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*Galapagos*  
Mechelen, Belgium

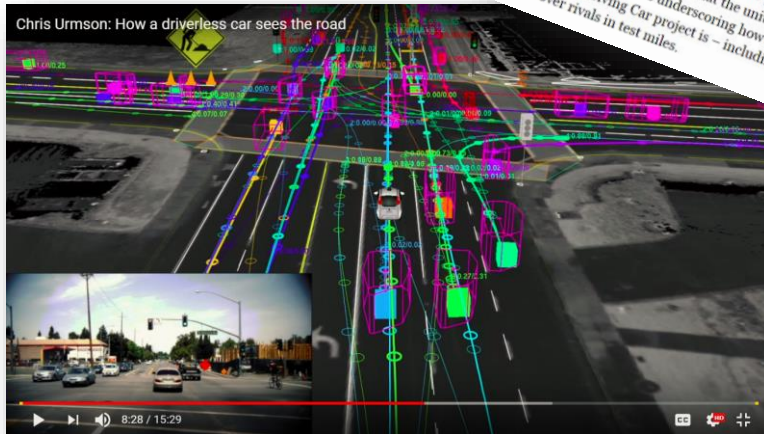
*"We always overestimate the change that will occur in the next two years and underestimate the change that will occur in the next 10."*

**- BILL GATES**





# Artificial Intelligence is disrupting society (?)



Sometime this year Waymo, Alphabet Inc.'s prized driverless car bet, starts a first of its kind revenue-generating robo-taxi service in Phoenix. Ahead of that the unit is maintaining a steady cadence of news underscoring how mature the former Google Self-Driving Car project is - including how big a lead it has over rivals in test miles.



ARTICLE

Mastering the game of Go with deep neural networks and tree search



AlphaGo's 4-1 victory in Seoul, South Korea, in March 2016 was watched by over 200 million people worldwide. It was a landmark achievement that experts agreed was a **decade ahead of its time**, and earned AlphaGo a 9 dan professional ranking (the highest certification) - the first time a computer Go player had ever received the accolade.

During the games, AlphaGo played a handful of **highly inventive winning moves**, several of which - including move 37 in game two - were **so surprising they overturned hundreds of years of received wisdom**, and have since been examined extensively by players of all levels. In the

# Artificial Intelligence is disrupting society (?)

## 2004 Grand Challenge [\[ edit \]](#)

*Main article: [DARPA Grand Challenge \(2004\)](#)*

The first competition of the DARPA Grand Challenge was held on March 13, 2004 in the [Mojave Desert](#) region of the United States, along a 150-mile (240 km) route that follows along the path of [Interstate 15](#) from just before [Barstow, California](#) to just past the [California–Nevada](#) border in [Primm](#). **None of the robot vehicles finished** the route. [Carnegie Mellon University](#)'s Red Team and car Sandstorm (a converted Humvee) traveled the farthest distance, completing 11.78 km (7.32 mi) of the course before getting hung up on a rock after making a switchback turn. No winner was declared, and the cash prize was not given. Therefore, a second DARPA Grand Challenge event was scheduled for 2005.

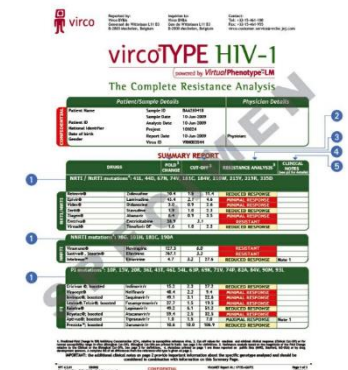
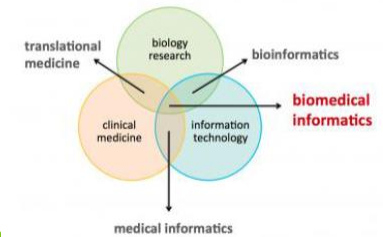
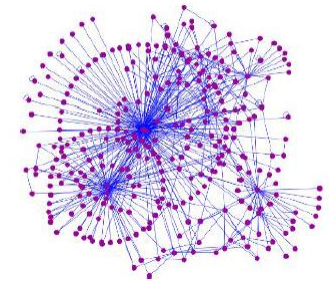


