AI for Drug Discovery
Landscape Overview 2017

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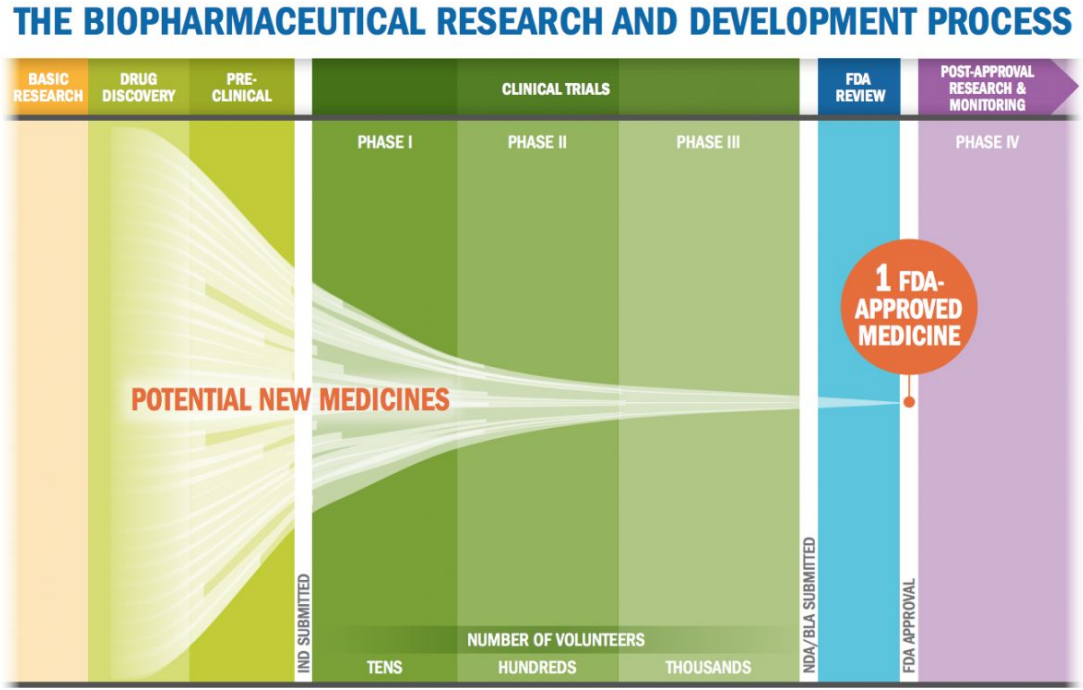
DEEP
KNOWLEDGE
VENTURES

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.



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

Drug makers need to find a more efficient way of developing medicines.
Artificial Intelligence (AI) can speed up drug discovery, cut R&D costs, decrease failure rates in drug trials and eventually create better medicines.

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 has been actively growing since 2015. But 2017 became year of cambrian explosion of AI in Healthcare industry.

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

106 STARTUPS TRANSFORMING HEALTHCARE WITH AI

The Application of AI within the Drug Discovery Process

Technologies increasing efficiency and reducing manual work

- aggregation and analysis of biomedical information
- improved decision-making
- form and qualify hypotheses
- analyze medical records to find patients for clinical trials

