



AI FOR DRUG DISCOVERY, BIOMARKER DEVELOPMENT AND ADVANCED R&D LANDSCAPE OVERVIEW 2017

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AI Will Redesign Healthcare

Healthcare will be the lead area of the Fourth Industrial Revolution and one of the major catalysts for change is going to be artificial intelligence (AI).

AI in health represents a collection of multiple technologies enabling machines to sense, comprehend, act and learn so they can perform administrative and clinical healthcare functions. Unlike legacy technologies that are only algorithms/tools that complement a human, health AI today can truly augment human activity.

AI has already found several areas in healthcare to revolutionize starting from the design of treatment plans through the assistance in repetitive jobs to medication management or drug creation. And it is only the beginning.



Source: <http://medicalfuturist.com/top-artificial-intelligence-companies-in-healthcare/>

The Rise of AI in Healthcare

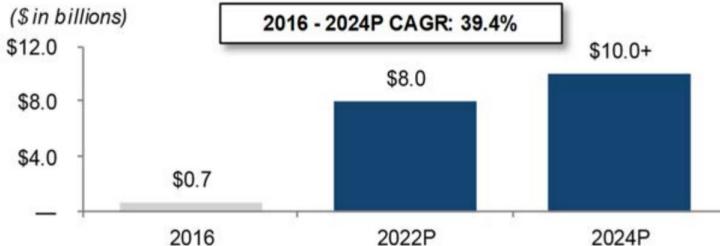
The number of startups entering the healthcare AI space has increased in recent years, with over 50 companies raising their first equity rounds since January 2015. Deals to healthcare-focused AI startups went up from less than 20 in 2012 to nearly 70 in 2016.

The field of AI for Healthcare has been actively growing since 2015. The market is primarily being driven by factors like the rise of personalized medicine in tests for clinical decision-making and big data in healthcare industry and the growing adoption of AI in genetics. Also, AI created real-time monitoring system, and healthcare wearables are playing a crucial role in digital healthcare monitoring.

AI in Healthcare:

- Drug Discovery
- Wearables
- Medical Imaging and Diagnostics
- Research
- Mental Health
- Lifestyle Management
- Digital Health Monitoring
- Patient Data and Risk Analytics
- Virtual Assistants
- Surgery
- Hospital Management

Global Healthcare AI Market Growth Through 2024



Source: Markets and Markets; Global Market Insights, Inc.

The U.S. healthcare AI market exceeded \$320 million in 2016, and is estimated to grow by more than a 38% CAGR through 2024 (Global Market Insights, "Healthcare AI Market Size, Competitive Market Share & Forecast, 2024").

The Global Healthcare AI market, among the AI industry's fastest growing sub-sectors, is expected to grow at a 39.4% CAGR to over \$10 billion in worldwide revenue by 2024.

Source: TM Capital "The Next Generation of Medicine: Artificial Intelligence and Machine Learning" Report



Top 10 AI Applications

APPLICATION	VALUE*	
Robot-Assisted Surgery**	\$40B	Connected Machines
Virtual Nursing Assistants	\$20B	Clinical Trial Participant Identifier
Administrative Workflow Assistance	\$18B	Preliminary Diagnosis
Fraud Detection	\$17B	Automated Image Diagnosis
Dosage Error Reduction	\$16B	Cybersecurity
		TOTAL = -\$150B

Source: Accenture analysis

* "Value" is the estimated potential annual benefits for each application by 2026.

** Orthopedic surgery specific



106 STARTUPS TRANSFORMING HEALTHCARE WITH AI



AI for Drug Discovery, Biomarker Development and Advanced R&D

- The global healthcare AI market is highly fragmented and is characterized by the presence of a large number of industry players.
- In this report we conducted specific analysis of the most crucial and important sectors of application AI in Healthcare:
 - Advanced R&D
 - Drug Discovery
 - in silico Clinical Trials
 - Diagnostics and Biomarker development
 - NeuroTech
 - Surgery
- We landscaped:
 - 40 leading AI companies working in these 5 sectors.
 - 100 investors that invested in these 40 startups.
 - 20 leading Pharma and IT-corporations exploring AI in Healthcare.

