able to interpret them and update the model.

Notwithstanding all the above difficulties, the progress in the area of pharmaceutical AI is tremendous, with many proof-of-concept studies confirming that the technology is maturing and gaining a commercial level and apparent disrupting potential for healthcare innovation.

The pharmaceutical artificial intelligence ecosystem is growing, including more and more AI-vendors, AI-driven biotech startups, and corporations that start building in-house capabilities and expand external partnerships with AI-labs and companies. The below image illustrates the key groups of organizations,.involved in the advancement and adoption of AI research and tech in drug discovery and medical R&D:



Next, let's review some of the notable industry developments in what relates to various artificial intelligence technologies, such as deep neural networks, and natural language processing being applied in drug discovery and clinical research. The focus here is on major investment rounds, important R&D partnerships between AI-vendors and big pharma/CROs, new AI-startups founded in 2020, and the important role of AI in tackling the COVID-19 pandemics. This is not meant to be a comprehensive overview, rather -- an illustrative list of developments and reflections on where things are moving forward.

The abundance of venture capital, major funding rounds

Biotech investors have been increasingly optimistic about the promise of AI in drug discovery, pouring more money into leading AI-driven biotech firms compared to previous periods. According to a report by Deep Pharma Intelligence, the total amount of VC funding in AI-biotech startups increased in 2020 (as of November) by around 23%, compared to 2019, approaching a total of $1.9B, which is also more than in 2015, 2016 and 2017 combined. There is an increasing number of late-stage mega-rounds (e.g. B, C),

including hundreds of millions of dollars.

XtalPi

XtalPi, an American-Chinese biotech company, raised a formidable $319M in the financial round C, which was led by SoftBank's Vision Fund. The company, founded in 2014, is developing approaches in which quantum physics, AI and cloud computing are intersecting. Based on this, its Intelligent Digital Drug Discovery and Development (ID4) platform provides prediction of small molecules candidates properties, solid-form selection, and other services.

Insitro

Insitro**,** a data-driven drug discovery company co-founded in 2018 by Prof. Daphne Koller, has recently raised $143M in Series B financing. The round was led by Andreessen Horowitz, CPP Investments, and others. The company differs from other AI companies as it has built its own cutting-edge laboratory that allows collecting massive amounts of data to train their ML engine. Additionally, Insitro entered a strategic collaboration with Gilead last year with the goal of developing new therapies for nonalcoholic steatohepatitis (NASH).

Tempus

In March, Tempus announced it received $100M in Series G financing. The investors included Baillie Gifford, Franklin Templeton, NEA, Novo Holdings, and funds and accounts managed by T. Rowe Price. The company's main focus is advancing precision medicine and applying AI in healthcare. With the additional funding Tempus continues to expand its operations to various diseases areas, including diabetes, depression, and cardiology. Since its founding in 2015, the company has raised in total $620 M of financing.

Exscientia

In May, Exscientia, a British start-up, announced it raised $60M in Series C round led by Novo Holdings, Evotec, Bristol Myers Squibb, and GT Healthcare Capital. Exscientia uses AI for small molecule drug design using its Centaur Chemist™ platform**.** The company already has a drug candidate in Phase 1 clinical trial for the treatment of obsessive-compulsive disorder (OCD). Together with Sumitomo Dainippon Pharma, Exscientia developed and brought the drug to clinical trials in one year, claiming its end-to-end AI capability to be the major contributing factor of this speedy timeline. Exscientia has already participated in multiple projects together with Bristol Myers Squibb, Bayer, Sanofi, Rallybio, and joined the COVID-19 initiative. With the above-mentioned financing, Exscientia hopes to expand its representation to the USA.

Owkin

Owkin, a medical research company that pulled two significant investments one by one in May and June, bringing in a total of $43M in 2020. This funding included $25M from Bpifrance, Cathay Innovation, MACSF, and $18M from Bpifrance and Mubadala Capital. Their AI-powered collaborative platform Owkin's Studio implements an alternative approach to healthcare data storage that is used by big tech companies, such as Amazon, Microsoft, and Google. Owkin’s task is to decentralize research and to make it more collaborative. For it the start-up uses federated machine learning, which allows training the algorithms from disparate sources (research laboratories, biotech companies), without needing to aggregate data together in one source.

Deep Genomics

Deep Genomics is a Toronto-based start-up, which raised $40M in Series B in January. The round was led by Future Ventures with the participation of Amplitude Ventures, Khosla Ventures, Magnetic Ventures, and True Ventures. This financial resource supports the advancement of Deep Genomics’ AI-based drug discovery platform and the development of treatment for rare genetic diseases. The Deep Genomics software, Saturn, is used to identify and better understand drug targets, especially targets that are thought to be undruggable.