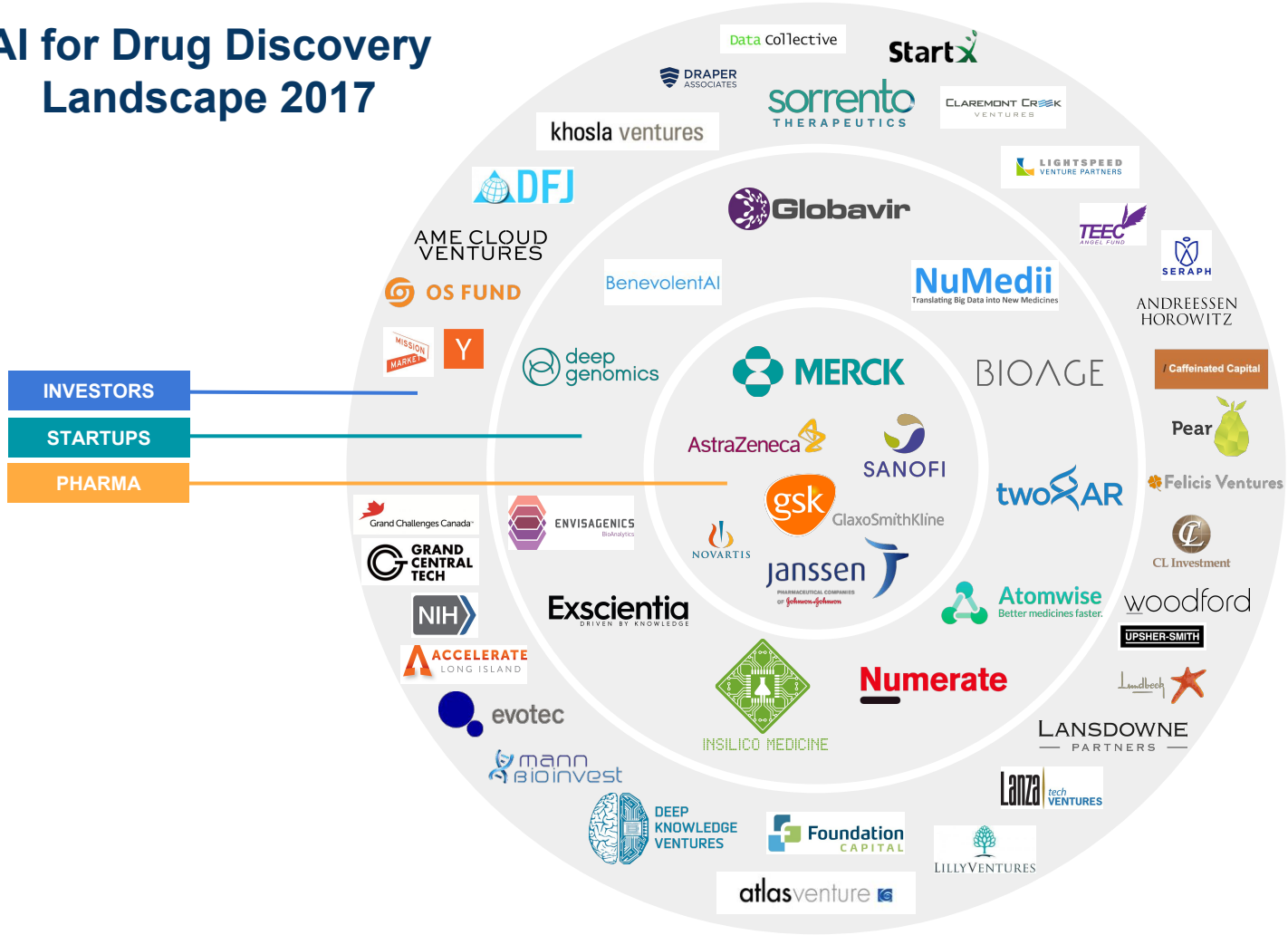
Development of new therapeutic molecules

- small molecules and biologics
- efficacy prediction
- drug combinations
- drug repositioning
- protein features and characteristics

Identification of new pathways and targets using “omics” analysis

- generate novel biomarkers and therapeutic targets
- personalized medicine based on omics markers
- discover connections between drugs and diseases

