

# Creating the Engine of Scientific Discovery

Hiroaki Kitano

# COVID-19 AI and Simulation Project

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## Project Overview

### Research Areas

- RA1 Simulation and visualization of droplet and aerosol diffusion
- RA2 Use of ICT to reduce infection risk
- RA3 SARS-CoV-2 testing standard and technologies
- RA4 Simulation of COVID-19 spread, suppression, and resource optimization
- RA5 BioMedical Countermeasures (diagnosis, biomarker discovery, virus mutation analysis)

## Project Overview

### Overview of the COVID-19 AI and Simulation Project

The spread of COVID-19, which is caused by the SARS-CoV-2 virus infection, continue pose a serious threat to our health and society both domestically and globally; hence, we must remain vigilant in relation to future developments. In the light of this situation, very high priority is being given to policies related to effective infection prevention, restriction of its spread, risk prediction, and swift development of treatment methods. Development and deployment of sophisticated, systematic, and flexible countermeasures at the earliest possible timing is the highest national priority.

The current aim of the project is to deploy a multiple layers of defense lines and supporting measures and a series of platforms to support them, as shown in Figure 1.

## Multiple layers of defense and supporting lines

Reducing high risk contacts

Reducing infection at risky places

Early detection & treatment

Preventing aggravation

Treating patients with sever status

Follow up of recovered patients

## A framework for rapid and preemptive responses

International standard for testing methods and precision

Simulation of spreading, countermeasures, medical resources

Studies on COVID-19 pathology, prevention, and treatment

Studies to prepare future Pandemic

An integrated data platform and real-time monitoring system

# COVID-19 AI and Simulation Project

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# COVID-19 AI and Simulation Project Call for Proposal on Research and Contributing Data



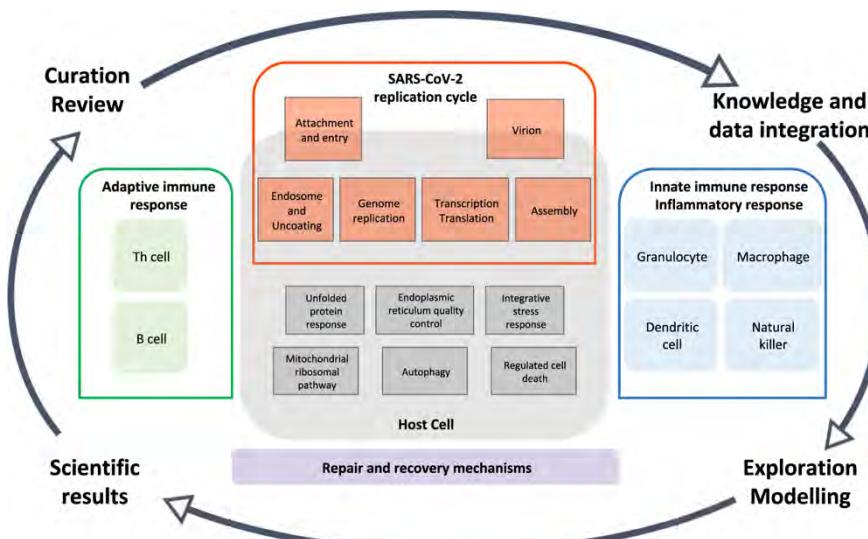
In the Office for Novel Coronavirus Disease Control, Cabinet Secretariat, we are collecting the knowledge and wisdom available in our country, evolving countermeasures, and making a wide appeal for proposals of research topics and data that are effective for COVID-19 counter-measures including simulation, AI, and other technologies, to prevent the spread of infection and enable economic activity.

# COVID-19 Disease Map, building a computational repository of SARS-CoV-2 virus-host interaction mechanisms

Marek Ostaszewski, Alexander Mazein, Marc E. Gillespie, Inna Kuperstein, Anna Niarakis, Henning Hermjakob, Alexander R. Pico, Egon L. Willighagen, Chris T. Evelo, Jan Hasenauer, Falk Schreiber, Andreas Dräger, Emek Demir, Olaf Wolkenhauer, Laura I. Furlong, Emmanuel Barillot, Joaquin Dopazo, Aurelio Ortega-Resendiz, Francesco Messina, Alfonso Valencia, Akira Funahashi, Hiroaki Kitano, Charles Auffray, Rudi Balling & Reinhard Schneider✉

