TRANSFORMING THE PHARMACEUTICAL INDUSTRY AND THE FUTURE OF LONGEVITY WITH NEXT-GENERATION ARTIFICIAL INTELLIGENCE

Insilico Medicine, Inc
Emerging Technology Centers
Johns Hopkins University
B301, 1101 33rd Street
Baltimore, MD, 21218

- **Drug Discovery**
- **Drug Repurposing**
- **Biomarker Development**
- **Clin. Trials Predictors**
- **Aging Research**
- **AI Solutions for Blockchain**

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ai.100
CBINSIGHTS
2018

Top 100 AI Companies 2018

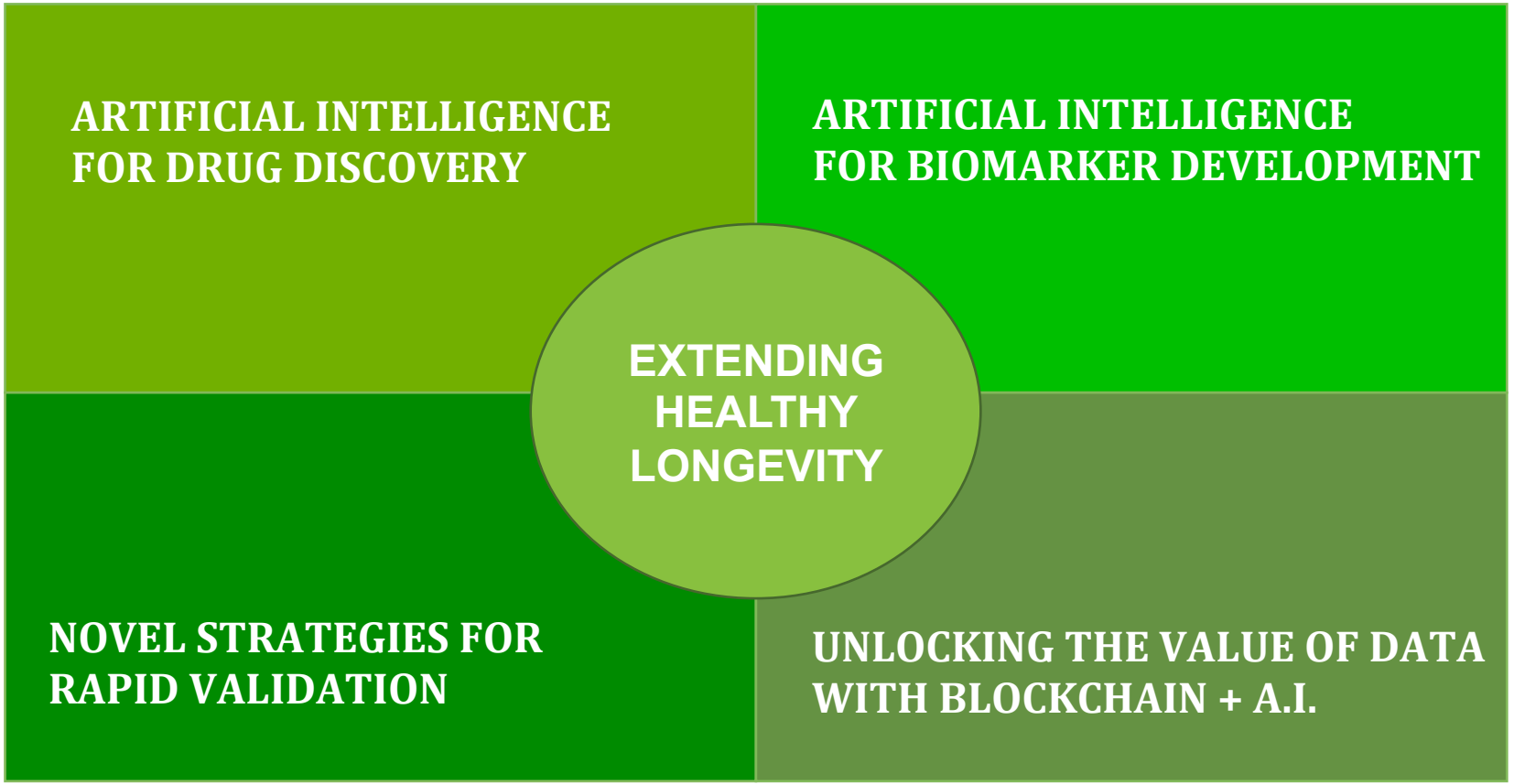
ALEX ZHAVORONKOV, PHD
alex@insilico.com

www.insilico.com

@biogerontology

WE AIM TO MAKE LONGEVITY BUSINESS CREDIBLE, EFFECTIE, SUSTAINABLE AND PROFITABLE

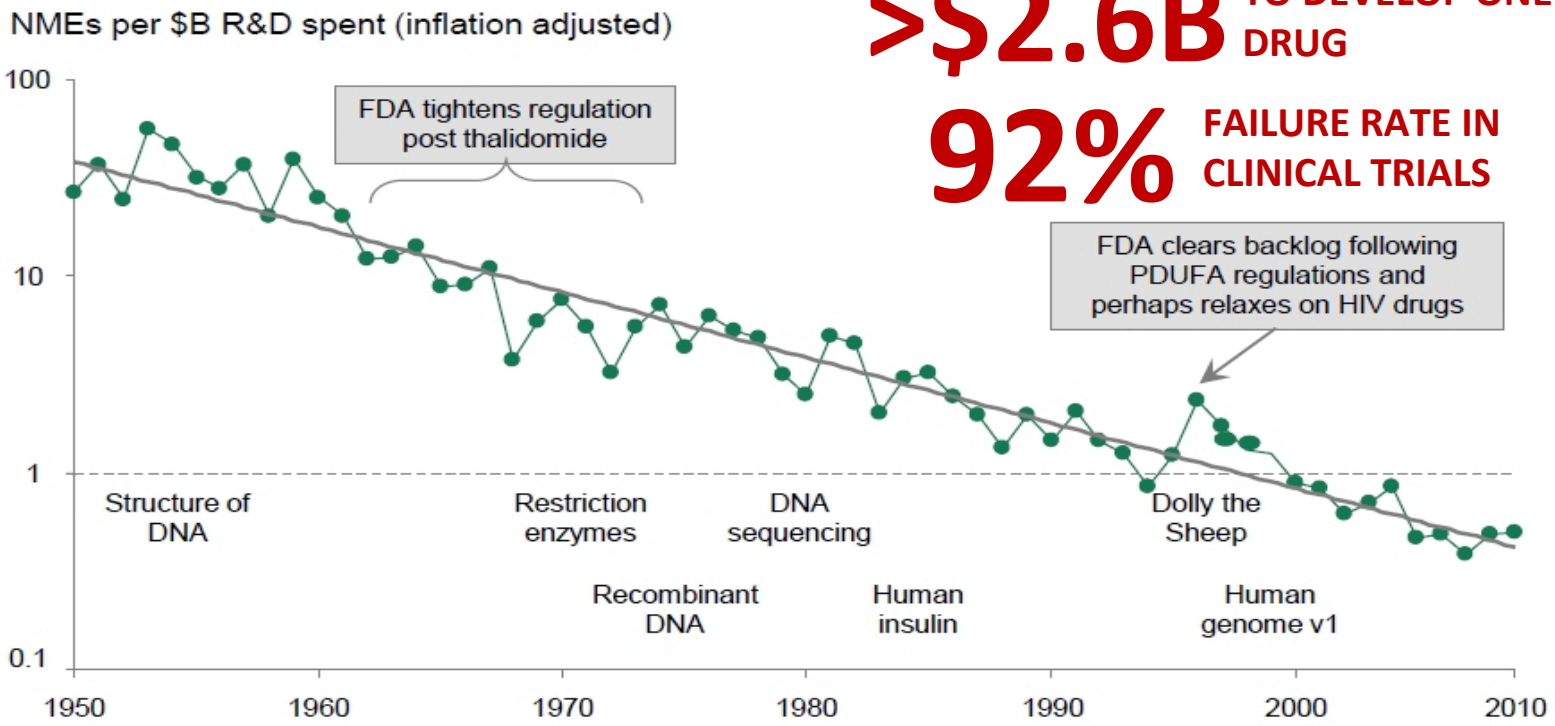
INSILICO MEDICINE AIMS TO EXTEND PRODUCTIVE LONGEVITY BY BUILDING SIGNATURES OF AGING AND AGE-RELATED DISEASES AND GENERATING NOVEL MOLECULES USING ARTIFICIAL INTELLIGENCE


