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Top Target Treatments

TOP TARGET TREATMENTS, *F. LEGA*
PRECISION HEALTH AND POPULATION HEALTH: CAN THEY INTERSECT EFFECTIVELY? *T. RASSAF ET AL.*
PERSONALISED MEDICINE: THE ROAD AHEAD, *D. PRITCHARD*
A HUMAN-CENTRIC APPROACH FOR DATA COLLECTION, *I. RÄSÄNEN & J. SINIPURO*
ENHANCING PRECISION MEDICINE: SHARING AND REUSING DATA, *C. PARRA-CALDERÓN*
PERSONALISED MEDICINE AND CARDIOVASCULAR DISEASE, *D. MUNDRA*
LEVERAGING ADVANCED METHODS TO EVALUATE AI-PHARMA COMPANIES, *M. COLANGELO & D. KAMINSKIY*

EUROSON 2019 WELCOMES WORLD OF ULTRASOUND, *P. SIDHU*

BREXIT MEANS BREXIT: RADIOLOGISTS WITHOUT BORDERS, *V. PAPALOIS*

FIGHTING CYBER THREATS WITH A GLOBAL COMMUNITY, *D. ANDERSON*

WHEN DOES STRIKING OUT ALONE WORK BEST? *D. MICHAELIDES*

VALUE-ORIENTED MANAGEMENT, *W. VON EIFF*

SEX AND GENDER IN MEDICINE, *N. KUMAR & T. ROHR-KIRCHGRABER*

SECRETS OF INNOVATION SUCCESS, *N. HENKE & R. BARTLETT*

NEW HOSPITAL POLICIES AND PROCEDURES REQUIRED FOR PATIENT SAFETY, *M. RAMSAY*

PEOPLE POWERED HEALTH MOVEMENT FOR PATIENTS, *L. THOMPSON*

HEALTHCARE AND INDUSTRY PARTNER FOR TECH INNOVATION, *A. FREJD*

NURSING ON THE MOVE: CROSS-BORDER HIRING, *I. MEYENBURG-ALTWARG*

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Leveraging advanced methods to evaluate AI-Pharma companies

The level of sophistication used in due diligence should be on par with the level of complexity in a given industry.

AI-Pharma companies are 100 times as complex as FinTech companies. Methodologies used to assess them should be 100 times as rigorous.

Margaretta Colangelo
Managing Partner
Deep Knowledge Ventures,
San Francisco, United States

mc@dkv.global

@RealMargaretta
@DeepTech_VC

Dmitry Kaminskiy
General Partner
Deep Knowledge Ventures
London, UK

dk@dkv.global

@DeepTech_VC

Discovering new drugs using AI is one of the most challenging areas in biological sciences. Top tier AI for Drug Discovery companies have distinguishing characteristics that include high levels of expertise in biopharmaceutical science, advanced proficiency in AI, very specialised teams, and constantly evolving internal knowledge. Companies in this sector are developing very advanced AI techniques that may enable them to produce the next blockbuster drugs, making them the new unicorns of the Pharma industry.

Due to the complexity, companies in this sector sometimes appear to be enigmatic black boxes to investors. Since most investment funds have not developed sufficiently robust methods to evaluate AI for Drug Discovery companies, they erroneously treat these companies as traditional biotech companies. There could be and should be better assessment methods for evaluating these companies. Even the most advanced companies should be scrutinised, and many parameters should be taken into account. Very few investment firms are capable of applying efficient due diligence to assess investment targets in this sector because they fail to use approaches that match the sophistication of the sector.

The drug discovery environment

The drug discovery environment is big. It includes advanced AI for drug discovery teams and startups, pharmaceutical companies, venture investors, healthcare providers and governments. Interactions in this environment are extremely inefficient. There are very few examples of high functioning relationships between AI startups, pharmaceutical companies and healthcare systems. Most of the venture investors are profiting on disproportions and inconsistencies in the sector, rather than through proactive adoption and use of the most advanced technologies available. This is why venture capital firms can generate profits without being sophisticated investors in this area. This scenario is far from ideal.