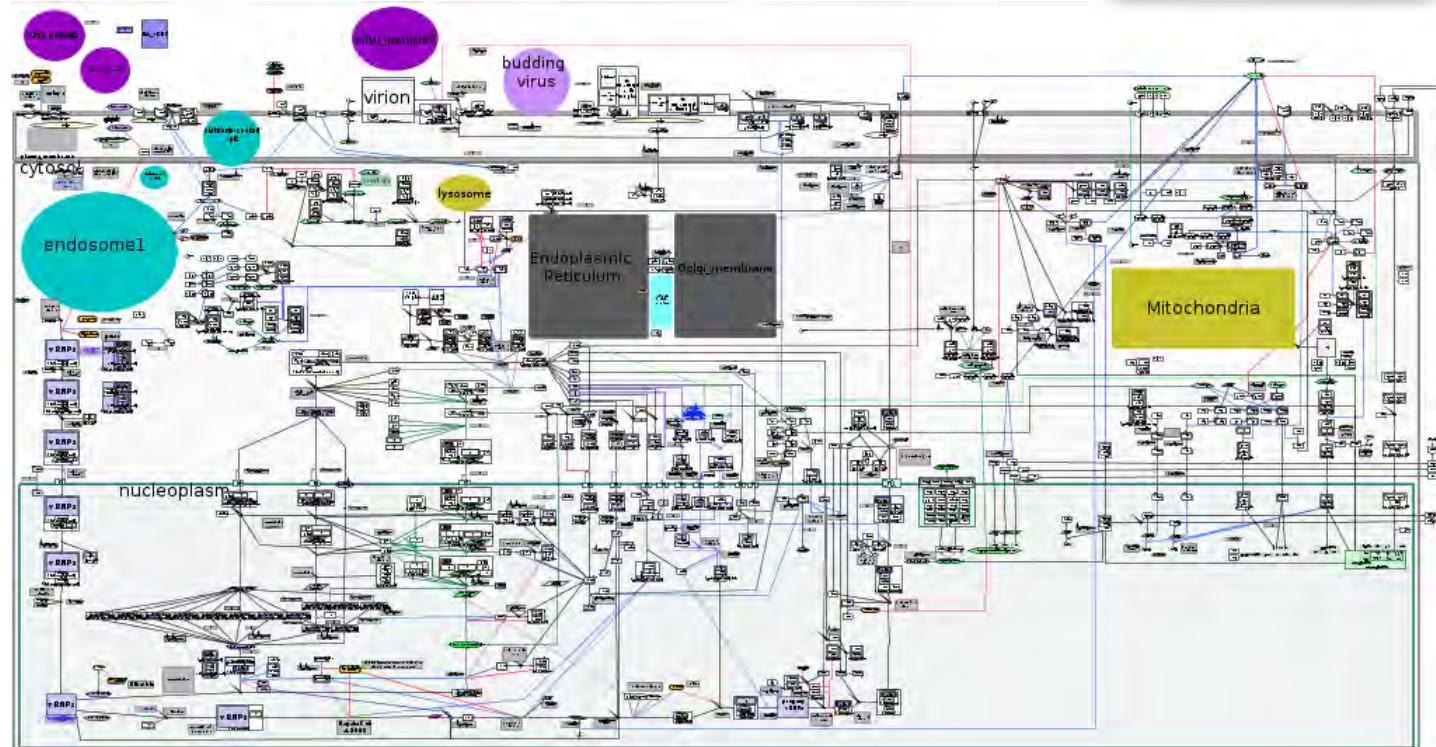
Scientific Data 7, Article number: 136 (2020) | Cite this article

4425 Accesses | 161 Altmetric | Metrics



JST ERATO 北野共生システムプロジェクト並びに、  
JST ERATO河岡宿主応答ネットワークプロジェクト  
の成果を基盤に国際連携が行われている。

ERATO



**SBI** The Systems Biology Institute 5

# Taxila COVID-19 AI/NLP Service (<https://covid19.taxila.io/>)

**TAXILA 2.0.0** CHANNEL GEO TRENDS ANALYSIS ▾

Type your search item here and explore

4098

Welcome to COVID-19 Taxila

You have access to 50645 articles. 886 of them were published in the last week.

\* Click And Drag on the graph to select specified time range

456

Apr 10, 20 May 09, 20

10 Apr, 2020 – 09 May, 2020

1m 3m 6m 1yr All

Tag Type Filter

# LATEST PUBMED ARTICLES

**PubMed.gov**

**Current State of Knowledge About SARS-CoV-2 and COVID-19 Disease in Pregnant Women**

During any epidemic of infectious diseases, pregnant women constitute an extremely sensitive group due to altered physiology and immune functions, and thus altered susceptibility to infection. With regard to the management of pregnant COVID-19 patients, in addition to the treatment of the infection

May 09, 2020

0 Likes 0 Saves

# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

**Optimal control of an SIR epidemic through finite-time non-pharmaceutical intervention**

We consider the problem of controlling an SIR-model epidemic by temporarily reducing the rate of contact within a population. The control takes the form of a multiplicative reduction in the contact rate of infectious individuals. The control is allowed to be applied only over a finite time interval.

May 09, 2020

0 Likes 0 Saves

# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

**Comprehensive Testing Highlights Racial, Ethnic, and Age Disparities in the COVID-19 Outbreak**

The United States (US), which is currently the epicenter for the COVID-19 pandemic, is a country whose demographic composition differs from that of other highly-impacted countries. US-based descriptions of SARS-CoV-2 infections have, for the most part, focused on patient populations with severe disease

May 09, 2020

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# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

**Severe obesity is associated with higher in-hospital mortality in a cohort of patients with COVID-19 in the Bronx, New York**

Background & Aims: New York is the current epicenter of Coronavirus disease 2019 (COVID-19) pandemic. The underrepresented minorities, where the prevalence of obesity is higher, appear to be affected disproportionately. Our objectives were to assess the characteristics and early outcomes of patients

May 09, 2020

0 Likes 0 Saves

# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

**BCG vaccine-induced protection from COVID-19 infection, wishful thinking or a game changer?**

A series of epidemiological explorations have suggested a negative association between national BCG vaccination policy and the prevalence and mortality of COVID-19. Nevertheless, these comparisons are difficult to validate due to broad differences between countries such as socioeconomic status, demog

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# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

**Identification and Analysis of Shared Risk Factors in Sepsis and High Mortality Risk COVID-19 Patients**

BACKGROUND Coronavirus disease 2019 (COVID-19) is a novel coronavirus strain disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). The disease is highly transmissible and severe disease including viral sepsis has been reported in up to 16% of hospitalized cases. The admissio