AI for Drug Discovery Landscape 2017

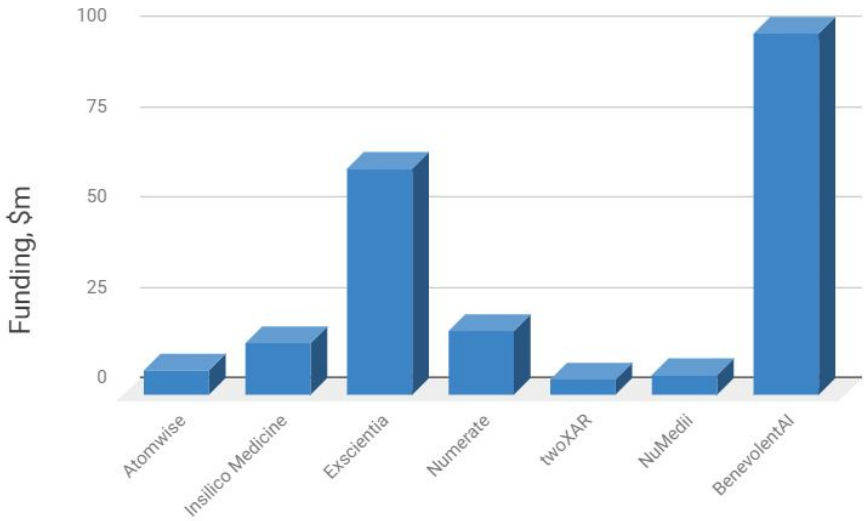


Comparison of AI for Drug Discovery Companies

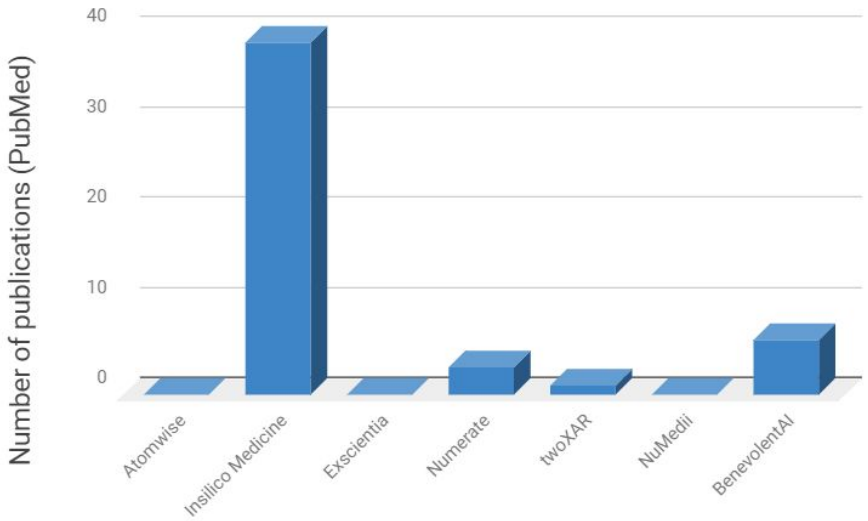
Company	Scientific publications covering AI for drug discovery	Number of AI experts in the team / total number of employees	Public talks on AI for drug discovery	Validation	Use GANs/RL
Atomwise	+	11/13	+	n/a	n/a
Cloud Pharmaceuticals	+	n/a	+	n/a	n/a
Benevolent.AI	+	18/74	+	n/a	n/a
Globavir	-	1/4	-	n/a	n/a
Envisagenics	-	n/a	+	n/a	n/a
Numerate	-	4/15	+	+	n/a
NuMedii	+	4/9	+	+	n/a
twoXar	+	1/15	+	n/a	n/a
Exscientia	+	2/12	+	+	n/a
BioAge Labs	+	1/5	+	n/a	n/a
Insilico Medicine	+	24/43	+	+	+

Comparison of AI for Drug Discovery Companies

Funding*, $m



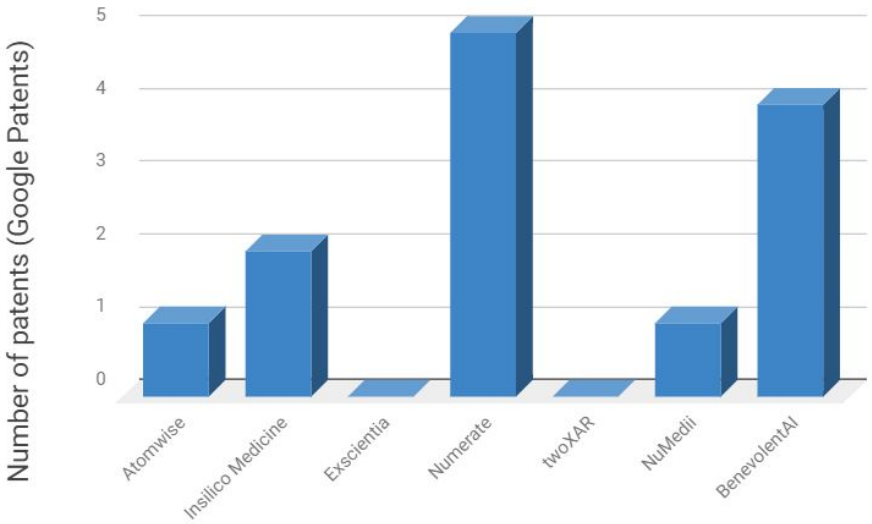
Number of Publications (PubMed)