AI for Advanced R&D

- The broad field of AI in Healthcare has already experienced a significant rise during 2016, especially in the application of computer vision, text analysis and chatbot technologies. Since all these techniques were first developed in the IT-sector, it was possible to easily repurpose them for the healthcare sector.
- However, the segment of applying AI for advanced R&D is limited to companies and researchers with very high levels of expertise. This creates a specific scarcity for AI specialists in this niche.
- 2018 is expected to become the year in which AI will be recognized as the most powerful driver of progress in solving the crucial challenges in the most advanced sectors of science and R&D in the healthcare and Biotech industries.
- Applying AI for advanced R&D, biomarker development and for drug discovery will bring the most disruptive impact on the business model of the Pharma and entire Biotech industry.
- This is why the players from the AI for drug discovery market can become new game changers and significantly influence the capitalization of pharma companies.

The Broken Model of BioPharma

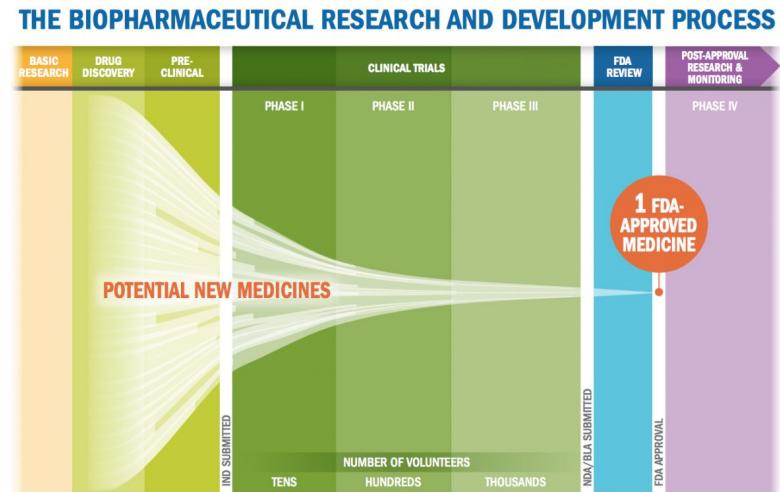
The efficiency of research and development (R&D), defined as the number of successfully approved drugs given the budget allocated to new drug development, has declined for decades.

The cost of drug discovery and subsequent development is a massive challenge in the pharmaceutical industry.

A typical drug can cost upwards of \$2.5 billion and a decade or more to identify and test a new drug candidate. Today, only about one in ten drugs that enter phase 1 clinical trials reaches patients.

Drug makers need to find a more efficient way of developing medicines.