May 09, 2020

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# BIORXIV AND MEDRXIV

**medRxiv** THE PREPRINT SERVER FOR HEALTH SCIENCES

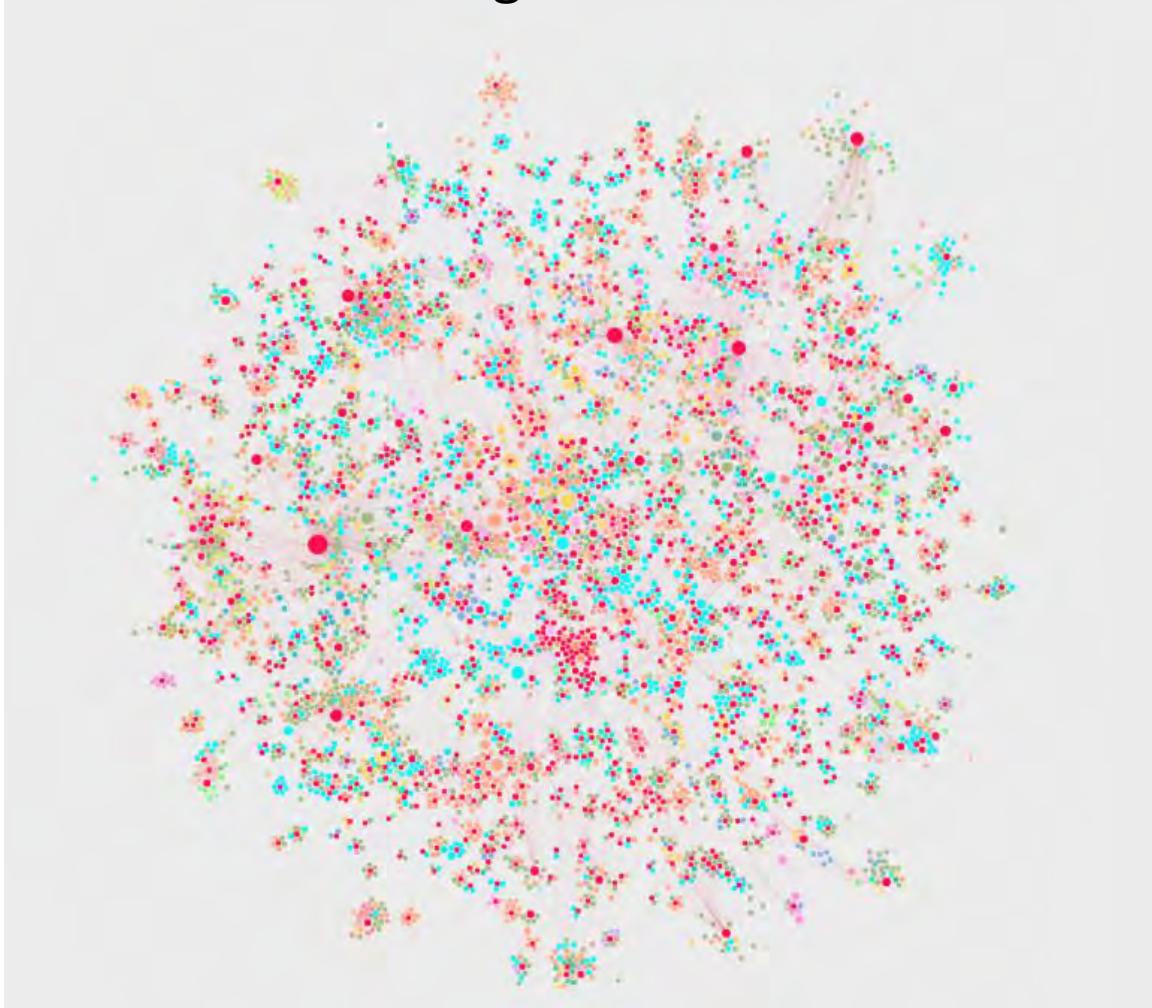
**Containing Covid-19 outbreaks with spatially targeted short-term lockdowns and mass-testing**

We assess the efficacy of spatially targeted lockdown or mass-testing and case-isolation in individual