> “MOST INVESTMENT FUNDS ERRONEOUSLY TREAT AI FOR DRUG DISCOVERY COMPANIES AS TRADITIONAL BIOTECH COMPANIES”

The pace of innovation in AI for Drug Discovery is unprecedented. These companies are using fundamentally different techniques than those used as standard practice 20 years ago. At the same time, the majority of investment funds are still using the same techniques that were used 20 years ago. The venture investment industry is not evolving at the pace required to match the rate of progress in DeepTech. The pace of progress in the investment technology industry (InvestTech) must keep up with the

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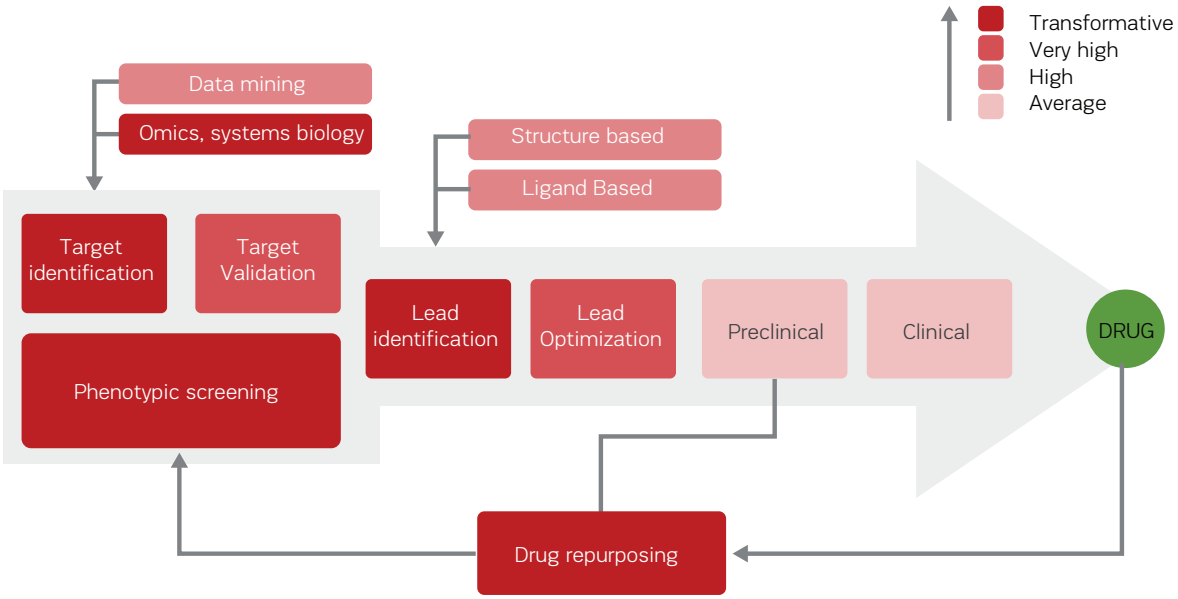
The Heat Map of AI Potential Value for Various R&D Areas



pace of progress in advanced science and technology. Investment funds that leverage progressive techniques to update their business models, exit strategies, and underlying assessment methodologies, will have a big advantage over funds that don't.

Specialised metrics for valuation and forecasting

Although there are about 150 AI companies in the Drug Discovery space, very few of them are capable of building end-to-end solutions. Companies such as WuXi NextCODE, BenevolentAI, DeepMind Health, and Insilico Medicine are leaders in this area. Insilico Medicine was the first company to apply generative adversarial networks for generating new molecular structures with specified parameters and published a seminal peer-reviewed paper (**oncotarget.com/index.php?journal=oncotarget&page=article&op=view&path%5B%5D=14073&path%5B%5D=44886**) submitted in June 2016.