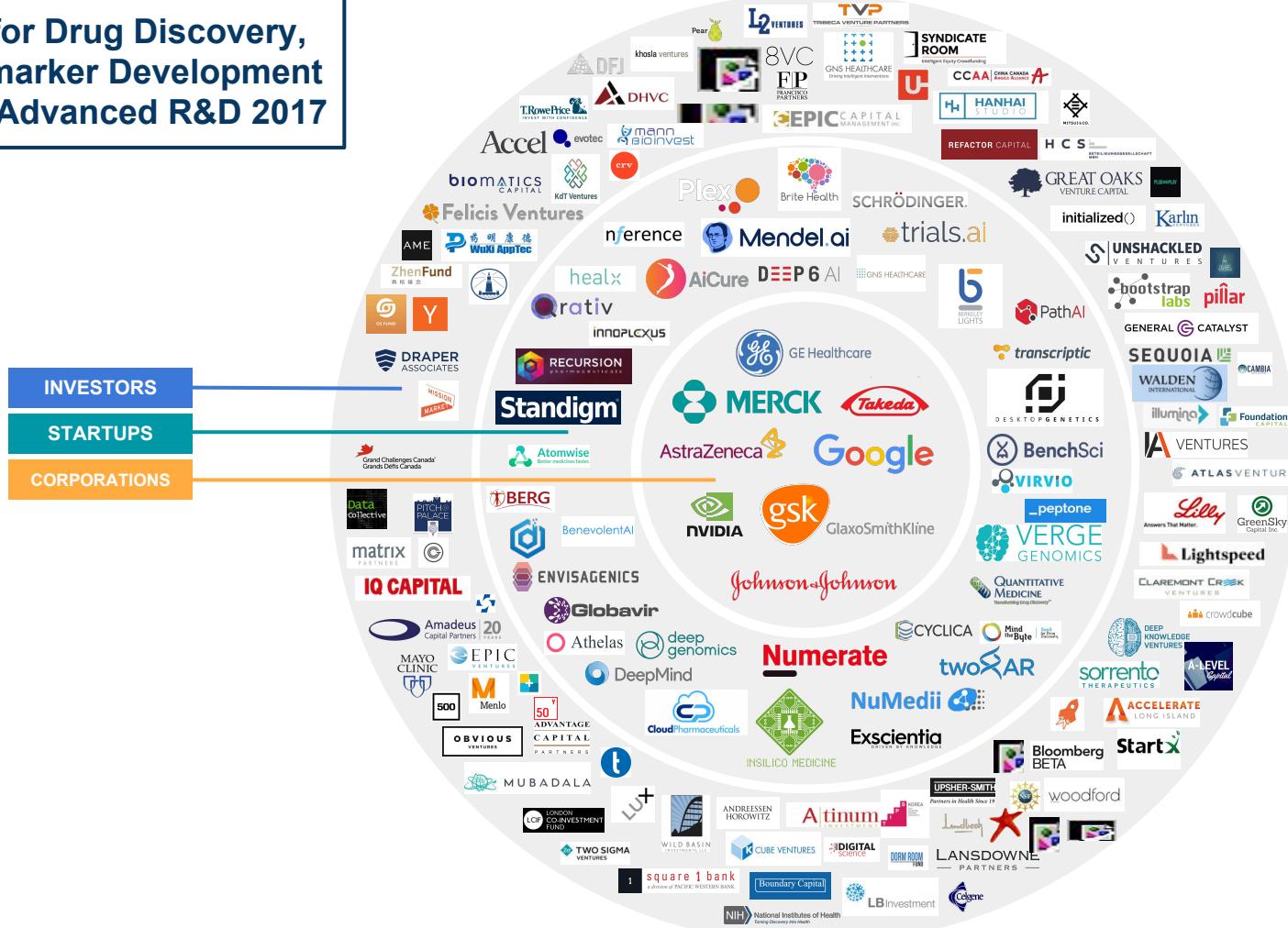
AI can speed up drug discovery, cut R&D costs, decrease failure rates in drug trials and eventually create better medicines.



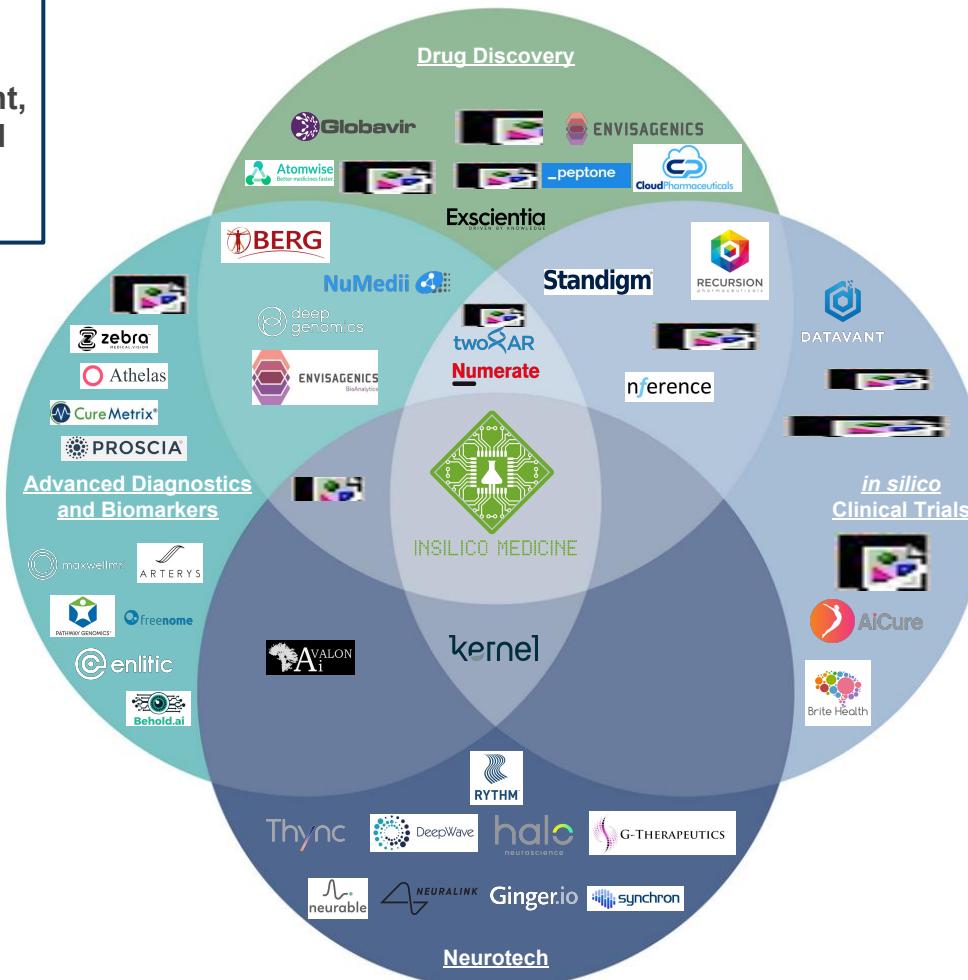
Source: PhRMA's 2015 "Biopharmaceutical Research & Development"