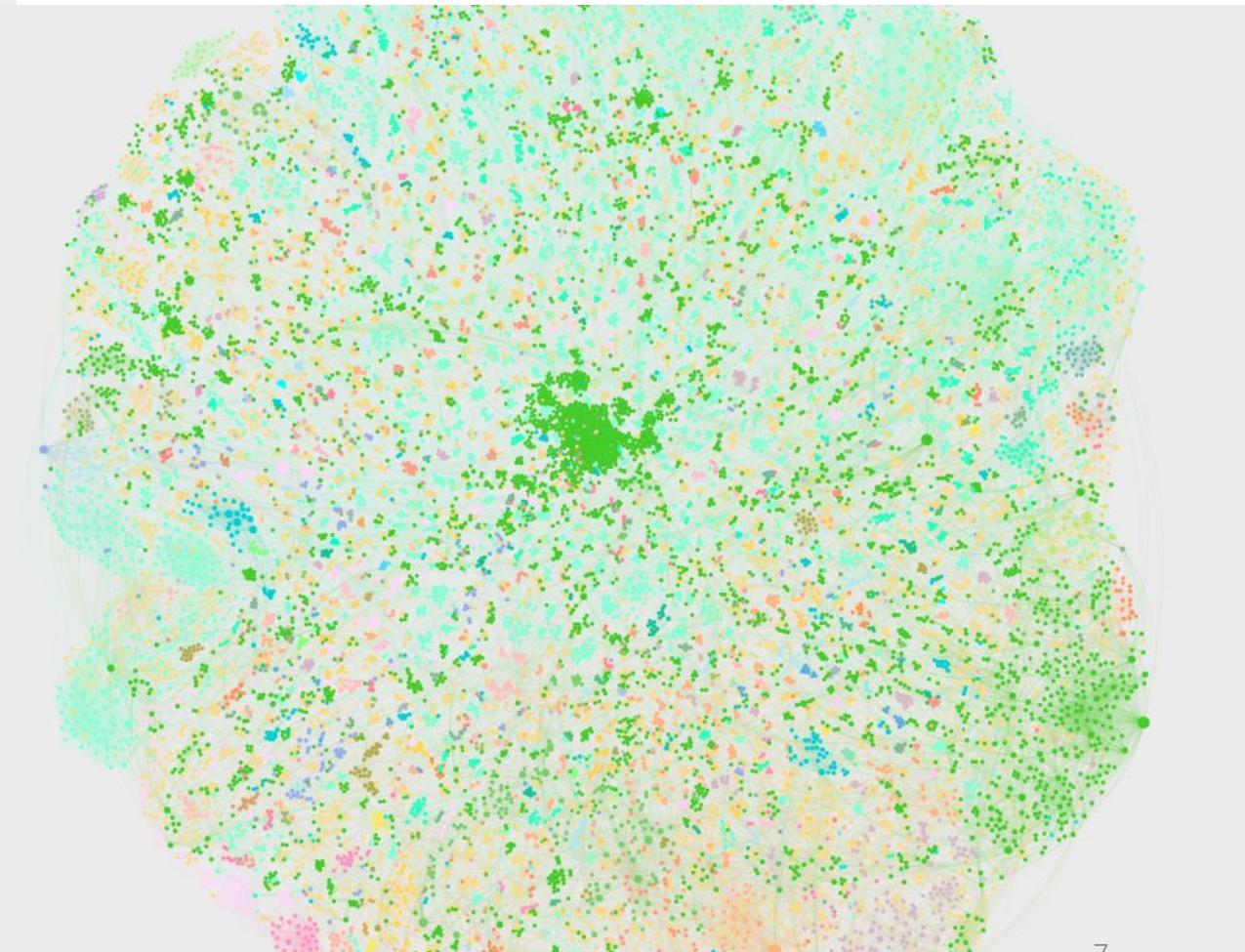
KT  
WC  
R

# Global Network of Researchers

Who is working on which molecule?

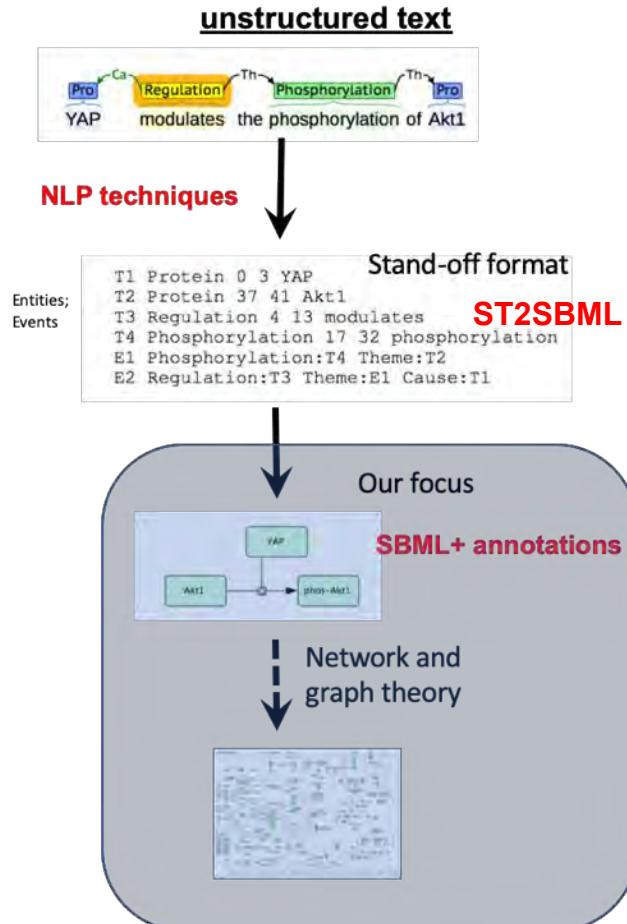


Who is working with who?

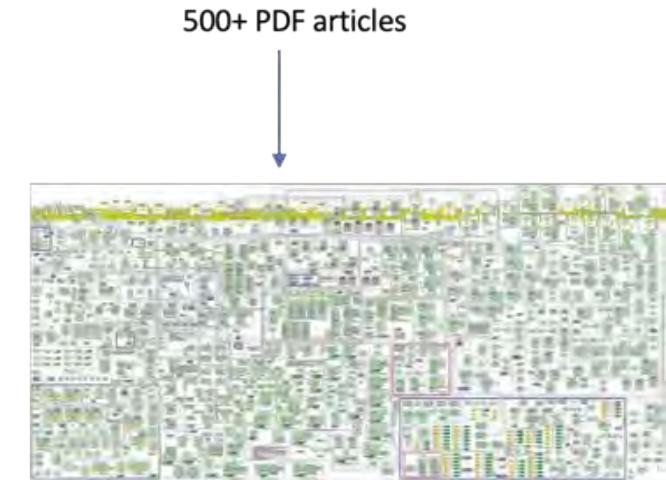
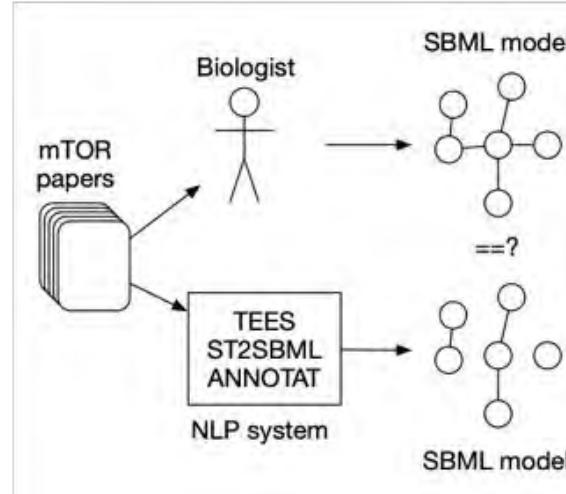