BenchSci

BenchSci is another Toronto-based start-up founded in 2015. Bench raised $22M in series B for future development. The round was led by F-Prime Capital, with participation from Northleaf Capital Partners and others. BenchSci is focusing on selecting relevant antibodies for experiments that significantly reduce the failure rates. Over 30 thousand scientists already used BenchSci's AI-Assisted Antibody Selection to plan their experiments. The company recently launched an AI-assisted reagent selection product, which encompasses such reagents as antibodies, RNAi, and recombinant proteins.

ImmunAi

A New-York city start-up, Immunai, raised $20M in seed funding from Viola Ventures and TLV Partners. ImmunAi intends to map the entire immune system with AI and single-cell analysis. Immunotherapies have been a hot topic in drug discovery in recent years, but it still needs more data to make therapies more efficient and safe. ImmunAi profiles hundreds of immune cell types, collecting data that will support biomarkers and better therapies discovery.

Cyclica

The Toronto-based AI-powered biotech Cyclica has closed $17M in series B financing. The round was led by Drive Capital with participation from Chiesi Farmaceutici, GreenSky Capital, and members of Cyclica's management team. The company has an ambitious plan to "create the biotech pipeline of the future" and will use the money to embody it. Cyclica designs lead molecules with a focus on preventing adverse effects through studying pharmacogenomics and gene polymorphisms.

Schrödinger

Finally, the beginning of 2020 was marked by a successful IPO in the sector of computational drug design -- New York-based Schrödinger closed its initial public offering in February, raising a total of $232.3 million in proceeds – more than originally planned.

New AI-driven biotech startups founded in 2020

There are quite a few new biotech startups founded in 2020, claiming to be developing or applying advanced data analytics platforms for drug design or other pharmaceutical R&D tasks. Those are typically based on deep learning, natural language processing and other AI technologies or their combinations with various fields of knowledge (e.g. quantum theory). Below I picked some notable startups to check:

Polaris Quantum Biotech**,** also known as Polarisqb, uses a combination of AI with quantum computing, Polarisqb intends to speed-up the drug discovery process from years to months. The company partners with UK-based Fujitsu to launch a new drug discovery platform, which combines quantum-inspired technology, machine learning, hybrid quantum mechanics, and molecular mechanics simulations (QM/MM). As Polaris says, their platform is 10.000 faster than any alternative product on the market and will be able to identify up to 100 drug blueprints per year. Recently the company received $250K to develop its platform.

Glamorous.AI The company is founded by a Syrian entrepreneur Dr. Noor Shaker. Glamorous.AI combines human chemistry insights (“human-in-the-loop”) and AI algorithms to augment drug discovery and enable applications where only limited data points are available. In April, Glamorous announced the collaboration with Cardiff University to discover Covid drugs. The partnership leverages Glamorous AI’s proprietary platform, Rosalind, to find inhibitors to Sars-Cov-2 main protease.

Transilico is a start-up from Florida that employs AI for biomedicine. Transilico’s team are experts with chemical, biomedical and computational backgrounds. The start-up applies graph convolutional neural networks (GCNN) for prediction of molecules activity. They have also developed an AMPDeep model for identifying Antimicrobial Peptide. The company’s website claims Transilico developed a new, non-toxic antimalarial (DC-9237), which will be experiencing lead optimization soon.

Pucho Life Sciences Inc started its activities with the search for the best compounds to treat Covid-19. On its website, Pucho states that it is a healthcare-focused startup that uses in-silico techniques, genetic algorithms, and machine learning (ML) to provide affordable treatment for all people.

Notable AI-focused collaborations involving “big pharma” players

The first half of 2020 illustrates the variation of niÑ■hes in which Big Pharma is making deals with AI companies. It includes partnerships on small molecules identification, drug repurposing, clinical trials and precision medicine, target identification, modulation of protein-protein interaction and many other use cases. Some of the illustrative R&D partnerships involving AI are listed below:

In January, Exscientia entered a $266 million agreement with Bayer. The partnership will leverage AI to accelerate drug discovery programs on oncology and cardiovascular diseases. Under the terms, Exscientia receives upfront fees, ongoing research funding and clinical milestone payments.

In the same month, Bayer signed a five-year partnership with Schrödinger to create new software that would screen and design synthetically feasible compounds. Under the agreement, Schrödinger will provide its machine learning capabilities and technologies for molecular design, while Bayer will share in silico models to predict ADMET properties.