Source: Biopharmaceutical Research & Development, PRMA
http://phrma-docs.phrma.org/sites/default/files/pdf/rd_brochure_022307.pdf

AI for Drug Discovery, Biomarker Development and Advanced R&D 2017



AI for Drug Discovery, Advanced Diagnostics and Biomarker Development, *in silico* Clinical Trials and Neurotech 2017



The Application of AI for Advanced R&D

Aggregate and Synthesize Information

- Extract knowledge from literature
- Generate insights from thousands of unrelated data sources
- Improve decision-making
- Eliminate blind spots in research
- Identify competitive whitespace

Generate Novel Drug Candidates

- Analyze data sets, form hypotheses and generate novel insights
- Identify novel drug candidates
- Analyze data from patient samples in both healthy and diseased states to generate novel biomarkers and therapeutic targets
- Predict binding affinity and other pharmacological properties of molecules
- Allow filtering for drug-like properties of molecules
- Reduce complexity in protein design

Repurpose Existing Drugs

- Rapidly identify new indications for many known drugs
- Match existing drugs with rare diseases
- Conduct experimental biology at scale by testing 1000+ of compounds on 100+ of cellular disease models in parallel
- Generate novel biomarkers and therapeutic targets

Design and Run Preclinical Experiments

- Reduce time, money, and uncertainty in planning experiments
- Decode open- and closed-access data on reagents and get actionable insights
- Automate selection, manipulation, and analysis of cells
- Expedite development of cell lines and automate manufacturing of cellular therapeutics
- Automate sample analysis with a robotic cloud laboratory

Clinical Trials

- Optimize clinical trial study design
- Transform diverse streams of biomedical and healthcare data into computer models representative of individual patients
- Deliver personalized medicine at scale, by revealing optimal health interventions for individual patients
- Analyze medical records to find patients for clinical trials
- Automate matching cancer patients to clinical trials through personal medical history and genetic analysis
- Improve pathology analysis
- Identify patients that would benefit from novel therapies

COMPARISON OF AI FOR HEALTHCARE COMPANIES

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
AiCure	AiCure uses artificial intelligence to visually confirm medication ingestion. The clinically-validated platform works on smartphones to reduce risk in clinical research and optimize patient behavior. AiCure has an extensive IP portfolio, comprising 26 awarded and 55 pending US and global patents.	2010	11-50	US	12.25	NIH
Athelas	Athelas utilizes deep learning and computer vision to rapidly analyze tissue samples for diagnostics. The product is used for immune monitoring, blood counts, and parasite diagnostics.	2016	11-50	US	3.62	n/a
Atomwise	Atomwise uses Deep Learning Neural Networks to help discover new medicines. Atomwise focuses on new drug hit discovery, binding affinity prediction, and toxicity detection. Atomwise predicts drug candidates for pharmaceutical companies, startups, and research institutions.	2012	10-15	US	6.57	Merck, AbbVie, Stanford University
BenchSci	BenchSci uses machine learning to decode open- and closed-access data and present published figures with actionable insights.	2015	11-50	Canada	n/a	n/a
BenevolentAI	BenevolentAI uses proprietary AI and machine learning technology to look deeply into vast scientific research data sets - rapidly forming and qualifying hypotheses, generating new insights and enabling scientific innovation.	2013	51-100	UK	100	Johnson & Johnson
Berg	BERG is a data driven biological research company. Berg focuses on three distinct areas of business to encompass the breadth of the pharmaceutical landscape: diagnostics, pharmaceutical research and development, health care analytics.	2006	251-500	US	n/a	AstraZeneca