Text driven  
network/ pathway  
reconstruction

# How good is automated curation vs expert curation?

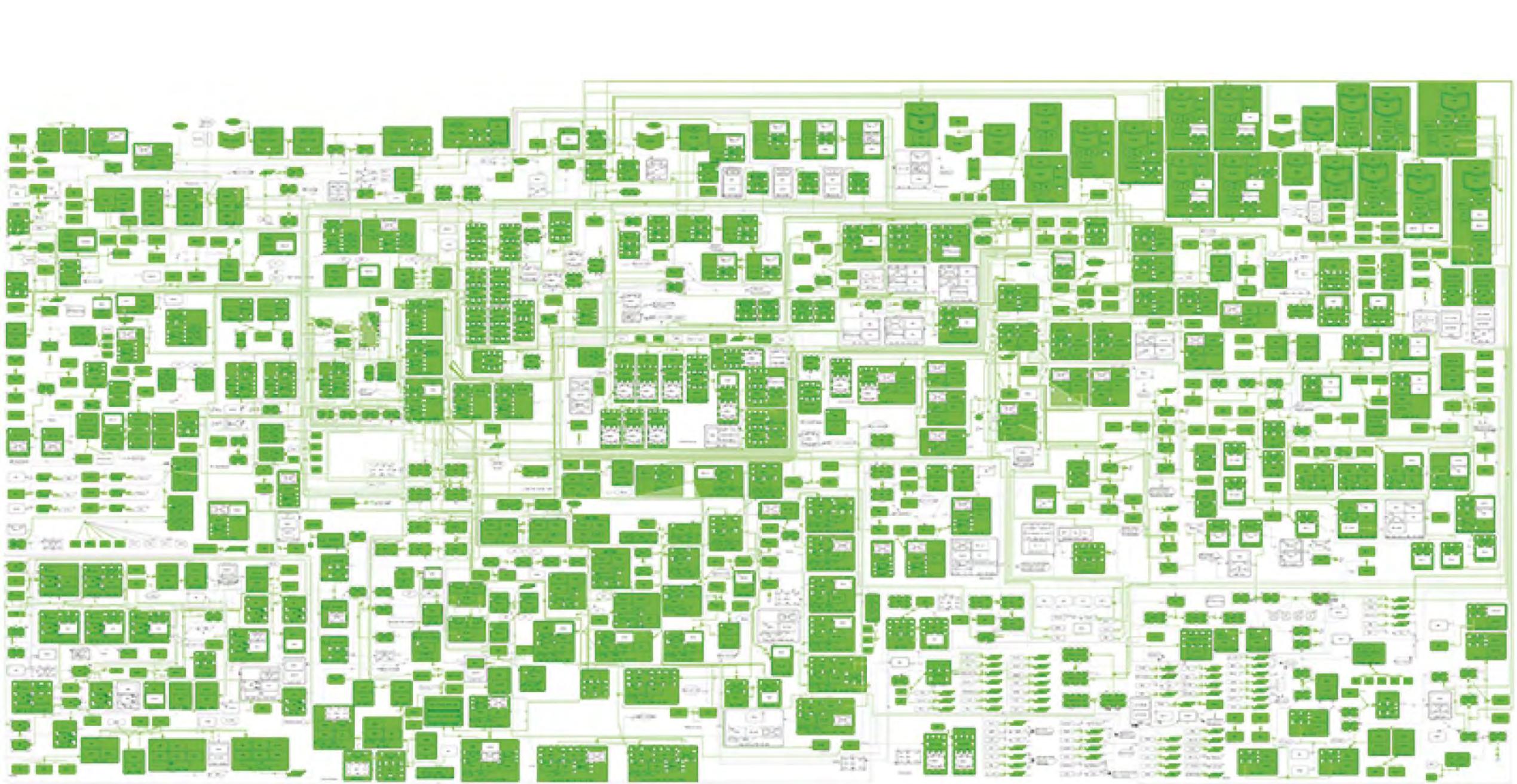


VS.