In January, Pfizer teamed up with Hong Kong-based computational biotech Insilico Medicine with a plan to identify new targets and biomarkers. Insilico has spent 6 years developing generative models and machine learning programs that the company applies for mining and analyzing omics data, hit discovery, target discovery, and biomarker development. In April, Insilico Medicine added another big pharma partner -- Boehringer Ingelheim. In this way, Boehringer deploys its Research Beyond Borders initiative, which expands the company's therapeutic areas and geographies. Insilico will leverage its new Pandomics platform to visualize genomics and proteomics data in order to elucidate cell signaling pathways and disease profiles.

In March, a Korean clinical-stage drug discovery company, Bridge Biotherapeutics partnered with Atomwise to participate in 13 small molecule programs connected to inflammation. Atomwise will use AI to evaluate and initiate programs for Pellino proteins. According to the agreement terms, Atomwise can potentially receive up to $1B in case of success on all programs.

In March, Pfizer announced that it will use Saama's Life Science Analytics Cloud (LSAC) platform to improve clinical trial models and accelerate getting drugs to the market. Saama's platform uses Deep Learning to analyze, transform, and predict data. To train Saama's model Pfizer will provide its own clinical data.

In May, Boehringer Ingelheim added its second computational partner in a month -- BERG Health, clinical-stage biotech with its own state-of-the-art AI platform. The company has a web lab platform that allows it to generate its own data, it already has drugs in the clinic and applies a mathematical approach distinct from machine learning. The partnership investigates inflammatory bowel disease and Crohn's disease, its causes, biomarkers, drug targets, and therapies.

In June, Imagia partnered with Illumina on a project aimed to advance the development of precision medicine. The collaboration will leverage Imagia AI-enabled EVIDENS™ platform to investigate data through federated learning, and Illumina's DRAGEN™ Bio-IT Platform and Illumina Analytics Platform to facilitate data interoperability.

In July, Repurpose.AI partnered with LEO Pharma to find potential drug candidates for the LEO's dermatology program. Following the agreement, Repurpose.AI will sift through several thousand drug candidates that passed a Phase 1 clinical trial but might have not been commercialized, trying to identify drug repurposing opportunities.

In October, Roche Group's subsidiary Genentech tapped a startup drug-discovery firm Genesis Therapeutics to find potential drug candidates for a variety of diseases.

In November, Merck KGaA announced it will deploy Insilico Medicine's Chemistry42 AI platforms for generative chemistry. The platform will run on Merck's high-performance computing infrastructure in Germany.

Just weeks earlier, Insilico Medicine established a multi-target AI-powered drug discovery collaboration with Janssen, where Insilico's role will be to design small molecule hits for a number of targets of interest for Janssen.

Finally, **in December**, PostEra, a biotechnology company specializing in machine learning solutions for preclinical drug discovery, signed a multi-year strategic partnership with Pfizer to accelerating small molecule research programs via PostEra's generative chemistry platform.

AI adoption by the contract research organizations (CROs)

Contract research organizations (CRO) are also increasingly focused on adopting AI-based technologies as an additional value-adding component of their R&D services.

For example, IQVIA launched the Avacare Clinical Research Network™ platform powered by AI algorithms that serve to match patients to the clinical trial sites. Whereas, Parexel decided to acquire ready-made Natural Language Processing (NLP) technology assets and transfer key personnel from Roam Analytic. CMIC is another company that, together with SUSMED, has started to offer solutions for real-world data cleansing. These technologies allow acceleration of drug development at the clinical trial stage, but CROs also partner with companies supplying solutions for the prediction of molecular interaction, hit identification, and a wide range of other research tasks.

Read more about this trend in Contract Research Organizations Tap Into AI To Increase Value Proposition.

AI-designed drug candidates in clinical trials

There are a plethora of “AI-inspired” clinical-stage drug candidates out there, with a few examples below:

AI-biotech BioXcel Therapeutics, the company developing previously approved drugs for the treatment of new indications met endpoints in Two Phase 3 Trials and is going to file a New Drug Application with the U.S. FDA in the first quarter of 2021. The drug candidate BXCL501, also known as dexmedetomidine, has been repurposed to treat acute agitations appearing in schizophrenia and bipolar disorder. The company’s other drug candidate BXCL701, an innate immunity activator, is currently ongoing a Phase 2 clinical trial as a part of combinational therapy to treat several cancer types.

Another clinical-stage drug candidate, obtained via AI-assisted repurposing, is LAM-002A by AI Therapeutics and Yale School of Medicine -- a potential treatment against COVID-19.