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
Berkeley Lights	Berkeley Lights has brought to market a novel technology for single cell identification, measurement and manipulation aiming to revolutionize biopharma, diagnostics and life science research.	2011	101-250	US	86.22	Roche, UCSF
Bio Age Labs	Bio Age Labs couple omics data with machine learning to measure human aging and accelerate drug discovery.	2015	1-10	US	10.9	n/a
Brite Health	Brite Health provides an AI platform for clinical trials.	2015	1-10	US	n/a	n/a
Cloud Pharmaceuticals	Cloud Pharmaceuticals uses a proprietary design process that combines AI and cloud computing to search virtual molecular space and applies along molecular modeling to design novel drugs that are well-qualified for development from the outset and have original composition of matter IP.	2014	11-50	US	1.5	n/a
Cyclica	Cyclica harnesses biophysics, biological data, and AI to help pharmaceutical companies navigate the drug discovery pipeline by assessing the safety and efficacy of drugs.	2010	11-50	Canada	6.95	n/a
Datavant	Datavant is dedicated to accelerating the discovery, development, and commercialization of new medicines through machine learning. They aim to partner with biomedical research institutions to eliminate silos of information and unlock insights from healthcare data.	2017	11-50	US	n/a	n/a
Deep 6 AI	Deep 6 AI finds patients for clinical trials in minutes rather than months.	2015	11-50	US	n/a	n/a

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
Deep Genomics	Deep Genomics is building a biologically accurate data- and AI-driven platform that supports geneticists, molecular biologists and chemists in the development of therapies. Deep Genomics will use its platform to unlock new classes of antisense oligonucleotide therapies that were previously inaccessible or out of reach, and advance them for clinical evaluation.	2014	11-50	Canada	16.7	n/a
Desktop Genetics	Desktop Genetics specializes in genome editing technology. They have developed DESKGEN AI which powers their flagship DESKGEN CRISPR Library product range.	2012	11-50	UK	6.83	Illumina, Horizon Discovery
Envisagenics	Their mission is to reduce the complexity of biomedical data to accelerate the development of innovative therapeutic solutions through RNA splicing analytics and artificial intelligence. Envisagenics is Cold Spring Harbor Laboratory spinout company.	2014	1-10	US	3.1	NIH, Microsoft
Exscientia	Exscientia is applying AI and big data processing to accelerate drug discovery and development. Their AI driven systems learn best practice from vast repositories of discovery data and are further enhanced with knowledge acquired from drug hunters.	2012	11-50	Scotland	62.3	GlaxoSmithKline
Globavir	Globavir is committed to the development of therapeutics and diagnostics for the treatment of global infectious diseases. Globavir has identified candidate compounds with efficacy in viral indications, including dengue, West Nile, Japanese Encephalitis, Ebola, Marburg, and Hunta viruses.	2011	11-50	US	7.5	Stanford, Bio-Rad

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
GNS Healthcare	They focus on advancing and applying industrial-scale data analytics to empower key healthcare stakeholders to solve complex care, treatment and cost challenges. They are a multi-disciplinary group of physicists, actuaries, geneticists, engineers, business people, and computer scientists, passionate about extracting the evidence of what works in healthcare and for whom.	2000	101-250	US	54.26	Johnson & Johnson, Novartis, NIH, Genentech
Healx	They use machine learning algorithms and computational biology to identify novel drug applications for rare diseases. Healx works with patient groups and charities to help identify drug repurposing opportunities and help translate basic research into tangible potential treatments.	2014	1-10	UK	2M	n/a
Innoplexus	Innoplexus uses AI to generate insights from structured and unstructured private and public data. Their iPlexus platform helps to generate intelligence and insights across pre-clinical, clinical, regulatory and commercial stages of a drug.	2011	101-250	Germany	n/a	n/a
Insilico Medicine	Insilico Medicine utilizes advances in genomics, big-data analysis, and deep learning for in silico drug discovery and drug repurposing for aging and age-related diseases. Through its Pharma.AI division, Insilico provides advanced machine learning services to biotechnology, pharmaceutical, and skin care companies, foundations and national governments globally.	2014	11-50	US	14	GlaxoSmithKline, Johnson & Johnson, NVIDIA, Life Extension, Novartis, etc.
Mendel.ai	Mendel.ai automates matching cancer patients to clinical trials through personal medical history and genetic analysis.	2016	1-10	US	2	n/a