Deep Knowledge Ventures invested in Insilico Medicine in 2014, years before the AI for Drug Discovery sector rose to prominence. In 2018, Deep Knowledge Ventures' analytical subsidiary, Deep Knowledge Analytics, developed industry-specific due diligence methods to determine which AI for Drug Discovery companies are overvalued, balanced (from a technological and financial perspective) and undervalued (where technology significantly exceeds financials).

Deep comparative analysis

Deep Knowledge Analytics uses multiple parameters and applies quantified metrics to perform deep comparative analysis to differentiate levels of maturity, business development, scientific advantages, and technological levels in a very objective way.

Early stage startups are assessed using 100 parameters. Advanced stage companies are assessed using more than 300 parameters.

10 fundamental parameters used by Deep Knowledge Analytics

1.Team structure

The number of specialists and balance in the company's team structure. Generally the best structure is 1/3 biochemistry specialists, 1/3 AI specialists, and 1/3 business development and investment relations experts, including former Pharma executives to assist in establishing contact and cooperation with Pharma companies. In practice what constitutes a sufficient number depends on the scope of the company's target applications. As a general rule, the number of specialists should be more than 10.

2. Independent scientific validation

Evidence of independent scientific validation including peer-reviewed scientific papers published in high-impact journals, and visibility within the scientific community through frequent presentations at scientific conferences.

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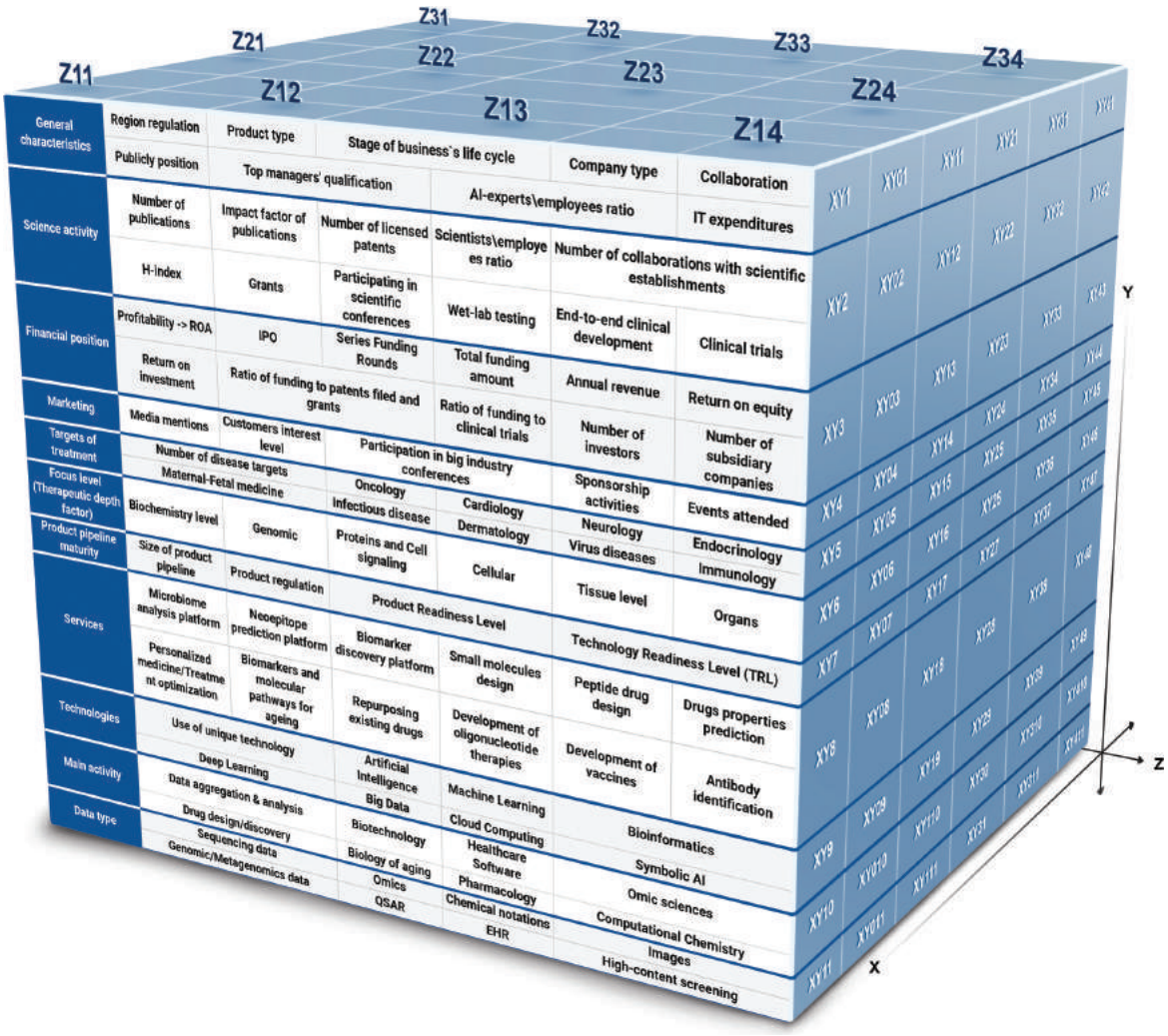