Exscientia has advanced its drug candidate, DSP-1181, toward entering clinical trials. Unlike in the case of repurposing, DSP-1181 was designed from scratch using the company's AI-driven end-to-end platform Centaur Chemist™. The treatment is intended to treat obsessive-compulsive disorder and is a product of collaboration with Sumitomo Dainippon Pharma.

Some other AI-biotech companies which have clinical-stage pipelines include BenevolentAI, BlackThorn Therapeutics, Berg Health, Lantern Pharmaceuticals, Recursion Pharmaceuticals, and other companies. The full list can be found in our report: A Landscape of Artificial Intelligence (AI) In Pharmaceutical R&D.

The emerging role of AI tech in fighting COVID-19

This post would have been incomplete without a brief review of how the ongoing global pandemics influenced the adoption of new technologies, in particular, artificial intelligence. Predictably, the urge to tackle pandemics on the one hand, and a suddenly opened landscape of opportunities -- on the other hand, prompted a true “biotech race” to develop anti-coronavirus therapeutics, vaccines, biomarkers, and commercial diagnostic tools. AI has rapidly become the important tool for researchers to fight COVID-19, in many roles -- from analyzing massive amounts of research literature generating disease hypotheses, to hit discovery, drug repurposing, biomarker discovery, and studying disease progression patterns to identify treatment relevance.

Many organizations provided free excess to their data for AI training or gave away certain research results for others to use for the public benefit.

It should also be noted that so-called “big tech” companies, such as Microsoft, Amazon, Google, and others have been increasingly active in 2020 in terms of establishing open collaborations with various biotech players -- a favorable opportunity for them to increase presence in the healthcare territory.

Below I summarized just several examples of companies using AI, among other technologies, to contribute to the global fight against coronavirus pandemics.

One case of drug repurposing to tackle COVID-19 was initiated by a UK-based startup**,** BenevolentAI, that predicted Eli Lilly’s drug “Olumiant” can stop the disease development. The drug is used for treating rheumatoid arthritis as it controls inflammation in patients. BenevolentAI suggested that the same mechanism will work in Covid-19 patients, moreover Olumiant has potential to prevent the virus from entering the lung cells. Eli Lilly has started a phase 3 clinical trial to find out whether AI prediction will work in real benefits.

Repurpose.AI partnered with Scripps research to find drug candidates to treat the coronavirus. Their joint collection of approved and investigational drugs accounted for nearly 8000 of compounds. The collaboration uses Repurpose.AI's ActivPred AI Drug Discovery Platform.

Many efforts are also made toward creating novel COVID-19 therapeutics, including attempts to block SARS-Cov-2 main protease. For example, PostEra initiated the Covid Moonshot project to crowdsource molecular design ideas. PostEra applied AI to prioritize ideas and find optimal synthesis routes. The project is funded via crowdfunding, philanthropy, and grants, establishing a strong case for open science drug discovery, where the public benefit will be derived via joint effort and not that of a particular commercial organization.

In June, UK-based startup Biorelate opened free access to its cloud-based platform GalacticAI, allowing researchers to use advanced ML algorithms to analyze millions of research text sources, extracting insights on targets, disease mechanisms, and existing drug options relevant to tackling COVID-19.

In March Microsoft Corporation announced the expansion of partnership with Adaptive Biotechnologies to study population-wide immune response to SARS-CoV-2. The data are collected from thousands of blood samples, with the help of Illumina platform Adaptive Biotechnologies indicates specific antibodies that induce immune response. These data are freely available on ImmuneCode, updating online in real time. Microsoft's hyperscale machine learning technology and the Azure cloud platform allow continuously refining the accuracy of the data. Another initiative included a grant, awarded by Microsoft AI to Mount Sinai Health System to support the newly-established COVID Informatics Center (MSCIC). MSCIC will use Microsoft Azure cloud computing enabling the development of AI tools that can improve care and evidence-based medicine treatment for coronavirus patients.

In response to the urgent need to navigate through tons of information about COVID-19, Amazon Web Services (AWS) launched ML enabled CORD-19 Search website. It is based on Allen Institute for AI's CORD-19 open research dataset that contains about 128,000 scientific materials. Researchers can easily search the information on the website, as relevant information has been already extracted by the provided ML algorithms.

In June, Schrödinger announced advanced COVID-19 drug discovery efforts with Google Cloud, a significant expansion of its work to discover novel antiviral therapeutics for COVID-19 as a part of a philanthropic global initiative. Google Cloud shared its parallel computing capabilities to increase screening pace to billions of molecules per week.