**mTOR pathway as a case study**

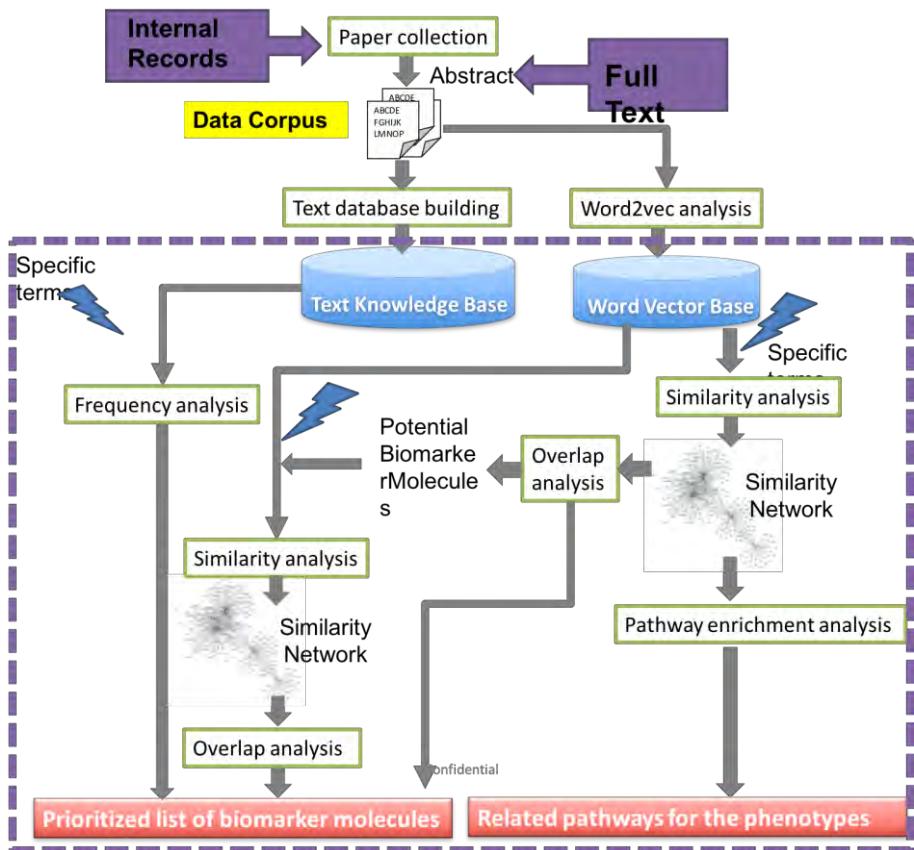
**Spranger, M., Palaniappan, S., Ghosh, S.: Measuring the state of the art of automated pathway curation using graph algorithms - a case study of the mtor pathway. BioNLP 2016, pp. 119–128. ACL**



# Key Case Studies

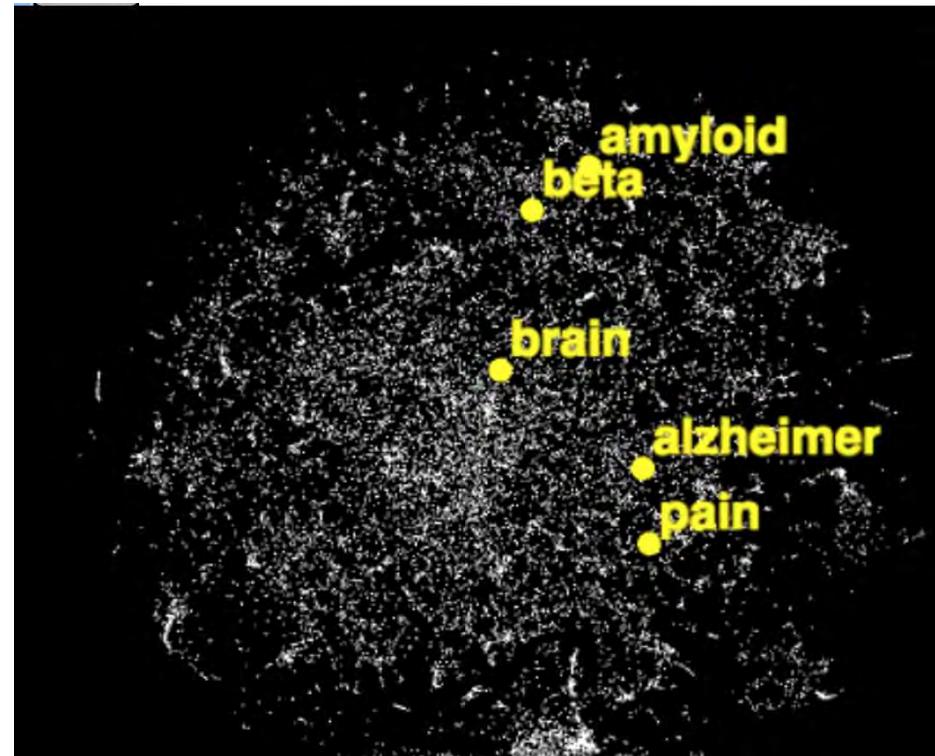
# Text mining approach for BioMarker Discovery