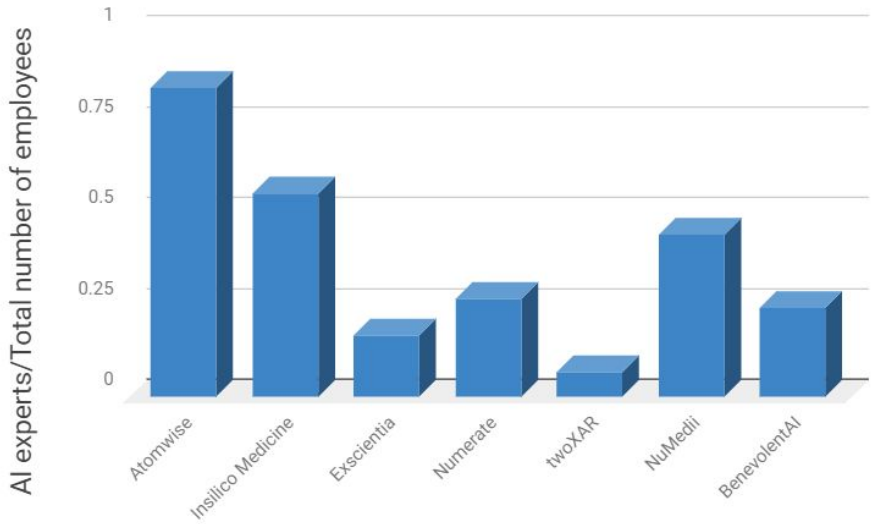
*According to Crunchbase or Company Website

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 a 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.

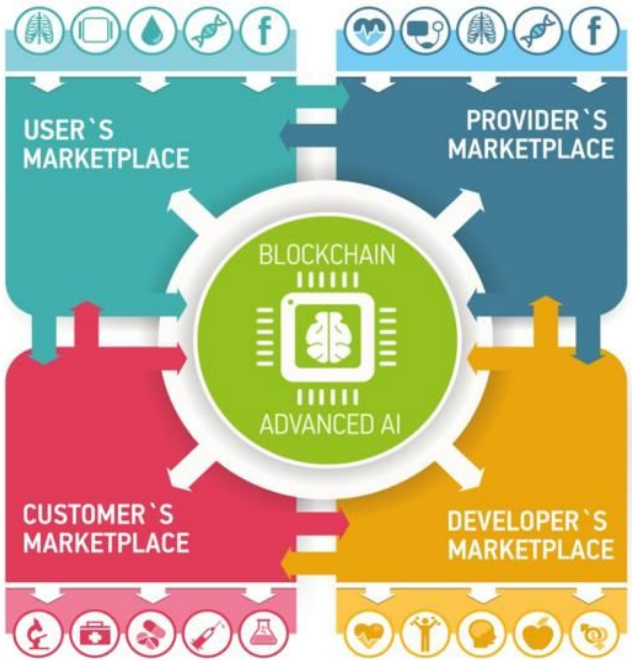
- This may reflect the inefficiency and of the organizations themselves and capital intensive barriers to entry more than the intrinsic intractability of complex biological systems - indeed, the most successful drugs historically have been discovered serendipitously. In any case, the sector shows signs 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 bet 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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APPENDIX

PROFILES

AI FOR
DRUG DISCOVERY
COMPANIES

TOP
BIO PHARMA
COMPANIES

AI FOR DRUG
DISCOVERY
CONFERENCES

Atomwise

Better medicines faster.

Atomwise is the creator of AtomNet, the first Deep Learning technology for novel small molecule discovery, characterized by its unprecedented speed, accuracy, and diversity.

Over the last 2 years, AtomNet has been deployed to help invent new potential medicines for 27 disease targets. They work with leading research groups at top organizations including Harvard University, Stanford University, Scripps Research Institute, and several large pharmaceutical companies, advancing the frontiers of human health.

Atomwise's notable successes have included promising compounds for the treatment of multiple sclerosis, Ebola, and botulinum neurotoxin, as well as work in cancer, malaria, and metabolic diseases. Today, Atomwise searches 1 million potential drug molecules every 24 hours.