# Overview

- AI introduction
- About me
- Three perspectives
  - Patient
  - Clinic/healthcare
  - Pharmaceutical industry
- Thoughts and discussion

## About me

- Civil engineer in physics (MSc) @UGent
- Master in Artificial Intelligence
- MBA
- Bioinformatics researcher @Tibotec  
modeling HIV drug resistance (genotype/phenotype)  
patent, *Virtual*Phenotype platform
- PhD bioinformatics @KULeuven  
systems biology; gene regulatory network inference
- Research coordinator biomedical informatics @University Hospital Antwerp
- Professor @University of Antwerp
- Co-founder of **biomina**
- Data Sciences @Janssen Pharmaceuticals
- **Head of Bioinformatics** @Galapagos
- Maker (3d printing, Arduino, Raspberry Pi, ...), art/sculpting, photography, travel, reading, and much more





**patients**



## Three perspectives: patients

# Deep learning algorithm does as well as dermatologists in identifying skin cancer

*In hopes of creating better access to medical care, Stanford researchers have trained an algorithm to diagnose skin cancer.*

Every year there are about 5.4 million new cases of skin cancer in the United States, and while the five-year survival rate for melanoma detected in its earliest states is around 97 percent, that drops to approximately 14 percent if it's detected in its latest stages. Early detection could likely have an enormous impact on skin cancer outcomes.



# Three perspectives: patients

## ■ Fabry's disease

- Rare disease
- Difficult to understand, often misdiagnosed
- Genetic, enzyme buildup
- pain, kidney, heart, skin, fatigue, neuropathy, tinnitus, vertigo, diarrhea, eye deviations, ...
- Extreme pain – organ failure – multiple organ failure
- 10-15 years to diagnose
- Treatment stops progression  
(200,000 dollar / year)