ARTIFICIAL INTELLIGENCE FOR DRUG DISCOVERY
ARTIFICIAL INTELLIGENCE FOR BIOMARKER DEVELOPMENT
EXTENDING HEALTHY LONGEVITY
NOVEL STRATEGIES FOR RAPID VALIDATION
UNLOCKING THE VALUE OF DATA WITH BLOCKCHAIN + A.I.

PHARMA EFFICIENCY IS DECLINING STEADILY

>$2.6B TO DEVELOP ONE DRUG

92% FAILURE RATE IN CLINICAL TRIALS



Bernstein Research: The Long View - R&D Productivity, 2010

DOES NOT SHARE EVEN OLDEST DATA

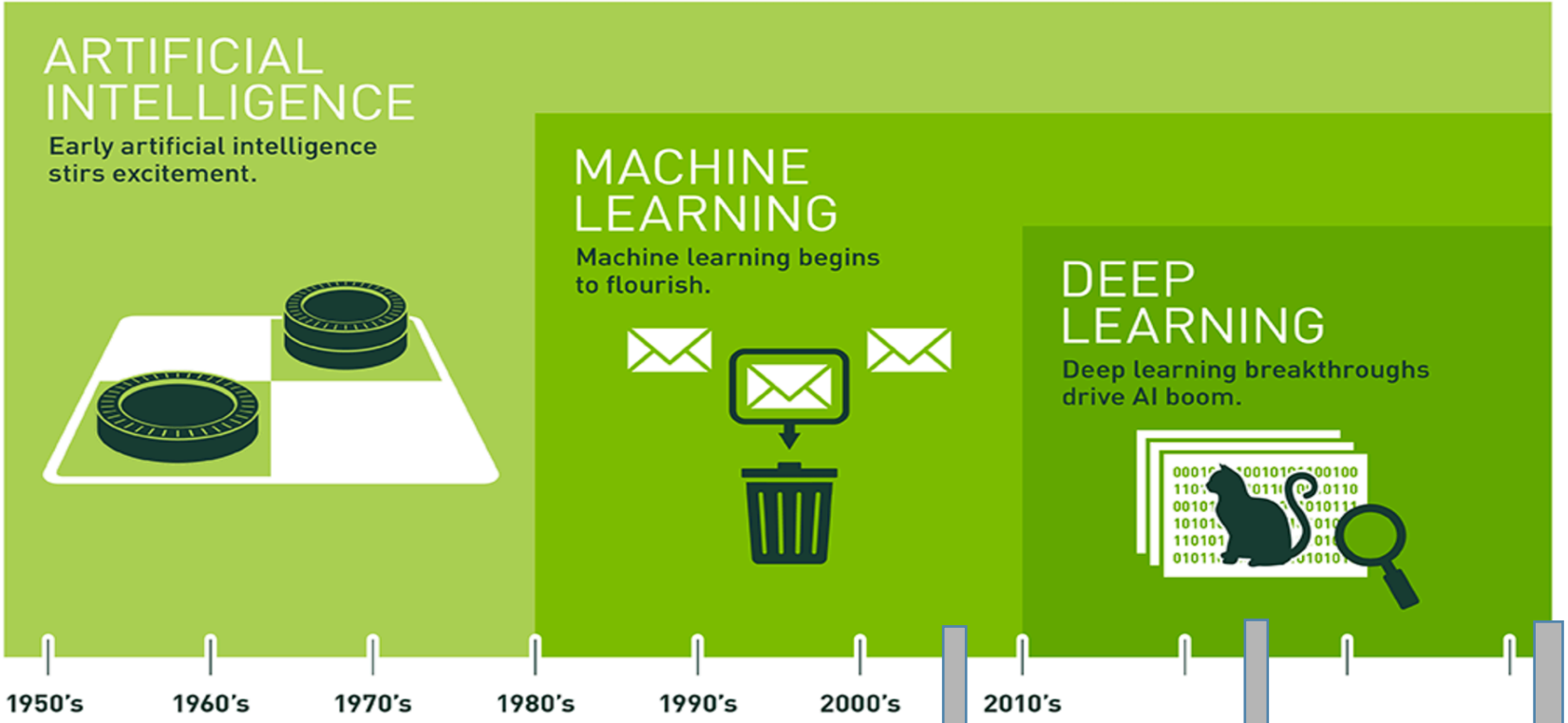
46 NEW DRUGS launched in 2014

GLOBAL SALES: >$1 Trillion

GLOBAL R&D: >$150 Billion

>$2.6B TO DEVELOP ONE DRUG

92% FAILURE RATE IN CLINICAL TRIALS



MOST OF THE "HYPE" IN AI IS DUE TO THE CREDIBLE ADVANCES IN DEEP LEARNING AND REINFORCEMENT LEARNING

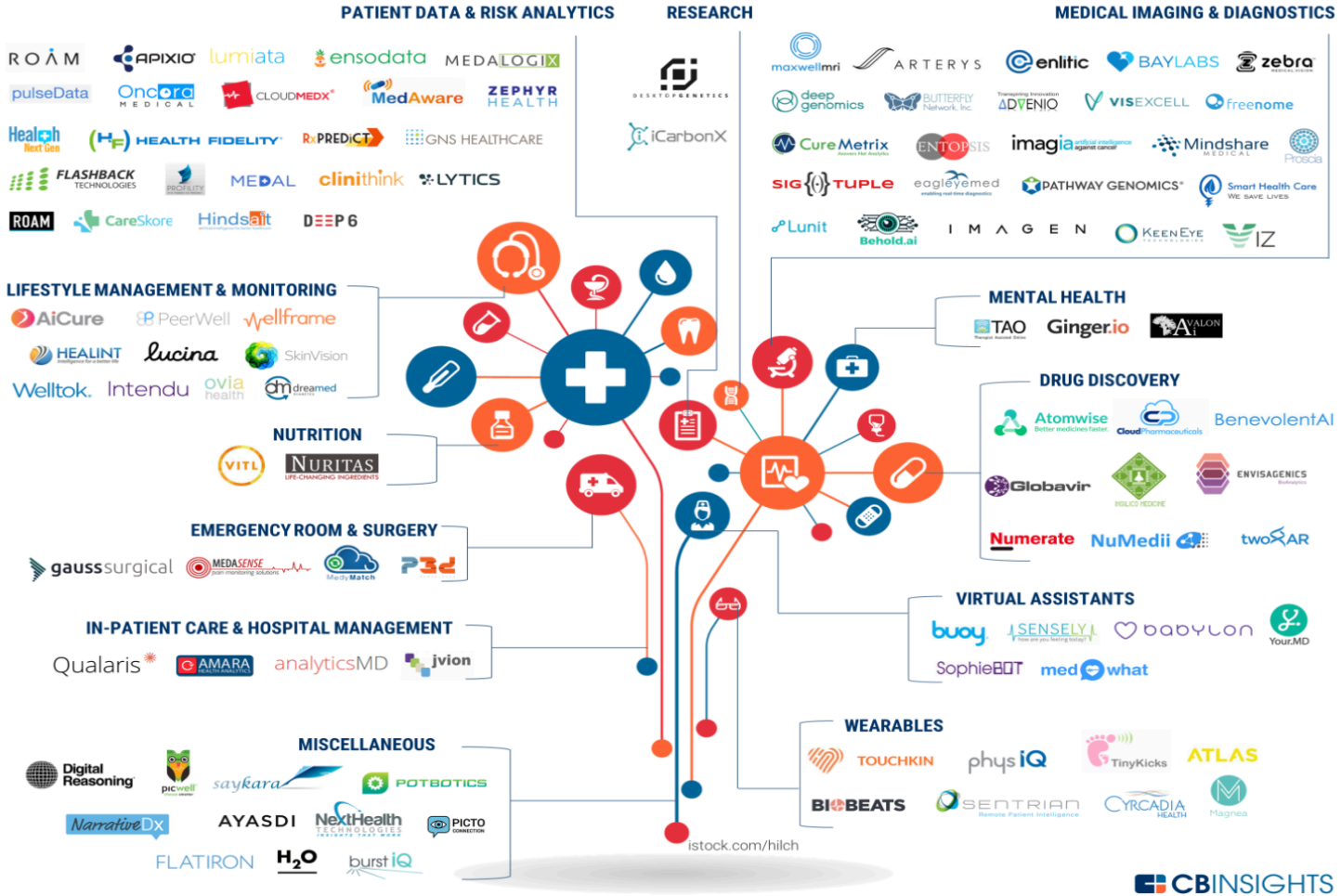
IBM WATSON

DEEP LEARNING REVOLUTION

DEEP LEARNING REVOLUTION IN DRUG DISCOVERY

Source of the original image: nvidia.com

106 STARTUPS TRANSFORMING HEALTHCARE WITH AI



CBINSIGHTS

THE WALL STREET JOURNAL.

HEALTH | JOURNAL REPORTS: HEALTH CARE

How AI Is Transforming Drug Creation

Pharmaceutical companies hope computers can help them find new medications that are faster, cheaper—and more likely to be effective

by Daniela Hernandez

Forbes

Contributor

Robin Seaton Jefferson

FULL BIO

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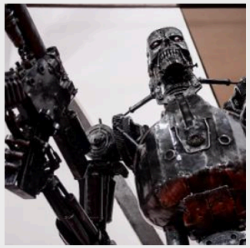
New Post *5 hours ago* **297** views



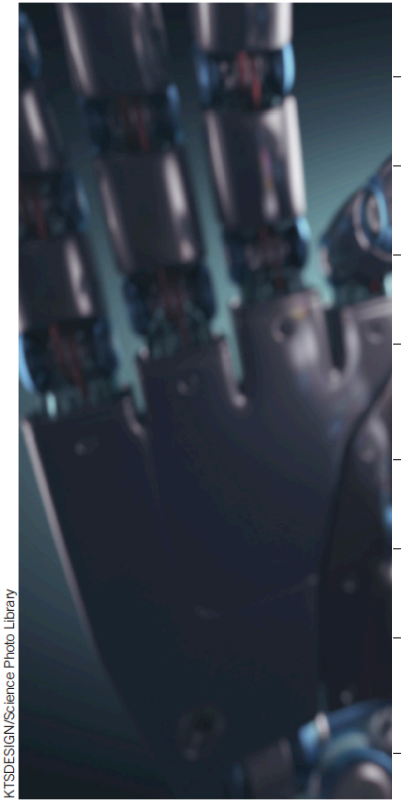
Company Seeks to Combat Aging And Disease With AI And Deep Learning

It's what movies were made of nearly four decades ago. Today, Artificial Intelligence and deep learning could very well change the world through drug discovery and the eradication of disease. And one Baltimore-based company is betting on it.

AI-powered drug discovery captures pharma interest

A drug-hunting deal inked last month, between Numerate, of San Bruno, California, and Takeda Pharmaceutical to use Numerate's artificial intelligence (AI) suite to discover small-molecule therapies for oncology, gastroenterology and central nervous system disorders, is the latest in a growing number of research alliances involving AI-powered computational drug development firms. Also last month, GNS Healthcare of Cambridge, Massachusetts announced a deal with Roche subsidiary Genentech of South San Francisco, California to use GNS's AI platform to better understand what affects the efficacy of known therapies in oncology. In May, Exscientia of Dundee, Scotland, signed a deal with Paris-based Sanofi that includes up to €250 ($280) million in milestone payments. Exscientia will provide the compound design and Sanofi the chemical synthesis of new drugs for diabetes and cardiovascular disease. The trend indicates that the pharma industry's long-running skepticism about AI is softening into genuine interest, driven by AI's promise to address the industry's principal pain point: clinical failure rates.