## Biomarker Knowledge Mining Pipeline



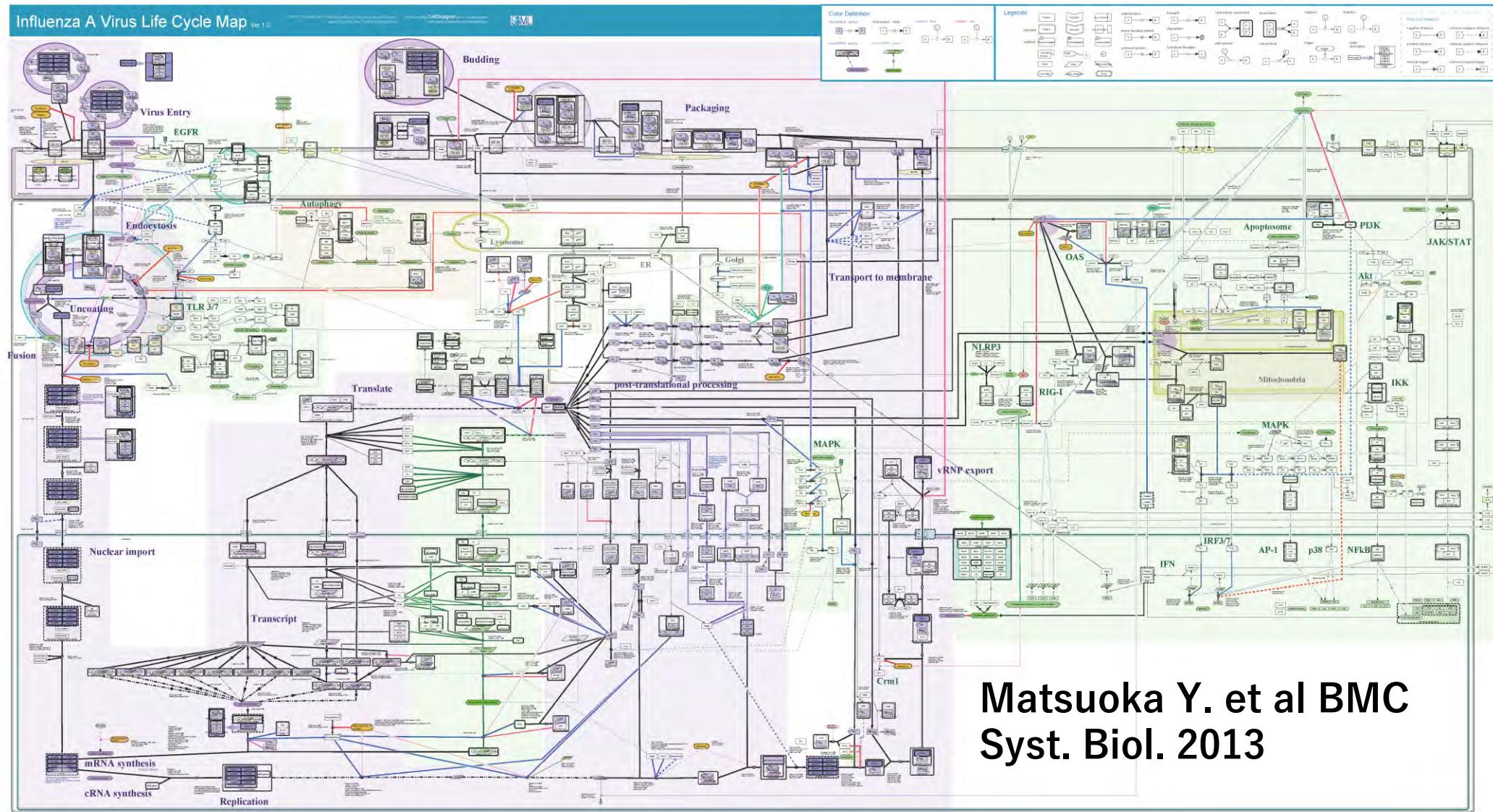
# Biomarker Galaxy

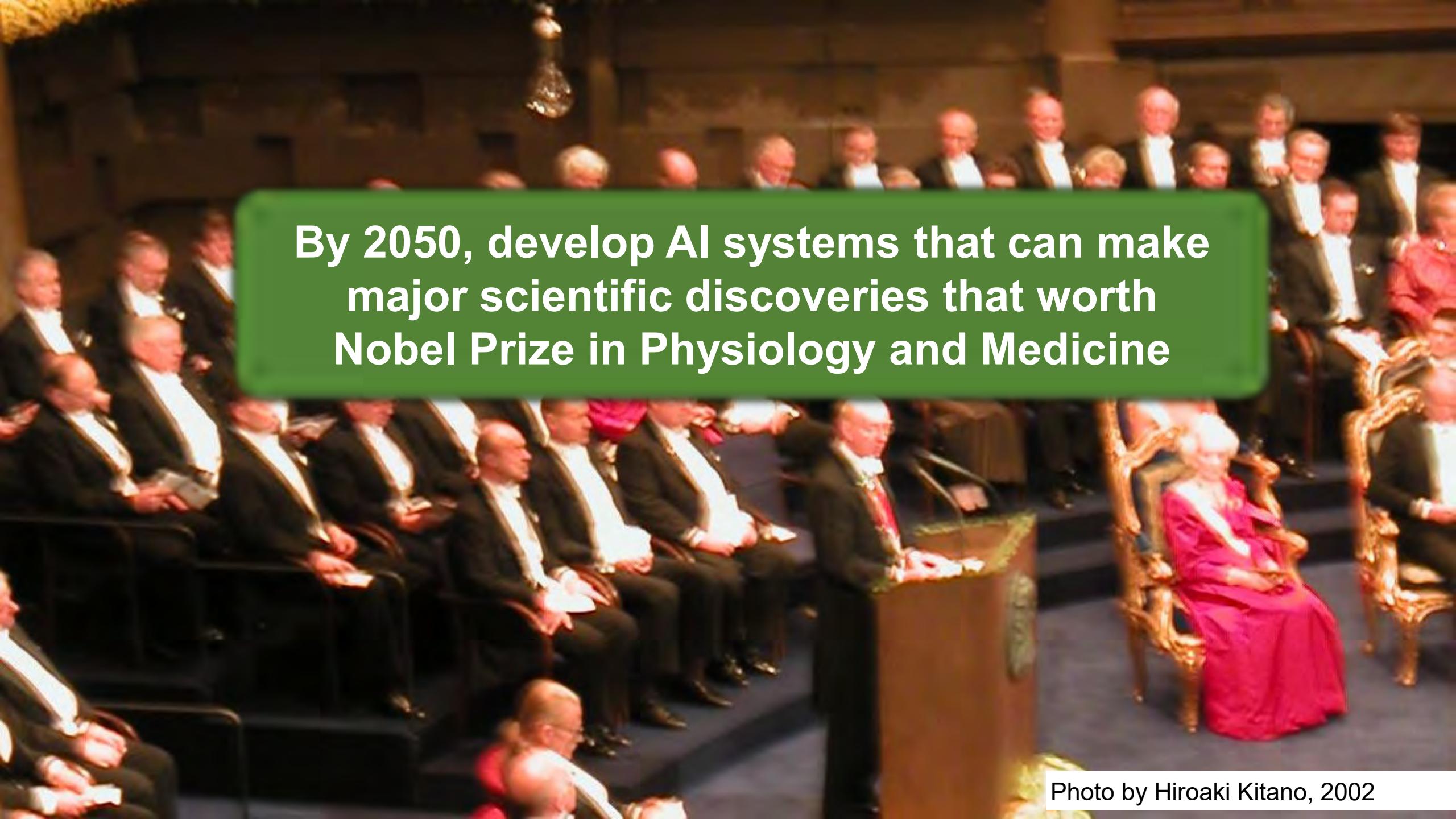
## Associate biomarkers with diseases



# Literature-driven Approach

## Influenza infection and replication network

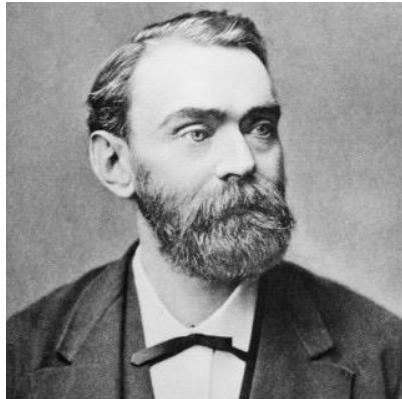