**clinic/healthcare**

# Three perspectives: clinic/healthcare

## ■ Top 10 health AI domains



Robot-Assisted  
Surgery\*\*

**\$40B**



Connected  
Machines

**\$14B**



Virtual Nursing  
Assistants

**\$20B**



Clinical Trial  
Participant  
Identifier

**\$13B**



Administrative  
Workflow  
Assistance

**\$18B**



Preliminary  
Diagnosis

**\$5B**



Fraud  
Detection

**\$17B**



Automated  
Image  
Diagnosis

**\$3B**



Dosage Error  
Reduction

**\$16B**



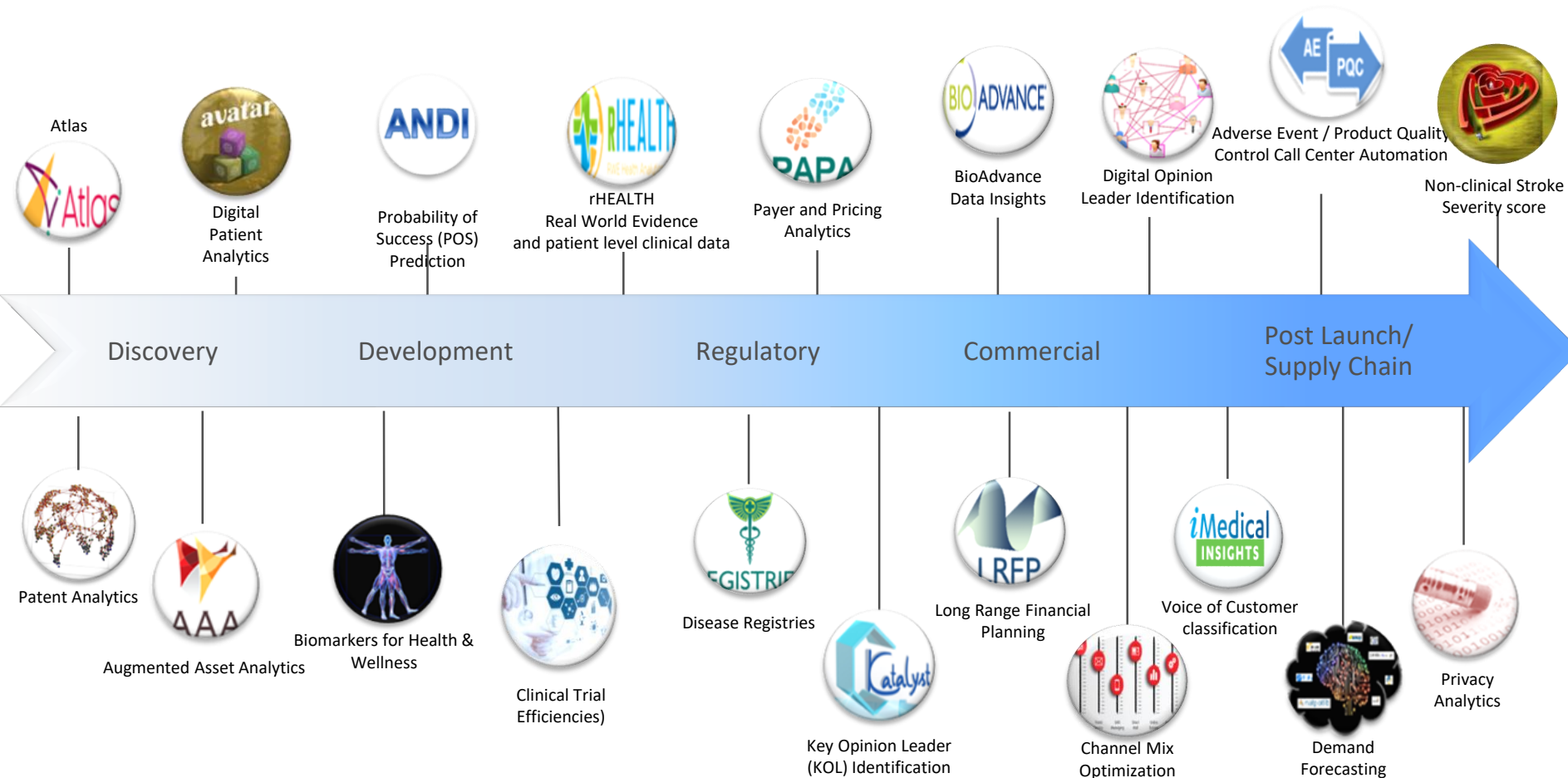
Cybersecurity

**\$2B**

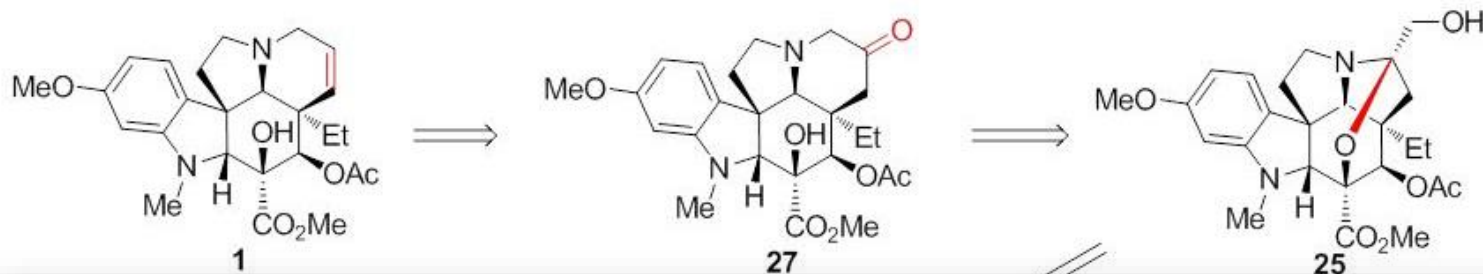
**pharmaceutical industry**



# Three perspectives: pharmaceutical industry



# Three perspectives: pharmaceutical industry



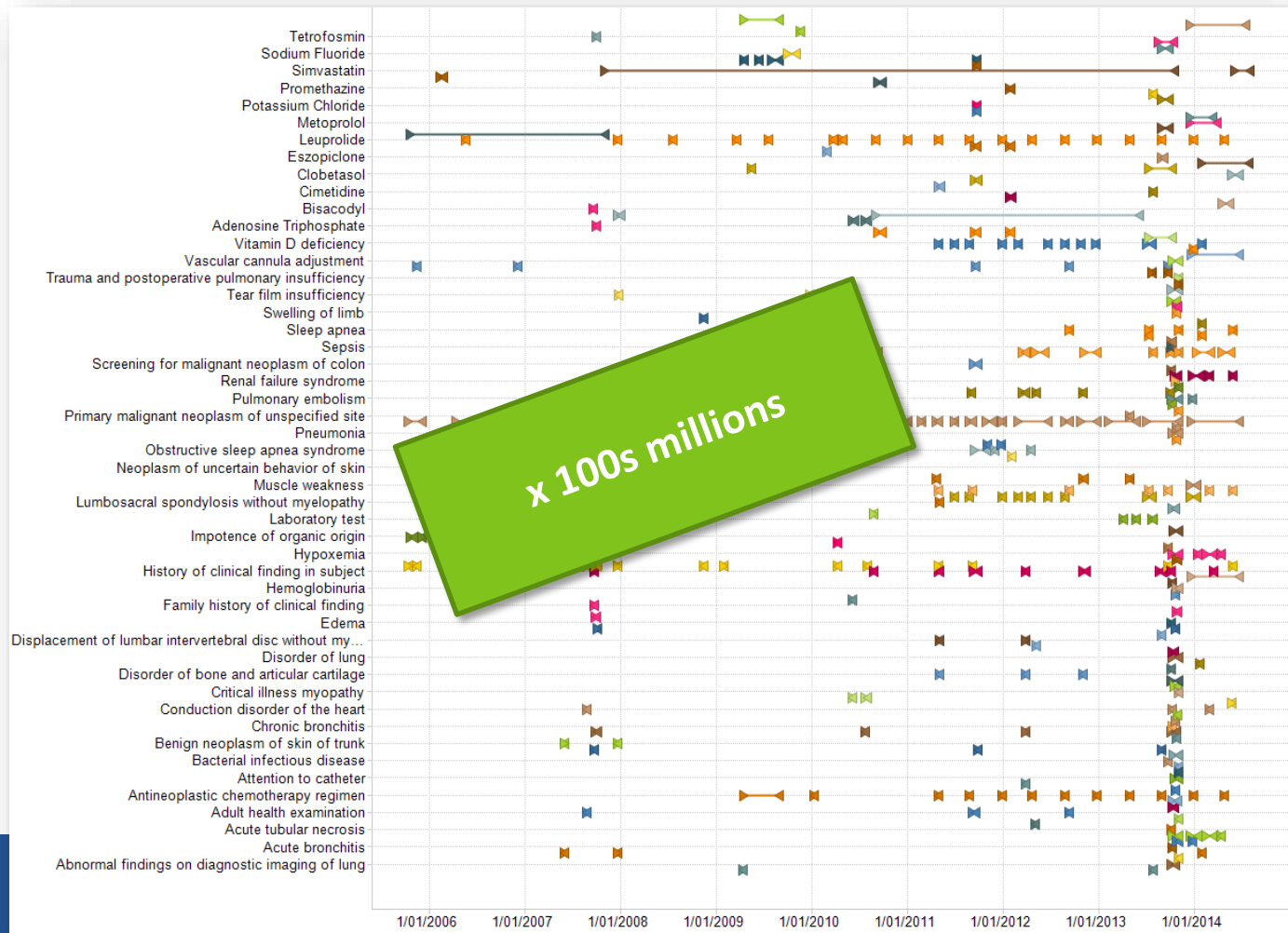
## Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler<sup>1,2</sup>, Mike Preuss<sup>3</sup> & Mark P. Waller<sup>4</sup>

To plan the syntheses of small organic molecules, chemists use retrosynthesis, a problem-solving technique in which target molecules are recursively transformed into increasingly simpler precursors. Computer-aided retrosynthesis would be a valuable tool but at present it is slow and provides results of unsatisfactory quality. Here we use Monte Carlo tree search and symbolic artificial intelligence (AI) to discover retrosynthetic routes. We combined Monte Carlo tree search with an expansion policy network that guides the search, and a filter network to pre-select the most promising retrosynthetic steps. These deep neural networks were trained on essentially all reactions ever published in organic chemistry. Our system solves for almost twice as many molecules, thirty times faster than the traditional computer-aided search method, which is based on extracted rules and hand-designed heuristics. In a double-blind AB test, chemists on average considered our computer-generated routes to be equivalent to reported literature routes.