The industry's willingness to consider AI approaches reflects the reality that drug discovery is laborious, time consuming and not particularly effective. A two-decade-long downward trend in clinical success rates has only recently



KTSDESIGN/Science Photo Library

Deep learning is starting to gain acolytes in the

Table 1 Selected collaborations in the AI-drug discovery space

AI company/ location	Technology	Announced partner/ location	Indication(s)	Deal date
Atomwise	Deep-learning screening from molecular structure data	Merck	Malaria	2015
BenevolentAI	Deep-learning and natural language processing of research literature	Janssen Pharmaceutica (Johnson & Johnson), Beerse, Belgium	Multiple	November 8, 2016
Berg, Framingham, Massachusetts	Deep-learning screening of biomarkers from patient data	None	Multiple	N/A
Exscientia	Bispecific compounds via Bayesian models of ligand activity from drug discovery data	Sanofi	Metabolic diseases	May 9, 2017
GNS Healthcare	Bayesian probabilistic inference for investigating efficacy	Genentech	Oncology	June 19, 2017
Insilico Medicine	Deep-learning screening from drug and disease databases	None	Age-related diseases	N/A
Numerate	Deep learning from phenotypic data	Takeda	Oncology, gastroenterology and central nervous system disorders	June 12, 2017
Recursion, Salt Lake City, Utah	Cellular phenotyping via image analysis	Sanofi	Rare genetic diseases	April 25, 2016
twoXAR, Palo Alto, California	Deep-learning screening from literature and assay data	Santen Pharmaceuticals, Osaka, Japan	Glaucoma	February 23, 2017

E. SMALEY, NATURE BIOTECHNOLOGY

NEW BUSINESS MODELS EMERGE AS PHARMA STARTS TESTING THE DEEP LEANING WATERS

GEN News Highlights

More »

May 9, 2017

Sanofi, Exscientia Ink Up to €250M Deal for Bispecific Drugs Against Metabolic Diseases

Sanofi and Exscientia signed a potentially €250 million (approximately $273 million) collaboration and license option deal to discover bispecific small-molecule drugs against metabolic diseases. Scotland-based Exscientia will use its artificial intelligence (AI)-driven platform and automated design capabilities to identify combinations of synergistic drug targets, and then apply its lead-finding platform to identify bispecific small molecules against those targets.