3. Partnerships with Pharma companies

The company should have several contracts in place with Pharma companies. This serves as additional validation that the company has something practical and tangible in its pipeline.

4. AI strength

There must be evidence that the company uses state-of-the-art AI techniques and consistently absorbs ongoing innovation in novel AI technologies and methodologies. If the company claims that it is an AI company, then it should be particularly strong in AI.

5. Investors

The company should have world-class investment funds as investors in their Series A or B rounds. There are fewer than 20 world-class investment funds recognised as being top funds globally by the entire investment community.

6. Molecules

The company should have a large number of target molecules discovered, and a sufficient number of molecules currently in clinical trials.

7. Target applications

The number of target applications the company pursuing (eg drug discovery, biomarker development, toxicity and ADME prediction, compound generation, compound binding, etc).

8. Technology development scope

Whether the company is developing an end-to-end clinical pipeline, or focusing on just one particular segment in the overall drug discovery and development process.

9. R&D depth

The proportion of the company's funds dedicated

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Company Profile

Key strengths	Key differentiations
Generative Adversarial Networks	High ratio of AI experts
Reinforcement Learning	Full range of AI for drug discovery services
Linking biology and chemistry	Focus on longevity and quantitative precision preventive medicine
Strong partnerships with top pharma companies	Personalized Medicine
Combination of advanced expertise in AI and drug discovery	Both AI for Healthcare and Drug Discovery projects

to its R&D activities, as opposed to completing the development of products near the end of their development cycle. A high proportion of funds devoted to R&D indicates proactive innovation and new technology adoption.

10. Ratio of investment to IP produced

The ratio of the amount of money invested in the company to the amount of IP produced by the company. This is indicative of the performance of the company's R&D activities and the company's future prospects, and reflects how intelligently and efficiently the company has utilised its funding to date.

Progressive InvestTech

The business model traditionally used by venture funds has stagnated and will be ineffective going forward. To achieve success, investment firms operating in DeepTech industries will need advanced science and technology assessment capabilities and new approaches to venture capital business models and exit strategies. Deep Knowledge Ventures is developing a novel InvestTech solution which will be particularly relevant for the AI for Drug Discovery sector. The thematic AI-Pharma investment fund is designed with one purpose - to invest in the best AI for Drug Discovery companies. The Pharma AI - Index Hedge Fund will use hybrid investment technologies combining the profitability of venture funds with the liquidity of hedge funds, significantly de-risking the interests of LPs and simultaneously providing the best and most promising AI companies with a relevant amount of investment.