Main Focus Areas: Structural Chemistry using Deep Learning

Number of employees: 13

Proof of concept publications:

- "AtomNet: A Deep Convolutional Neural Network for Bioactivity Prediction in Structure-based Drug Discovery" 2015 https://arxiv.org/abs/1510.02855
- "Systems and methods for applying a convolutional network to spatial data" 2016 https://www.google.com/patents/US9373059

Public talks on AI for drug discovery:

- October 3, 2017 "Computation and Synthetic Biology" Session at the SynBioBeta SF 2017
- June 29, 2017 "AtomNet: A deep convolutional neural network for bioactivity prediction in structure-based drug discovery" at the O'Reilly AI: Put AI to work
- June 27, 2017 "Panel Discussion: Accelerating Drug Discovery and Research with AI" at the AI in Healthcare Summit 2017
- September 23, 2016 "AtomNet: A Deep Convolutional Neural Network for Bioactivity Prediction in Structure-based Drug Discovery" at the 1st International Workshop on Deep Learning for Precision Medicine
- January 5, 2016 "Deep Learning to Discover Medicines" at Impact.tech SF
- "Atomwise: AI for drug discovery" at the 2015 Machine Learning and Market for Intelligence Conference

Cloud Pharmaceuticals is committed to improving health and well-being through the computational design and rapid development of new therapies. Cloud Pharmaceuticals' proprietary design process combines AI and cloud computing to search virtual molecular space and design novel drugs. These drugs are excellent candidates for further development and have novel composition of matter IP. The process enables faster drug development progress at lower cost and a higher success rate and better targeting of hard-to-drug indications.

Main Focus Areas: Ligand Chemistry, looking to develop two or more molecules

Number of employees: 4
Proof of concept publications::

- Speed the Discovery of Novel Drug Candidates with Quantum Molecular Design http://www.cloudpharmaceuticals.com/uploads/5/9/1/9/59199625/qmd_overview_815.pdf
- Accurate In Silico Prediction of Ligand Binding Potency in Therapeutic Targets using Quantum Molecular Design http://www.cloudpharmaceuticals.com/uploads/5/9/1/9/59199625/cloud_pharmaceuticals_white_paper.lie_2016.pdf
- Computational modeling and in-vitro/in-silico correlation of phospholipid-based prodrugs for targeted drug delivery in inflammatory bowel disease https://www.ncbi.nlm.nih.gov/pubmed/29101519
- In Silico Prediction of Ligand Binding Energies in Multiple Therapeutic Targets and Diverse Ligand Sets-A Case Study on BACE1, TYK2, HSP90, and PERK Proteins https://www.ncbi.nlm.nih.gov/pubmed/28759991

Public talks on AI for drug discovery:

- July 26-27, 2017 ''Discover: Showcasing the Utility of AI in Early Stages of R&D to Prove This Disruptive Technology's Validity'' at the AI Pharma Innovation
- September 27–28, 2017 ''Artificial Intelligence (AI) in Drug Discovery and Development'' Session at the Artificial Intelligence in Drug Development Congress

BenevolentAI

BenevolentAI uses proprietary AI and machine learning technology to look deeply into vast scientific research data sets. The company works primarily with the text data using semantic links in patents, publications and other data sets. BenevolentBio is focussed on applying the Company's technology in the bioscience industries. BenevolentTech is developing an advanced artificial intelligence platform that helps scientists make new discoveries and redefines how scientists gain access to, and use, all the data available to them to drive innovation. The technology is built upon a deep judgement system that learns and reasons from the interaction between human judgement and data.

Main Focus Areas: Text Mining using advanced Natural Language Processing (NLP)

Number of employees: 74

Proof of concept publications:

- Structural and Functional View of Polypharmacology https://www.ncbi.nlm.nih.gov/pubmed/28860623
- Classification and analysis of a large collection of in vivo bioassay descriptions https://www.ncbi.nlm.nih.gov/pubmed/28678787
- The druggable genome and support for target identification and validation in drug development https://www.ncbi.nlm.nih.gov/pubmed/28356508
- A comprehensive map of molecular drug targets https://www.ncbi.nlm.nih.gov/pubmed/27910877

Public talks on AI for drug discovery:

- Dec 8, 2017 ''Machine Learning for Molecules and Materials'' Workshop at the NIPS Conference
- Nov 30, 2017 ''"Can a machine cure brain disease" at the SLUSH
- Oct 30, 2017 ''Artificial Intelligence'' Panel at the Founders Forum
- Oct 16, 2017 "AI to enhance and accelerate global scientific discovery" at the Data Driven NYC
- Oct 11, 2017 "Why drug discovery needs artificial intelligence" at the What can Big Data do for Chemistry?
- Aug 21, 2017 ''Machine Learning for Drug Discovery'' at the Machine Learning Meet-up

Globavir is initially focused on the treatment of dengue virus infection, a potentially lethal disease infecting 390 million patients annually. Through the combination of their proprietary diagnostic technology and advanced therapeutic candidates, Globavir is ideally positioned to rapidly impact the clinical landscape for Dengue patients.

Globavir's platform discovery technologies have further identified candidate compounds with efficacy in additional viral indications, including West Nile, Japanese Encephalitis, Ebola, Marburg, and Hunta viruses.

Main Focus Areas: Antivirals

Number of employees: 4

Proof of concept publications:

- Safety and immunogenicity of different doses and schedules of a live attenuated tetravalent dengue vaccine (TDV) in healthy adults: A Phase 1b randomized study https://www.ncbi.nlm.nih.gov/pubmed/26384447
- Safety and Immunogenicity of a Tetravalent Dengue Vaccine Candidate in Healthy Children and Adults in Dengue-Endemic Regions: A Randomized, Placebo-Controlled Phase 2 Study https://www.ncbi.nlm.nih.gov/pubmed/26704612

Public talks on AI for drug discovery:

- September 19, 2017 ‘’Progress Towards Curative Therapies’’ at the Anti-Infectives Rx
- September 26, 2014 ‘’ Globavir's therapeutic candidates for Ebola and Dengue virus’’ at the Healthcare & Technology Conference

ENVISAGENICS
BioAnalytics

Envisagenics' 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.

Main Focus Areas: RNA splicing analytics

Number of employees: 7
Proof of concept publications:

- Differential connectivity of splicing activators and repressors to the human spliceosome, 2015 https://genomebiology.biomedcentral.com/articles/10.1186/s13059-015-0682-5
- Differentiation of mammary tumors and reduction in metastasis upon Malat1 lncRNA loss, 2015 http://genesdev.cshlp.org/content/30/1/34
- Differential connectivity of splicing activators and repressors to the human spliceosome, 2015 https://genomebiology.biomedcentral.com/articles/10.1186/s13059-015-0682-5
- SpliceTrap: a method to quantify alternative splicing under single cellular conditions https://academic.oup.com/bioinformatics/article-lookup/doi/10.1093/bioinformatics/btr508

Public talks on AI for drug discovery:

- Dec 12, 2017 "How Advances in Biomarkers and Big Data are Transforming Clinical Trials and Clinical Applications" Session at the Technology for Precision Health Summit

Numerate

Numerate is a privately-held computational drug design company that is transforming the discovery of new medicines that fill significant therapeutic gaps by harnessing the vast computational power of the cloud and the ever-increasing amounts of drug discovery data by applying proprietary artificial intelligence algorithms. Numerate's drug design platform combines advances in computer science and statistics with traditional medicinal chemistry approaches to overcome major challenges in small molecule drug discovery and significantly accelerate candidate selection and optimization. Using this platform, coupled with innovative funding and partnership models, Numerate is developing a therapeutic pipeline focused on producing first-in-class candidates against emerging targets addressing major unmet medical needs in cardiovascular, metabolic and neurodegenerative disease.

Main Focus Areas: Ligand Chemistry, ADME, combination of machine learning with classical approaches

Number of employees: 15

Proof of concept publications:

- In press

Public talks on AI for drug discovery:

- December 1, 2017 "AI in drug discovery: Current state and opportunities" at the Global Pharma R&D Informatics Congress
- November 30, 2017 ''Artificial Intelligence Applied to CB Threat Characterization and Mitigation'' at the CHEMICAL AND BIOLOGICAL DEFENSE SCIENCE & TECHNOLOGY CONFERENCE
- November 2, 2017 "Data & Algorithm Challenges Facing Research in Applying AI to Pharmaceutical R&D" at the Einstein AI and Deep Learning Summit
- September 17-18, 2017 ''Artificial Intelligence'' Session at the Artificial Intelligence Innovation Summit
- September 10-13, 2017 ''How Artificial Intelligence is transforming drug discovery'' at the Basel Life
- July 26, 2017 "How AI can be Implemented in Key Areas of Failure Along the R&D Pipeline: A Technology Perspective" at the AI Pharma Innovation