Source: Genetic Engineering & Biotechnology News

FierceBiotech

BIOTECH RESEARCH IT CRO MEDTECH

MedTech

GlaxoSmithKline taps Baltimore's Insilico for AI-based drug discovery

by *Amirah Al Idrus* | Aug 16, 2017 10:06am

GEN News Highlights

More »

June 12, 2017

Numerate to Use AI Platform in Developing Drugs for Takeda

Computational drug design company Numerate said today it will use its artificial intelligence (AI) platform to identify and deliver multiple clinical candidates for Takeda Pharmaceutical Company, through a collaboration whose value was not disclosed.

GEN News Highlights

More »

July 5, 2017

GSK Launches Up-to-$43M AI-Focused Collaboration with Exscientia

GlaxoSmithKline (GSK) will use the artificial intelligence (AI)-enabled platform of Exscientia to develop new drugs, through a collaboration that could generate up to £33 million (about $43 million) in milestone payments for the British AI-focused drug discovery and design company.

NEW AI-POWERED LONGEVITY-FOCUSED PHARMA EMERGES

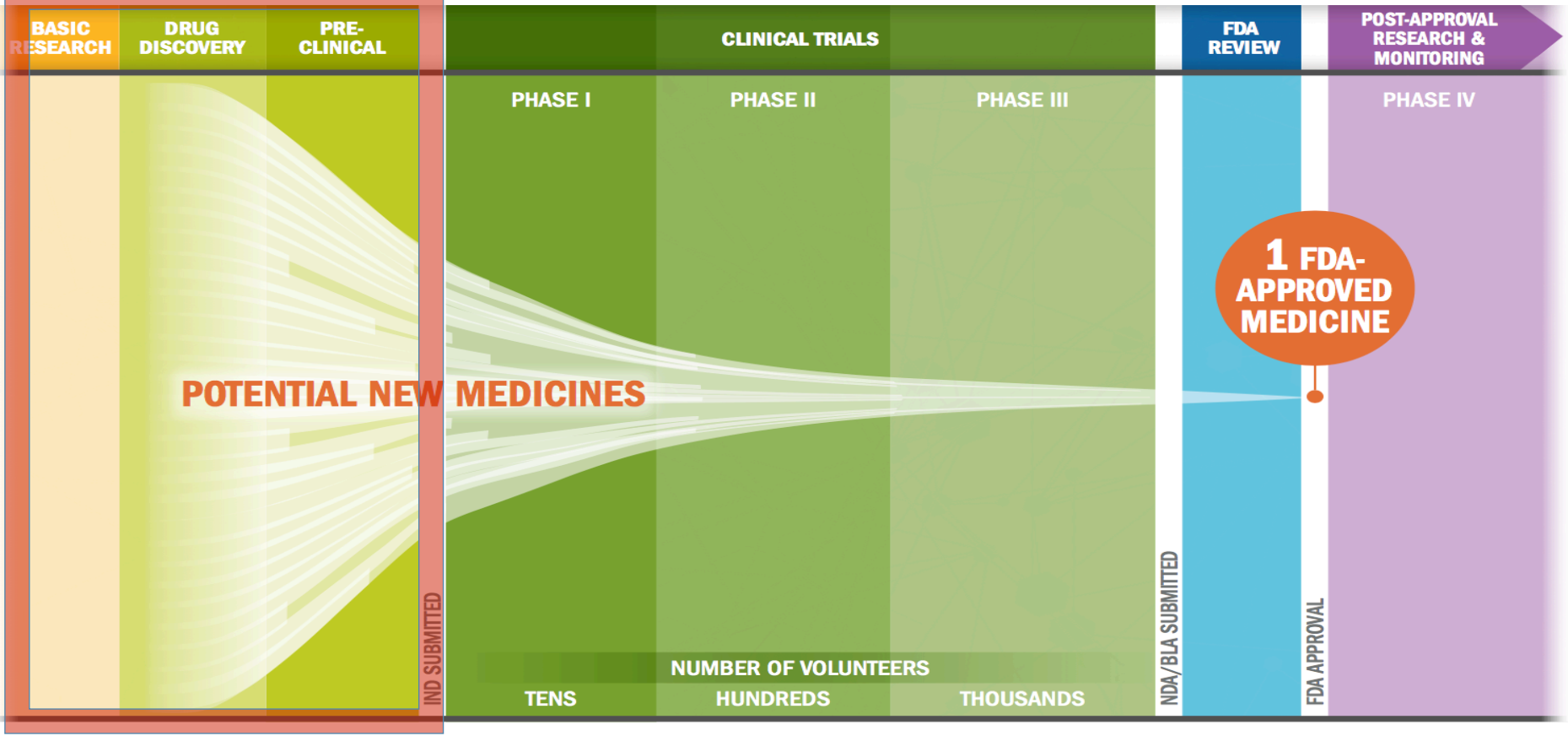
JUVENESCENCE
THE BOOK & THE COMPANY

Gregory Bailey, MD
MediqVentures

Jim Mellon
British "Warren Buffet"

Declan Doogan, MD
developed Zoloft, Lipitor and Viagra

THE BIOPHARMACEUTICAL RESEARCH AND DEVELOPMENT PROCESS



Key: IND: Investigational New Drug Application, NDA: New Drug Application, BLA: Biologics License Application

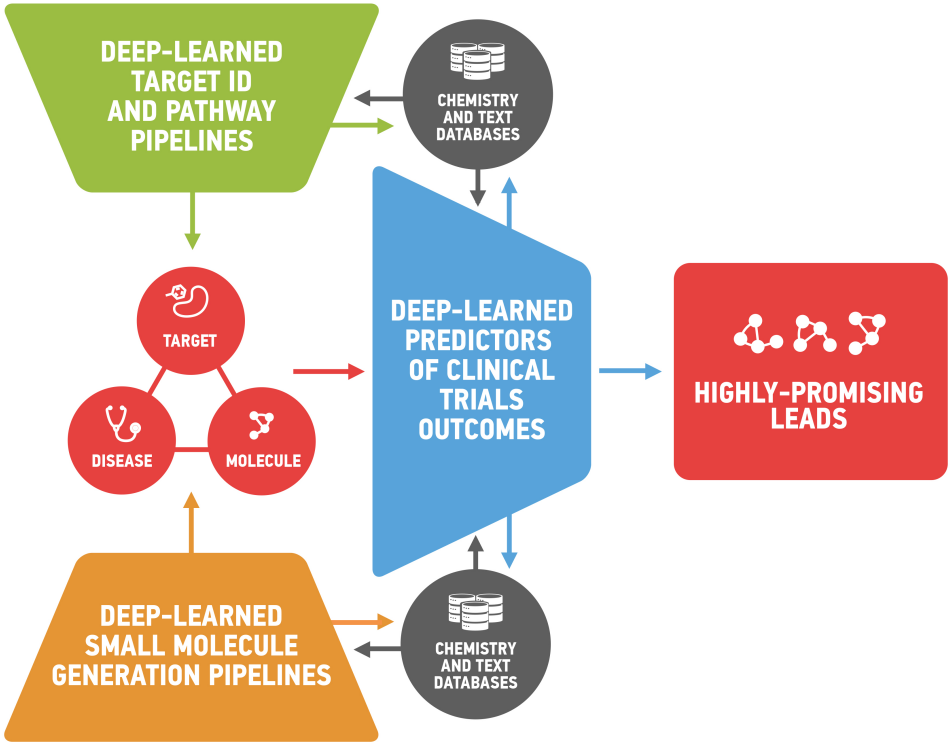
Source: Biopharmaceutical Research & Development, PRMA http://phrma-docs.phrma.org/sites/default/files/pdf/rd_brochure_022307.pdf