Deep Knowledge Analytics reports

Deep Knowledge Analytics, a subsidiary of Deep Knowledge Ventures, regularly produces comprehensive quarterly reports on multiple topics including DeepTech, AI, Longevity, and AI for Drug Discovery. Deep Knowledge Analytics, a subsidiary of Deep Knowledge Ventures, regularly produces comprehensive quarterly reports on multiple topics including DeepTech, AI, Longevity, and AI for Drug Discovery.

On April 12, 2019 Deep Knowledge Analytics published a new open-access quarterly report on the AI for Drug Discovery Industry. This 108 page report provides a comprehensive overview of the AI Pharma landscape through Q1 2019. This report features analysis of 350 investors, 50 corporations and 150 companies active in the sector, and features a list of 30 leading R&D centres that provide important research in this area. The report also covers the

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most important events that took place in the industry in Q1 2019.

Deep Knowledge Analytics' 108 page open-access Q1 report on the AI for Drug Discovery Industry provides a comprehensive overview of the AI Pharma landscape through Q1 2019. This report features analysis of 350 investors, 50 corporations and 150 companies active in the sector, and features a list of 30 leading R&D centers that provide important research in this area. The report also covers the most important events that took place in the industry in Q1 2019.

> "ALTHOUGH THERE IS NO CONSENSUS SO FAR AMONG ANALYSTS REGARDING THE EXPECTED VALUATION OF THE INDUSTRY, ESTIMATES RANGE FROM $5 BILLION TO $20 BILLION BY 2024"

Q1 2019 report highlights

- Investment in AI for Drug Discovery startups increased from $200 million in 2015 to over $700 million in 2018.
- The number of AI for Drug Discovery companies increased by 20 companies.
- The report shows 350 investors identified in Q1 2019, which is 30 more investors than Q4 2018.
- There are 350 investment funds investing in the sector including Google Ventures, Tencent, Wuxi, Andreessen Horowitz, Khosla Ventures, and Sequoia Ventures.
- Although there is no consensus so far among analysts regarding the expected valuation of the industry, estimates range from $5 billion to $20 billion by 2024.
- Cost of R&D per drug is growing exponentially, but sales per asset are definitely not increasing.
- An additional 10 new research centers were recorded since Q4 2018.
- Regional proportion remained almost the same, despite an increased number of entities and a growing interest from China.
- Declining R&D efficiency of Biopharma Companies remains a major concern among all parties in the industry with a continuous decline recorded during the last 8 years.
- Demand for AI technologies and AI talent is growing in the Pharma and healthcare industries and driving the formation of a new interdisciplinary field — data-driven drug discovery/healthcare.

Download the Q1 2019 report here: AI for Drug Discovery Landscape Overview Q1/2019 (**ai-pharma.dka.global/quarter-1-2019**)

To see a complete list of reports please visit: Deep Knowledge Analytics (**ai-pharma.dka.global**)

Deep Knowledge Ventures is an investment fund focused on DeepTech. Investment sectors include AI, Precision Medicine, Longevity, and Neurotech. Deep Knowledge Ventures led Insilico Medicine's seed funding round in 2014 and has remained a close advisor in the company's journey towards becoming a global leader in the application of advanced AI, particularly deep learning and GANs. Deep Knowledge Analytics, a subsidiary of Deep Knowledge Ventures, regularly produces comprehensive open access analytical reports on topics related to DeepTech including AI in Drug Discovery and AI in Healthcare. ■

Conflicts of interest

Deep Knowledge Ventures led Insilico Medicine's seed funding round in 2014 and has remained a close advisor in the company's journey towards becoming a global leader in the application of advanced AI, particularly deep learning and GANs.

KEY POINTS

- ✓ The pace of innovation in AI for Drug Discovery is unprecedented.
- ✓ Discovering new drugs using AI is one of the most challenging areas in biological sciences.
- ✓ AI-Pharma companies are 100 times as complex as FinTech companies. Methodologies used to assess them should be 100 times as rigorous.
- ✓ Companies in this sector are developing very advanced AI techniques that may enable them to produce the next blockbuster drugs, making them the new unicorns of the Pharma industry.

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