NuMedii

Translating Big Data into New Medicines

NuMedii discovers and de-risks effective new drugs by translating Life Sciences Big Data into therapies with a higher probability of therapeutic success. The company's proprietary and dynamic Big Data technology, developed in Atul Butte's lab at Stanford University and licensed exclusively to NuMedii, consists of hundreds of millions of human, biological, pharmacological and clinical data points that the company has normalized and annotated. The company integrates these data with proprietary network-based algorithms to find both drug candidates and biomarkers predictive of efficacy for diseases.

Main Focus Areas: Gene and Protein Expression Analysis, Pathway Analysis

Number of employees: 9

Proof of concept publications:

- A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors, 2013 https://www.ncbi.nlm.nih.gov/pubmed/24078773
- Exploiting drug-disease relationships for computational drug repositioning, 2011 https://www.ncbi.nlm.nih.gov/pubmed/21690101
- Computational repositioning of the anticonvulsant topiramate for inflammatory bowel disease, 2011 https://www.ncbi.nlm.nih.gov/pubmed/21849664
- Discovery and preclinical validation of drug indications using compendia of public gene expression data, 2011
- https://www.ncbi.nlm.nih.gov/pubmed/21849665
- Drug discovery in a multidimensional world: systems, patterns, and networks, 2010 https://www.ncbi.nlm.nih.gov/pubmed/20677029

Public talks on AI for drug discovery:

- December 8, 2017 at the ML4H: Machine Learning for Health
- January 26, 2016 "Turning Big Data into Smart Data" at the PMWC 2016
- February 16, 2015 "Drug Repositioning in the Era of Precision Medicine" at the Bioinformatics for Big Data

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. twoXAR is financially backed by Andreessen Horowitz and the Stanford-StartX Fund and engaged in collaborations with leading academic research and biopharma R&D organizations.

Main Focus Areas: Gene and Protein Expression Analysis

Number of employees: 15

Proof of concept publications:

- Synergistic drug combinations from electronic health records and gene expression , 2017

https://academic.oup.com/jamia/article/24/3/565/2664593/Synergistic-drug-combinations-from-electronic

- An Integrative Bioinformatics Approach Rapidly Identifies in vivo-validated Drug Candidates with Novel Mechanisms of Action in Rheumatoid Arthritis

https://uploads.strikinglycdn.com/files/1e42a126-c024-478a-afd1-76121b6620a6/twoXAR%20-%20Rheumatoid%20Arthritis%20Supplementary%20Material%20-%20Stanford%20Drug%20Discovery%20Conference.pdf

Public talks on AI for drug discovery:

- October 4, 2017 “Computational Drug Design” Panel at Stanford SPARK
- June 27, 2017 “Panel Discussion: Accelerating Drug Discovery and Research with AI” at the AI in Healthcare Summit 2017
- April 24, 2017 ‘’An integrative bioinformatics approach identifies in vivo validated drug candidates with novel mechanisms of action in rheumatoid arthritis’’ at the Stanford Drug Discovery Conference
- September 16-17, 2015 “twoXAR: Drug Discovery in a Few Minutes, A Computational Approach” at the MIT Digital Health Conference

Exscientia
DRIVEN BY KNOWLEDGE

Exscientia's AI driven systems actively learn best practice from vast repositories of discovery data and are further enhanced with knowledge acquired from seasoned drug hunters. With better information to hand than any researcher could acquire individually, their knowledge-driven systems design millions of novel, project-specific compounds and pre-assess each for predicted potency, selectivity, ADME and other key criteria.
From this, a selection of the best, information-rich compounds are selected for synthesis and assay.
With new experimental data generated, the results are integrated and the next design cycle initiated.
Rapid design-make-test cycles ensure unparalleled progress towards desired project goals.
Exscientia has already delivered exceptional productivity, generating candidates in roughly one-quarter of the time of traditional approaches.