STRATEGIES FOR AI-POWERED DRUG DISCOVERY

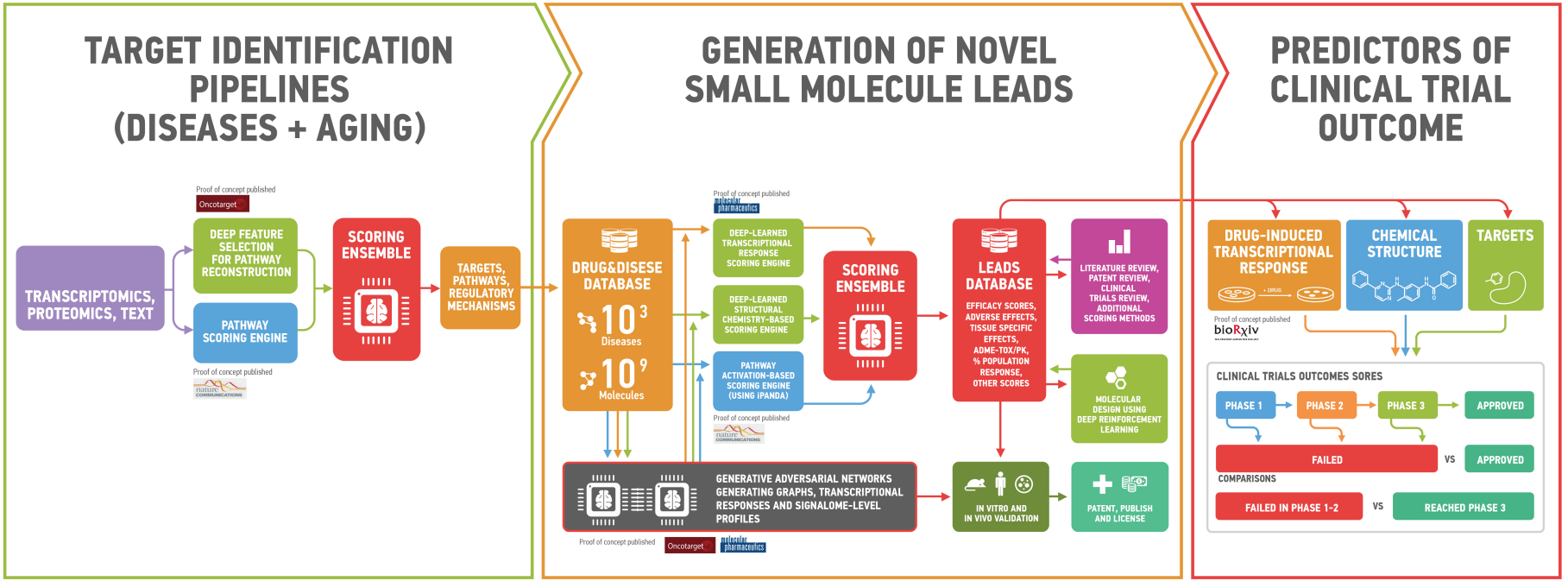
LOOKING FOR A NEEDLE IN A HAYSTACK

GENERATE PERFECT NEEDLES

INTEGRATED TOP-DOWN AND BOTTOM-UP TARGET ID AND DRUG DISCOVERY PIPELINES



THE MOST COMPREHENSIVE END-TO-END DRUG DISCOVERY PIPELINE IN THE INDUSTRY UTILIZING NEXT-GENERATION ARTIFICIAL INTELLIGENCE



GENERATIVE ADVERSARIAL NETWORKS (GANs)

Computer Science > Neural and Evolutionary Computing

Generative Adversarial Text to Image Synthesis

Scott Reed, Zeynep Akata, Xinchen Yan, Lajanugen Logeswaran, Bernt Schiele, Honglak Lee

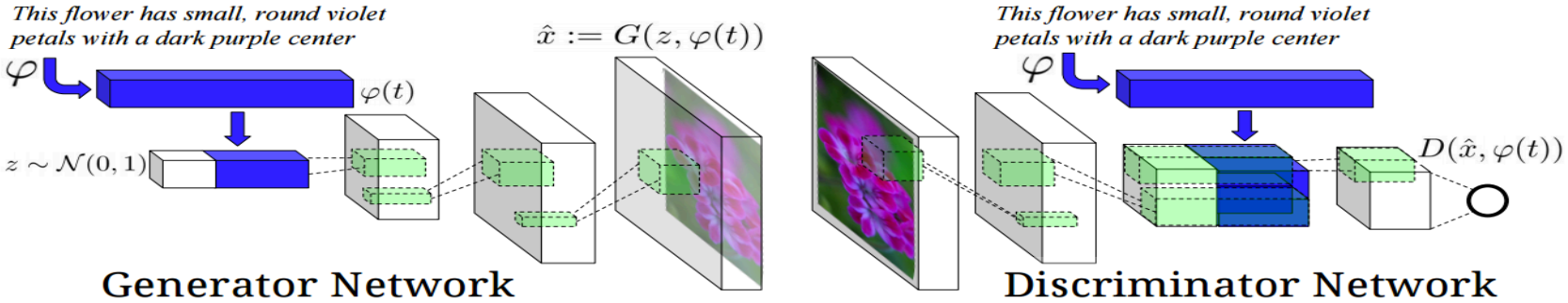
(Submitted on 17 May 2016 (v1), last revised 5 Jun 2016 (this version, v2))

Automatic synthesis of realistic images from text would be interesting and useful, but current AI systems are still far from this goal. However, in recent years generic and powerful recurrent neural network architectures have been developed to learn discriminative text feature representations. Meanwhile, deep convolutional generative adversarial networks (GANs) have begun to generate highly compelling images of specific categories, such as faces, album covers, and room interiors. In this work, we develop a novel deep architecture and GAN formulation to effectively bridge these advances in text and image model- ing, translating visual concepts from characters to pixels. We demonstrate the capability of our model to generate plausible images of birds and flowers from detailed text descriptions.

Comments: ICML 2016
Subjects: **Neural and Evolutionary Computing (cs.NE)**; Computer Vision and Pattern Recognition (cs.CV)
Cite as: **arXiv:1605.05396 [cs.NE]**
(or **arXiv:1605.05396v2 [cs.NE]** for this version)

Submission history

From: Scott Reed [view email]
[v1] Tue, 17 May 2016 23:09:15 GMT (2146kb,D)
[v2] Sun, 5 Jun 2016 13:39:27 GMT (2147kb,D)



this small bird has a pink breast and crown, and black primaries and secondaries.

this magnificent fellow is almost all black with a red crest, and white cheek patch.

the flower has petals that are bright pinkish purple with white stigma

this white and yellow flower have thin white petals and a round yellow stamen

Figure 1. Examples of generated images from text descriptions. Left: captions are from zero-shot (held out) categories, unseen text. Right: captions are from the training set.