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
Mind the Byte	Mind the Byte is a bioinformatics company specializing in computational drug design using a pay-per-use SaaS platform. They have developed a versatile set of applications using cloud computing which lowers the entry barrier to the technology	2011	1-10	Spain	0.63	Amazon Web Services
nference	Their knowledge synthesis platform - nferX - uses state-of-the-art Neural Networks for real-time, automated extraction of knowledge from the commercial, scientific, and regulatory body of literature. The platform enables a diverse set of applications ranging from R&D to commercial strategy and operations in the life sciences ecosystem.	2013	51-100	US	3M	Mayo Clinic
NuMedii	NuMedii's Big Data technology consists of hundreds of millions of normalized and annotated human, biological, pharmacological and clinical data points. They integrate these data with network-based algorithms to find both drug candidates and biomarkers predictive of efficacy for diseases.	2008	11-50	US	5.5	Astellas, Boehringer Ingelheim
Numerate	Numerate has developed a computational platform that can predict how a potential drug will behave in the lab and the body. They use this platform to process large spaces of chemistry while searching for therapies for some of the world's most important diseases, such as, obesity, heart failure, Alzheimer's, and Huntington's disease.	2007	11-50	US	17.42	Takeda
PathAI	PathAI's platform provides end-to-end data-driven pathology analysis, resulting in fast, accurate and standardized pathologic diagnoses. Their deep-learning solutions drive discovery and predictive diagnostics in drug-development.	2016	11-50	US	15.2	Philips

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
Peptone	Peptone accelerates the lengthy process of protein lead optimisation and design through AI coupled with experimental cross-validation.	2016	1-10	The Netherlands	n/a	NVIDIA
Plex Research	Their search engine helps to analyse compound's mechanism of action/toxicity, select/characterize/prioritize hits, optimize leads, repurpose drugs, generate focused screening sets for selected targets, pathways, therapeutic indications, and phenotypes.	2009	1-10	US	11M	n/a
Qrativ	Qrativ combines nference's AI-driven knowledge synthesis capabilities with the clinical expertise and proprietary data of Mayo Clinic for reinventing the way treatments for diseases with unmet medical need are discovered.	2017	11-50	US	8.3M	Mayo Clinic
Quantitative Medicine	They apply machine learning techniques from three complementary informatics technologies: Supervised Learning, Transfer Learning and Active Learning, to efficiently solve multi-parameter optimization problems in a series of discrete discovery cycles.	2012	1-10	US	0.563	n/a
Recursion Pharmaceuticals	Recursion Pharmaceuticals is combining high-throughput experimental biology, bioinformatics, and machine learning to rapidly identify new indications for many known drugs and shelved assets. Their focus initially is in the orphan disease space, but their core technology has applications in oncology, infectious disease, and inflammation.	2013	1-10	US	84.33	Takeda

Company	About	Founded Year	Number of Employees	Country	Disclosed Funding, \$	Collaborations with Corporations
Standigm	Standigm applies cutting-edge AI technologies to drug discovery. Standigm generated tens of drug candidates for cancers, Parkinson's disease (PD), autism, fatty liver diseases (NASH) and more.	2015	1-10	South Korea	3.69	n/a
Transcriptic	Transcriptic is the robotic cloud laboratory for life sciences. Transcriptic's automated cellular and molecular biology platform enables scalable life science research, with flexibility and precision.	2012	11-50	US	27.77	Agilent Technologies
Trials.ai	Trials.ai is an eClinical platform that uses AI to help companies conduct and manage clinical trials. It directs its users through the study, from collecting informed consent to patient visits and follow-ups, to study closeout that allows its system to understand the exact tasks that are impacting its users' study in real-time, giving sponsors and CROs better insights and clarity.	2015	1-10	US	n/a	n/a
twoXAR	twoXAR is an artificial intelligence-driven drug discovery company. They leverage their computational platform to identify promising drug candidates, validate & de-risk them through preclinical studies, and progress candidates to the clinic through industry and investor partnerships.	2014	11-50	US	4.3	Stanford, Santen
Verge Genomics	They use machine learning and human genomic data to accelerate the discovery of new treatments for patients with neurodegenerative diseases.	2015	11-50	US	4	USC, Johns Hopkins Medicine
Virvio	Virvio is a synthetic biology company developing designer mini-protein biotherapeutics.	2015	n/a	US	0.21	NIH, Google Compute Engine

