

# 2018 Brings A Surge Of Activity In The “AI For Drug Discovery” Space

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The idea of using artificial intelligence (AI) to accelerate drug discovery process and boost a success rate of pharmaceutical research programs has inspired a notable amount of activity over the last several years with a considerable number of initiated research collaborations between AI-driven R&D vendors and top pharmaceutical companies in 2016-2017.

(For a detailed review of the topic, read Biopharma's Hunt For Artificial Intelligence: Who Does What?).

A busy beginning of 2018 shows that the area is getting even “hotter” and things start unfolding faster in the emerging “AI for drug discovery” space. Below is a brief summary of some of the most notable events of this year so far:

## Atomwise

Atomwise, which was founded in 2012 and pioneered the use of deep neural networks for structure-based drug design, just raised \$45 M round A investment to advance its AI-driven drug discovery technology. The company is focusing on addressing chemical challenges of the drug discovery process -- identifying in silico best small molecules for specific drug targets, and further computationally optimizing them into potent and safe drug candidates with optimal properties (lead optimization). The company says it currently screens 10 million small molecules each day and uses its proprietary platform AtomNet, utilizing deep learning algorithms, to analyze molecules and predict their potency as medications, toxicity, and side effects.

Atomwise now has more than 50 molecular discovery programs, allowing to rapidly improve its AI-based models, and is partnering with top pharma companies, like Merck and AbbVie, as well as prominent research institutions, including Harvard, Duke, Stanford and Baylor College of Medicine.

## Sirenas and Bristol-Myers Squibb

Sirenas, a biotech company applying machine-learning based computational approaches to discover therapeutics derived from the global microbiome, entered a multi-target research collaboration agreement with Bristol-Myers Squibb to apply its proprietary drug discovery platform against a series of undisclosed but challenging therapeutic targets. The research collaboration leverages Sirenas' expertise in applying its proprietary data mining technology ATLANTIS™ to identify potential drug candidates among Sirenas' proprietary chemical library isolated from global microbiome collections. It is important to note another area of Sirenas' expertise -- state-of-the-art organic synthesis, which makes it possible for the company to deliver not only computational predictions but also chemical compounds with unusual nature-inspired scaffolds.

## Juvenescence and Insilico Medicine

Another quite notable move was made by Juvenescence Ltd, a young biotech company focusing on developing therapies to increase healthy human longevity, Juvenescence has licensed its first compound family from AI-driven drug discovery Insilico Medicine for further clinical development.

“JAI-001 and its analogs, have demonstrated in-vitro activity in assays directly relevant to aging and age-related diseases”, as said in a recent press release.

The selected compounds are pure “AI-born” drug candidates, so this deal might be among the first “historical” proofs of concept for AI-driven drug discovery, in the case of success of the future clinical trials with JAI-001 and its analogs. Let's stay tuned for the updates.

## Datavant and Verge Genomics

A fresh US-based AI-driven startup Datavant is focused on organizing and structuring healthcare data for deriving actionable insights for the design and interpretation of clinical trials. In the beginning of January, it announced a strategic alliance with Verge Genomics, a company using artificial intelligence to discover and develop new therapeutics. The newly formed partnership aims at unlocking the value of pharmaceutical datasets in a possession of Datavant -- clinical trial data, claims, pharmacy history, electronic health records and genomics data on patients.-- to accelerate discovery and development of new medications.

So far, Datavant has two more partnerships besides Verge -- with Duke Clinical Research Institute (DCRI), Global Genomics Group (G3) -- all aiming at combining drug discovery expertise, biological big data, and novel data analytical technologies, such as AI, to boost innovation in the field of pharmaceutical research.

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## Engine Biosciences

Engine Biosciences is a San Francisco and Singapore based biotech firm, which just announced a \$10 M funding round to advance its AI-based platform for drug discovery, development of combination therapeutics, and cellular reprogramming. The company's technology allows researchers and drug developers to reveal gene interactions and biological networks, and provide test therapies specifically targeting genetic interactions. The company's AI platform can assist in target discovery, drug repurposing, and analysis for precision medicine applications.

## XtalPi

Founded in 2014 by a group of quantum physicists at MIT, XtalPi is a U.S.-China biotech firm which has just raised a Series B round of \$15M from several investors, including Google and Sequoia China among the others. The company is claiming that it can quickly and accurately predict numerous important characteristics of small-molecule drugs and solid forms by combining artificial intelligence, quantum physics, and high-performance cloud computing. Using this sophisticated interplay of technologies, the company will be able to provide "time-saving insights into the safety, stability, and efficacy of drug candidates".

## Owkin

New York -Paris based Owkin, was founded in 2016 to apply machine learning for optimizing drug discovery process via better comprehending the overabundant biological data. Having started with a seed round of above \$2M in 2016, the company raised its Round A of as much as \$11M this January to scale its technology platform, called Owkin Socrates. The company is actively searching for pharma partners.

According to the company's website, the Owkin's platform can integrate molecular and imaging libraries with patient data to reveal patterns of biomarkers causing a disease. The company perceives a competitive advantage of its platform in a so-called transfer learning, which improved the learning capacities of the algorithm on a particular dataset after being exposed to other datasets.

## E-Therapeutics

Founded in 2003 in Oxford, e-Therapeutics is pioneering so-called network-driven drug discovery (NDD) approach, which is an alternative to a target based research paradigm, widely adopted by the pharmaceutical industry. Over the years, e-Therapeutics has created a drug discovery engine supported by large-scale, proprietary databases of biological and chemical information, combined with a suite of

computational tools. The company creates and analyses network models of a disease with the aim of identifying specific proteins that could effectively be disrupted to treat it. The approach of e-Therapeutics allows for target-agnostic discovery of new small-molecule drug candidates having potentially polypharmacological mechanisms of action.

In January 2018 e-Therapeutics announces partnerships with two AI-driven startups, Intellegens and Biorelate, to enhance and expand its own machine learning capabilities, and bridge the gaps in the data processing and analyzing workflows.

## Concluding remarks

Judging by the increasing activity in the “AI for drug discovery space” over the last two years, it is expected that 2018 will be a year of a more widespread curiosity among biopharma companies about AI-based technologies and tools. As a consequence, a growing number of new AI-vendors will be pitching in, offering solutions for novel use cases and more flexible collaboration models, and more research initiative will be launched on the side of “big” and “middle” pharma players. It means the market of R&D outsourcing will be growing even faster in 2018, at least in the segment of outsourcing AI, cloud and big data technologies and expertise. (For a more detailed review of the R&D outsourcing trends in biopharmaceutical industry, read [Pharma R&D Outsourcing Is On The Rise](#))

On the other hand, AI-vendors will face a more pressing challenge of finding ways to prove their value proposition for the pharmaceutical and biotech partners in more practical and measurable terms -- in order to overcome a growing skepticism fueled by sometimes irresponsibly overhyped claims about “AI revolution” in the mass media.

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- Engine Biosciences
- Insilico Medicine
- Sirenas
- Verge Genomics
- XtalPi
- e-therapeutics