Reed et al, ICML 2016

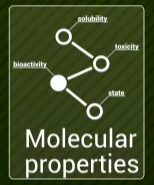
Zhang et al, StackGAN: Text to Photo-realistic Image Synthesis with Stacked Generative Adversarial Networks

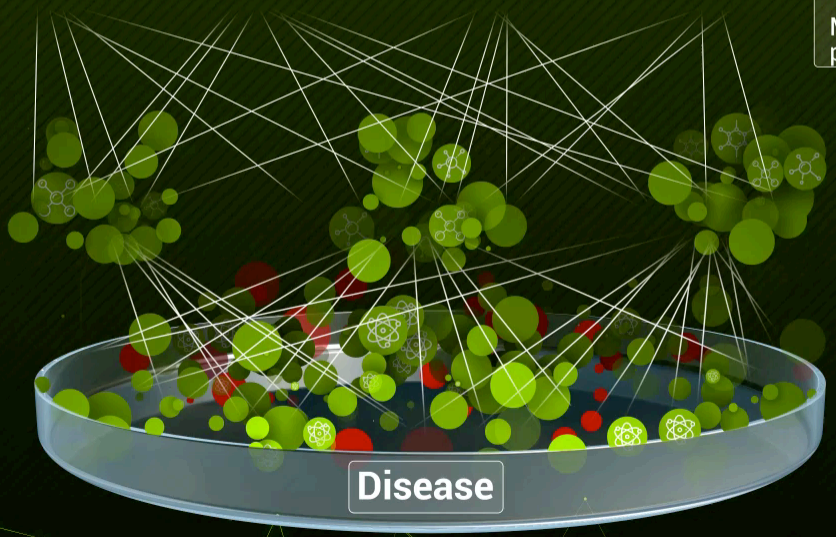
arXiv:1612.03242v1 [cs.CV] 10 Dec 2016

Drug Database

Drug candidates

discriminator





Generative Adversarial Networks

INSILICO MEDICINE

GAN/RL-BASED MOLECULAR GENERATORS WERE VALIDATED EXPERIMENTALLY AND ARE BEING FINE-TUNED

RESULTS WILL BE UNVEILED AT THE INTERNATIONAL CONFERENCE ON MACHINE LEARNING, JULY 10-15 2018 (INSILICO IS A GOLD SPONSOR)

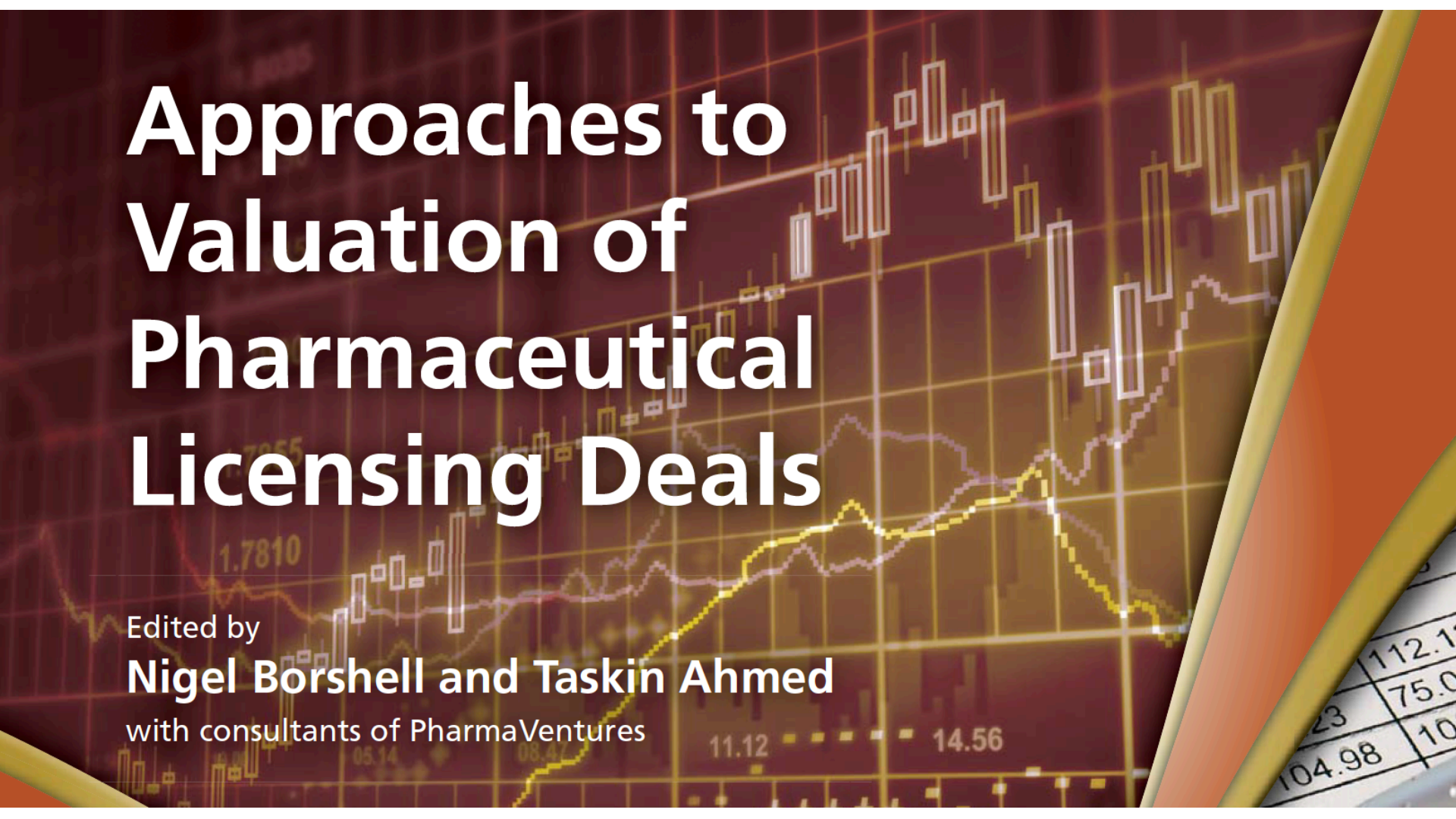
FOLLOW US ON PUBMED: INSILICO+MEDICINE

Type	Title
New 3D Struct. for AAE	3D Molecular Representations Based on the Wave Transform for Convolutional Neural Networks. *ACS Mol. Pharm, 2018*
Pathways for IO (training DNNs)	Bifunctional immune checkpoint-targeted antibody-ligand traps that simultaneously disable TGFβ enhance the efficacy of cancer immunotherapy. *Nature Communications, 2018*
DNNs for Age Prediction	Population specific biomarkers of human aging: a big data study using South Korean, Canadian and Eastern European patient populations. *Journal of Gerontology Section A, 2018*
GANs for Medicinal Chemistry	druGAN: An Advanced Generative Adversarial Autoencoder Model for de Novo Generation of New Molecules with Desired Molecular Properties In Silico. *ACS Molecular Pharmaceutics, 2017*
DNNs for Side Effects	Towards natural mimetics of metformin and rapamycin. *Aging, 2017*
DNNs for Target ID	Use of deep neural network ensembles to identify embryonic-fetal transition markers: repression of COX7A1 in embryonic and cancer cells, *Oncotarget, 2017*
DNNs and Blockchain for Data Exchange	Converging blockchain and next-generation artificial intelligence technologies to decentralize and accelerate biomedical research and healthcare. *Oncotarget, 2018*
GANs for Medicinal Chemistry	The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology. *Oncotarget, 2016*
Dimensionality Reduction Algorithm	In silico Pathway Activation Network Decomposition Analysis (iPANDA) as a method for biomarker development. *Nature Communications, 2016*
DNNs for Classification of Molecules	Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data. *ACS Molecular Pharmaceutics, 2016*
DNNs for Age Prediction	Deep biomarkers of human aging: Application of deep neural networks to biomarker development. *Aging, 2016*
Review	Applications of Deep Learning in Biomedicine. *ACS Molecular Pharmaceutics, 2016*