AI for Drug Discovery and Biomarker Development

- Applying AI for advanced R&D, biomarker development and drug discovery will bring the most disruptive impact on the business model of the Pharma and entire Biotech industry.
- Specific attention should be paid to those projects capable of applying Next Generation Artificial Intelligence techniques, Deep Learning and in particular GAN's (generative adversarial networks) and reinforcement learning for:
 - Drug Discovery and Drug Repurposing
 - Biomarker Development
 - Clinical Trials Predictors
 - Aging Research
 - AI Solutions in convergence with Blockchain
- The leading players in this specific niche can become new game changers for entire market and significantly influence the capitalization of pharma companies.

Comparison of AI for Drug Discovery Companies

Category	Number of individuals reporting any physical violence	Number of individuals reporting any sexual violence	Number of individuals reporting any emotional abuse	Number of individuals reporting any financial abuse	Number of individuals reporting any physical abuse	Number of individuals reporting any sexual abuse
Total	100	100	100	100	100	100
Male	50	50	50	50	50	50
Female	50	50	50	50	50	50
18-24 years	50	50	50	50	50	50
25-34 years	50	50	50	50	50	50
35-44 years	50	50	50	50	50	50
45-54 years	50	50	50	50	50	50
55-64 years	50	50	50	50	50	50
65+ years	50	50	50	50	50	50
White	50	50	50	50	50	50
Black	50	50	50	50	50	50
Asian	50	50	50	50	50	50
Other	50	50	50	50	50	50
Married	50	50	50	50	50	50
Not married	50	50	50	50	50	50
Employed	50	50	50	50	50	50
Not employed	50	50	50	50	50	50
High income	50	50	50	50	50	50
Low income	50	50	50	50	50	50

Comparison of AI for Drug Discovery Companies

Funding*, \$m

Number of Publications (PubMed)



*According to Crunchbase or Company Website

Comparison of AI for Drug Discovery Companies

Number of Patents (Google Patents)

AI experts/Total Number of Employees



AI in Healthcare and AI in Drug Discovery

- The global healthcare AI market is highly fragmented and is characterized by the presence of large number of industry players, while the AI for drug discovery segment has a comparatively lower level of competition because this market segment only accepts companies with very high levels of expertise. There are more than 100 AI in Healthcare companies, but only 10 of them are capable of entering the AI in Drug Discovery sector.
- The breakthroughs in AI for drug discovery will change the R&D process of Bio Pharma, and it will make tremendous impact on whole biopharma industry.
- That is why the players from the AI for drug discovery market can become new game changers and significantly influence the capitalization of pharma companies.

AI in BioPharma R&D: The Big GAP

- It will have a domino effect in the sense that Biopharma budgets are significantly related to spending on R&D and failures in clinical trials, meanwhile the breakthroughs in applying AI for drug discovery will have dramatic impact on not just Biopharma companies but all biotech startups and biotech VC funds. All of them will be disrupted.
- The major progress in these technologies is coming not from biotech side but from IT side.
- Due to the lack of AI specialists and promising AI & Drug Discovery startups, only a select few BigPharma players will emerge as the leaders of this trend.
- Meanwhile others, even with substantial budgets and the will to succeed in this area, will fail if they are even 1 year late to the race because all of the top AI specialists and AI in healthcare start-ups will have been acquired by then.
- The number of experts in the field of AI for drug discovery is insufficient to meet the demand of all big pharma companies, so only those few pharma companies and investors who will partner with the best AI for drug discovery companies in time will benefit from these collaborations and increase their capitalization accordingly.