Main Focus Areas: Computer-assisted Medicinal Chemistry

Number of employees: 7

Proof of concept publications::

- Design of molecules - US Patent App. 14/986,516, 2015
- Morpholino compounds, uses and methods - US Patent 9,079,895, 2015
- Automated design of ligands to polypharmacological profiles
  https://static1.squarespace.com/static/5809fdadd1758e887703526b/t/5881fee203596ec776739fc7/1484914404329/Nature-2012-Besnard.pdf

Public talks on AI for drug discovery:

- 2018 ''AI-driven Pre-clinical and Clinical Drug Design, Discovery, and Development'' at the PMWC

BIOAGE

BioAgeLabs couple omics data with machine learning to measure human aging and accelerate drug discovery.They're betting on the power of high-throughput human data, coupled with innovative machine learning, to substantially accelerate drug discovery for aging. BioAge Labs take a hybrid experimental and computational approach to identifying the molecular signatures that drive aging, working with multiple partners in academia and industry.

Main Focus Areas: Metabolomics

Number of employees: 5

Proof of concept publications:

- MortalityPredictors.org: a manually-curated database of published biomarkers of human all-cause mortality https://www.ncbi.nlm.nih.gov/pubmed/28858850
- In silico drug screen in mouse liver identifies candidate calorie restriction mimetics https://www.ncbi.nlm.nih.gov/pubmed/22533420
- Genome-Wide Scan Informed by Age-Related Disease Identifies Loci for Exceptional Human Longevity https://www.ncbi.nlm.nih.gov/pubmed/26677855
- Quantifying signaling pathway activation to monitor the quality of induced pluripotent stem cells https://www.ncbi.nlm.nih.gov/pubmed/26327604
- Prioritizing therapeutics for lung cancer: an integrative meta-analysis of cancer gene signatures and chemogenomic data https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4364883/
- Integrative computational biology for cancer research https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3179275/

Public talks on AI for drug discovery:

- September 11, 2017 "Metabolomic biomarkers of human aging" at the Basel Life
- June 23, 2017 "Whole-Genome Sequencing of the World's Oldest People" at the 4th Annual Clinical Genome Conference

INSILICO MEDICINE

Insilico Medicine, Inc. is a deep learning powerhouse headquartered at the Emerging Technology Centers at the Johns Hopkins University Eastern campus in Baltimore, with R&D centers in Russia, Taiwan and Hong Kong and R&D resources in Belgium and in the UK hiring top talent through hackathons and competitions. It pioneered the use of GANs and RL for generating novel molecular structures. The company pursues internal drug discovery programs in cancer, fibrosis, muscle wasting, diabetes, dermatological conditions and has multiple partnerships with the pharmaceutical companies, governments and academia.

Main Focus Areas: Gene and Protein Expression Analysis, GANs/GANRL for Novel Chemistry, Aging Research

Number of employees: 43

Proof of concept publications:

- A comparative review of computational methods for pathway perturbation analysis: dynamical and topological perspectives
- druGAN: An Advanced Generative Adversarial Autoencoder Model for de Novo Generation of New Molecules with Desired Molecular Properties in Silico
- The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology
- In silico Pathway Activation Network Decomposition Analysis (iPANDA) as a method for biomarker development
- In search for geroprotectors: in silico screening and in vitro validation of signalome-level mimetics of young healthy state
- Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data
- Deep biomarkers of human aging: Application of deep neural networks to biomarker development
- Applications of Deep Learning in Biomedicine

Public talks on AI for drug discovery:

- November 8, 2017 “Reinventing Pharma” at the Exponential Medicine
- September 12-13, 2017 “Artificial Intelligence for Drug Discovery and Biomarker Development” at the Basel Life
- May 10, 2017 “Applications of Generative Adversarial Networks to Drug Discovery in Oncology and Infectious Diseases” at the NVIDIA GTC
- April 26, 2017 “Artificial Intelligence in Drug Discovery and Aging Research” at the BioData World West
- February 28, 2017 “Application of Deep Neural Networks to Biomarker Development” at the Deep Learning for Healthcare Summit
- January 25, 2017 “Deep Learning for In Silico & Ab Initio Drug Discovery & Actionable Biomarker Development” at the Advanced Pharma Analytics

Top Pharma Companies*
Exploring the Potential of AI for Drug Discovery

*by 2017 market capitalization

Major AI for Drug Discovery Conferences