BUSINESS MODEL:

DISCOVER NEW MOLECULES USING AI, PRE-VALIDATE THE MOLECULES, LICENSE TO BIG PHARMACEUTICAL COMPANIES FOR DEVELOPMENT

Approaches to Valuation of Pharmaceutical Licensing Deals



Edited by
Nigel Borshell and Taskin Ahmed
with consultants of PharmaVentures

VALUATION OF A PRE-CLINICAL ASSET

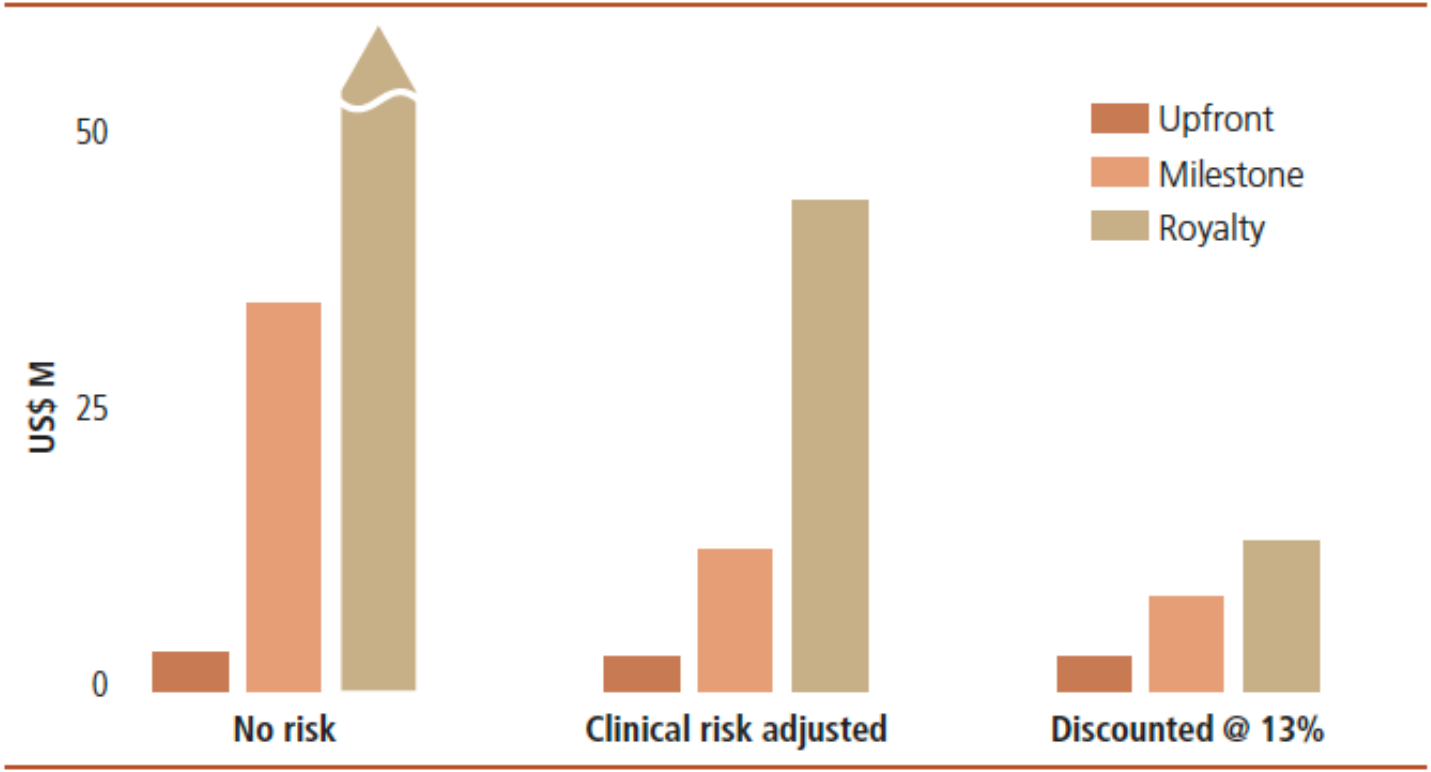


Figure 15 – The effect of time and risk on the value of deal components.

INSILICO PIPELINE

Approximate numbers as of December 2017 with new molecules generated every week

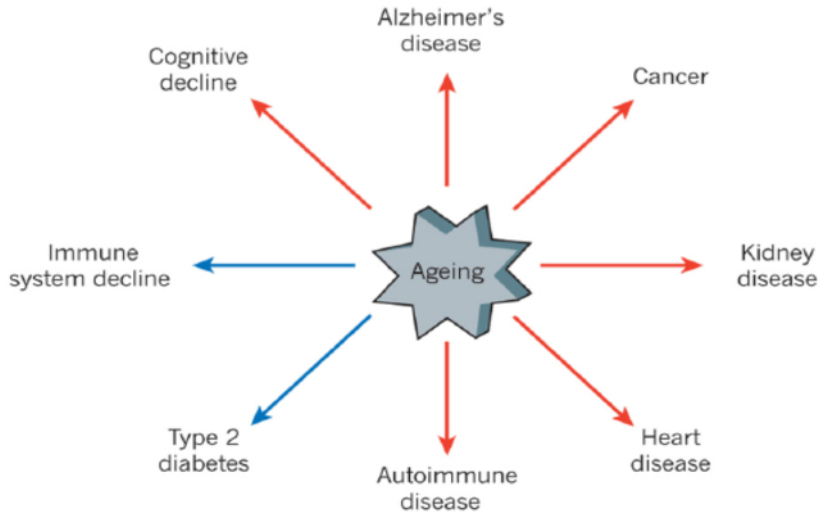
	Generated, profiled, scored	Target known, validation with simulations	Internal in vitro validation	In various stages of validation with Juvenescence.AI, biotech, pharma, academic collaborators and NGOs
Oncology	30 000	1221	52	24
Musculoskeletal disorders	5345	186	31	
Metabolic diseases	1708	201	8	
Fibrosis/Senofibrosis	975	78	25	12
Senescence	130	55	8	8
Neurodegenerative disorders	1601	305	55	7
Dermatological conditions	13334	774	115	8

FINANCING PLANS

CURRENTLY THERE ARE OVER 2,000 PROMISING PRE-CLINICAL LEADS IN THE PIPELINE (AVG. LICENSING DEAL IS $38 MIL)