BioPharma: The Road Forward

- Those Bio Pharma companies that will create strong AI for drug discovery divisions and that will succeed to acquire the best AI startups will become the leaders of the field as little as 3 to 5 years from now. *Consider the acquisition of DeepMind by Google for \$0.5B in 2014.*
- Those companies that will invest heavily in their AI for drug discovery departments will see their market capitalization skyrocket in coming years.
- Those Bio Pharma companies that do not accept AI will repeat the mistakes of Kodak, who were once the leader of their industry, but went to bankruptcy because they failed to embrace digital photography as the disruptive trend it was, even despite the fact that the digital camera was invented inside Kodak labs.
- If Bio Pharma would find the courage to spend 10% of their marketing budget on R&D in AI, they could blow IBM Watson out of the water by learning from their mistakes, reinventing themselves and coming one step closer to halting the looming threat of the Silver Tsunami.

BioPharma's Failure is Strategy, Not Capital

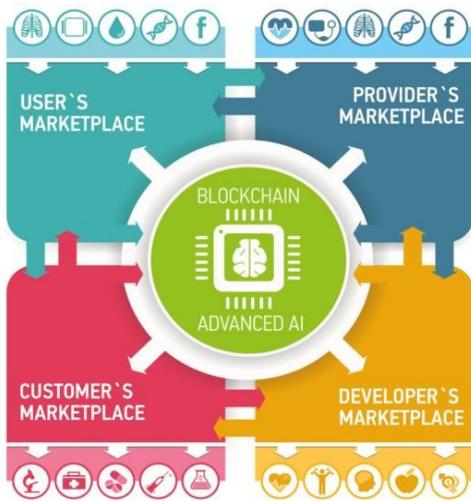
- The pharmaceutical industry has accumulated capital but remains conservative, bureaucratic and risk-averse in their investment strategy. As government budgets become ever more constrained, it is increasingly urgent that the roadblocks to medical advancement be eliminated.
- This may reflect the inefficiency and of the organizations themselves and capital intensive barriers to entry more than the intrinsic intractability of complex biological systems - indeed, the most successful drugs historically have been discovered serendipitously. In any case, the sector shows signs of sluggishness: twenty years ago, 20% of Swiss GDP was derived from pharmaceuticals — now it is down to 5.7% of GDP.
- Banks and IT giants are snapping up the best AI specialists and startups and it is inevitable that pharma will require the same scarce technology and talent. Biopharma must recruit advanced deep learning teams (as Google did with Deep Mind).

Invest & Short

- Banks have embraced machine learning quickly, looking more like IT firms with each passing day, but the executives of pharma have been less agile. Top managers are avoiding risk rather than showing results. They don't want to be the executive who reduced earnings by engaging in advanced IT spending. However, in neglecting disruptive technological risk, they are failing to hedge properly.
- Invest in AI in Healthcare sector because it will inevitably grow.
- Invest in AI for Drug Discovery, as it will have potentials for exponential growth 10x the potential for growth above AI for Healthcare ratio.
- Invest in the AI for Drug Discovery subsector, as it will have the potential for exponential growth 10x above the AI for Healthcare sector.
- Invest in smart BioPharma, which will transform themselves into AI-Biopharma giants, as NVIDIA and Google have transformed themselves from IT-companies into AI-leaders.
- Short those BioPharma that will be late to seize the passing opportunity to implement AI into the core of their R&D. They will fail in the way of Kodak and Yellow Cab, who were bankrupted by digital photography and Uber.

Next Generation AI for Drug Discovery and Biomarker Development

Convergence with Blockchain and Digital Medicine



- In 2018, even more extreme challengers and disruptors will arrive with the convergence of next generation AI, blockchain and precision medicine.
- Longenesis is a revolutionary blockchain-based personalized medicine Data Marketplace platform built by Insilico Medicine and Bitfury that provides modular toolsets coupled with integrated advanced Artificial Intelligence systems to store, manage, and trade life data: social network data, health data and medical records.
- Longenesis will redefine the relationships between healthcare companies and patients. By facilitating a fast and easy way to contribute or purchase data along with an integrated deep learning AI, enterprises can save much money on R&D while users will for the first time be compensated for their Life data efficiently and ethically.



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