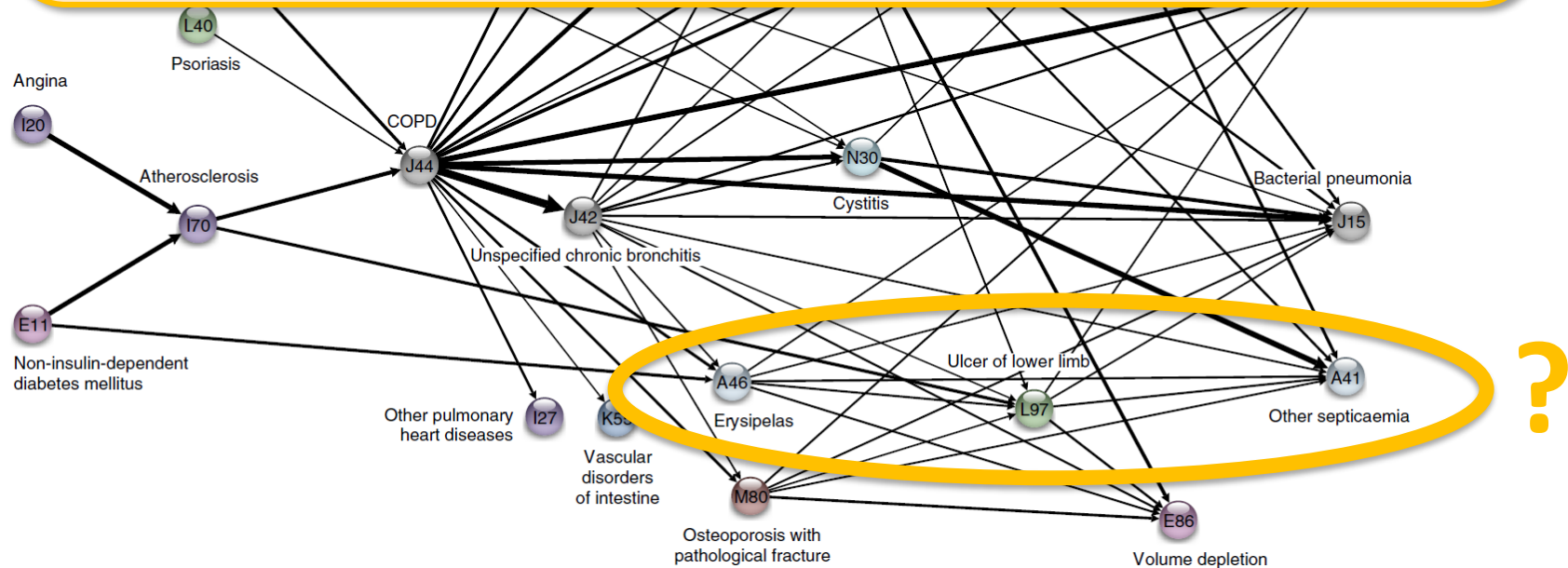
# Three perspectives: pharmaceutical industry

- Rich anonymized patient data available
  - Secondary use of reimbursement codes  
drug regimen(s), medical procedures, diagnostic codes, lab tests, ...



# Three perspectives: pharmaceutical industry

- Gain insights in patient treatment trajectories for:
  - Novel drug development
  - Improve clinical trial design
  - Identify/prevent adverse effects
- Better understand *real-life metrics* like 'Duration of Therapy', 'Compliance'







# Thoughts and discussion

- Integrating health apps in clinical flows
- Patient protection vs. innovation: when is legislation protecting patients? When is legislation preventing better treatment?
- Impact of informed consent on data use
- Machine learning and predictive models
  - Learning on distributed, heterogeneous, unclean, non-harmonized, multi-lingual EHR data?