PLANNING TO INITIATE THE FUNDING ROUND B IN APRIL-MAY 2018

5th ANNUAL AGING RESEARCH FOR DRUG DISCOVERY FORUM
2nd AI & BLOCKCHAIN FOR HEALTHCARE
AT EMBO/BASEL LIFE



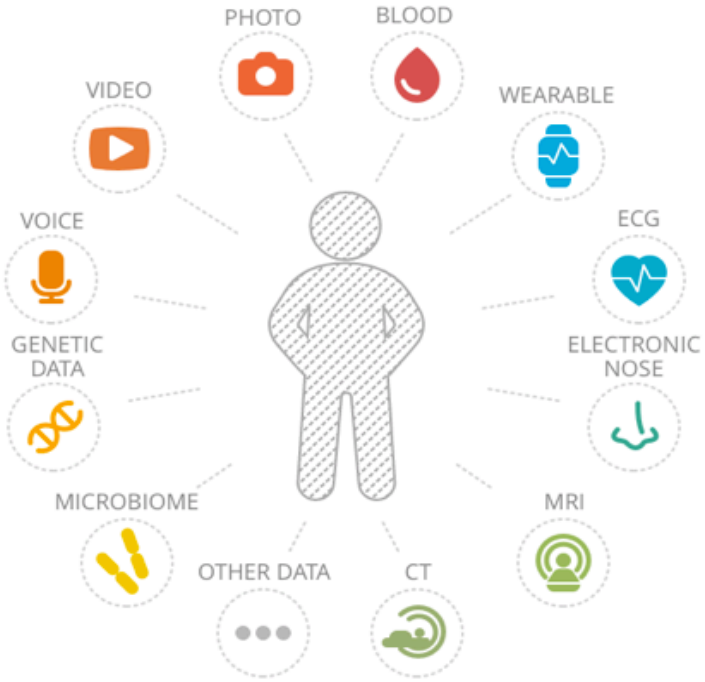
Source: Nature 493,17 January 2013

Basel, Switzerland

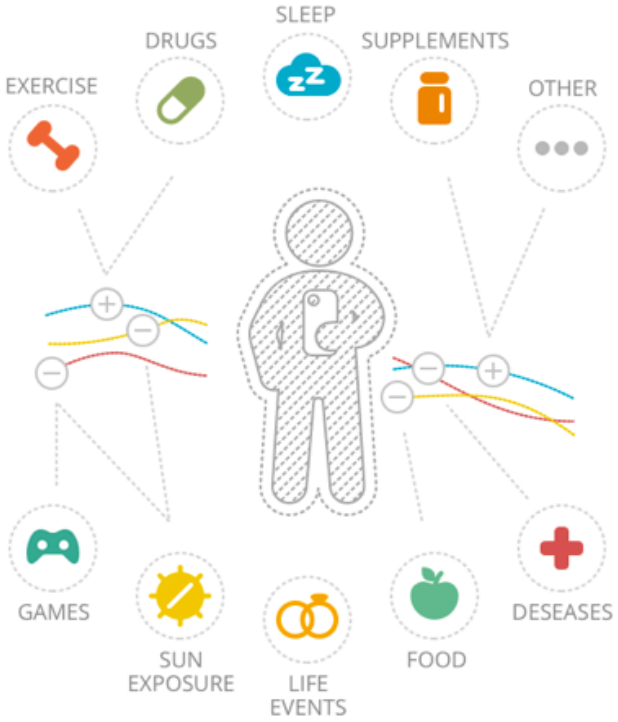
Basel Congress Center, Sept 11-14

www.BaselLife.Org

MEET US AT “THE LAB”
AT MASTER INVESTOR SHOW
FOR A DEMO OF YOUNG.AI AND LONGENESIS



Track your age at every level!



See what makes you younger or older!

alex19
38 years
Weight: 82 lb. Height: 182 in

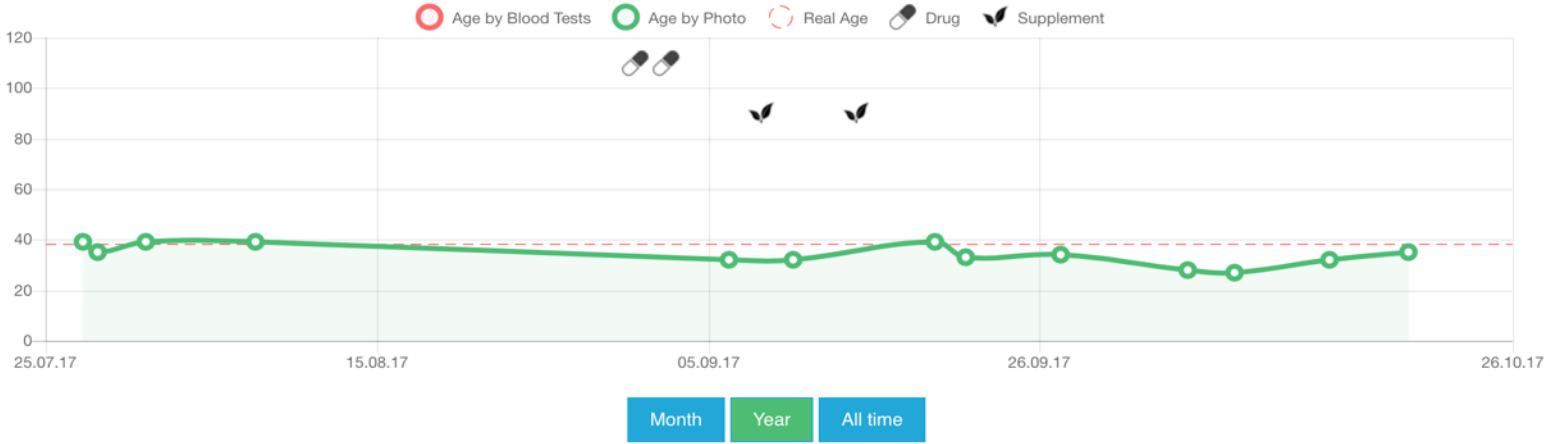
DASHBOARD
Dashboard
Blood Tests
Photo
Additional Tests
Advanced Blood Tests
Basic Urine Test
Transcriptome (blood)
Tissue Transcriptomes
Picture of the Hand
Picture of the Eye
Full Body Picture

Young.AI beta 1.0

Welcome to Young.AI biological age tracker.

Add blood test Add Photo

Track your age, daily activity



Glucose
Please, enter more data

RBC - red blood cells (Erythrocytes)
Please, enter more data

Cholesterol
Please, enter more data

Creatinine
Please, enter more data

alex19
38 years
Weight: 82 lb. Height: 182 in

DASHBOARD
Dashboard
Blood Tests
Photo
Additional Tests
Advanced Blood Tests
Basic Urine Test
Transcriptome (blood)
Tissue Transcriptomes
Picture of the Hand
Picture of the Eye
Full Body Picture

Photos

35 years
2017-10-20

32 years
2017-10-15

27 years
2017-10-09

28 years
2017-10-06

32 years
2017-09-28

36 years
2017-09-28

34 years
2017-09-22

32 years
2017-09-22

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Top 100 AI Companies 2018

ALEX ZHAVORONKOV, PHD
alex@insilico.com

www.insilico.com

@biogerontology