By 2050, develop AI systems that can make major scientific discoveries that worth Nobel Prize in Physiology and Medicine

# Nobel Turing Challenge

The Nobel Committee to give AI system the Nobel Prize without noticing it is an AI system, not a human scientist.



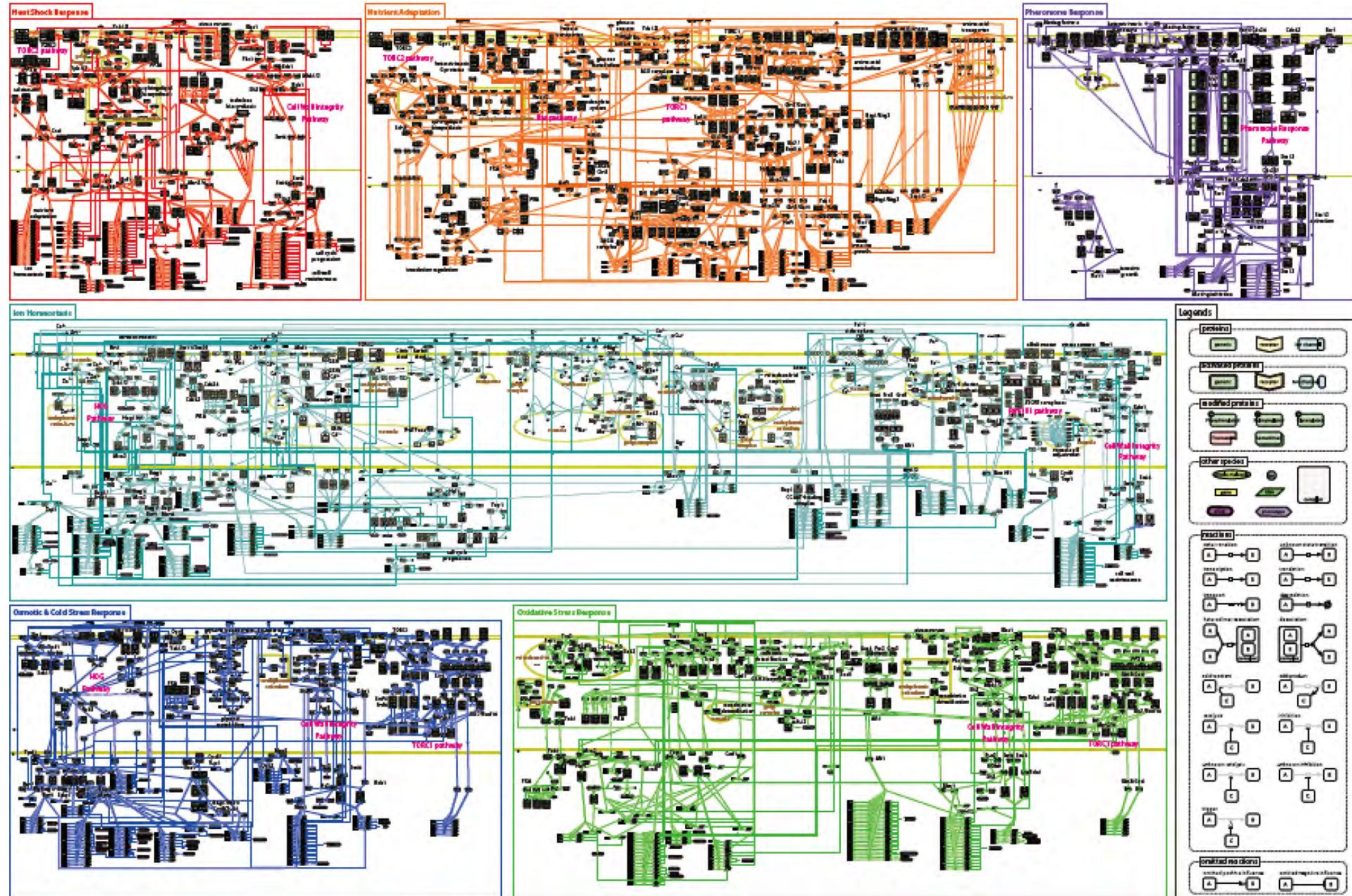
Alfred Nobel

The Turing Test at the Nobel-quality scientific activities

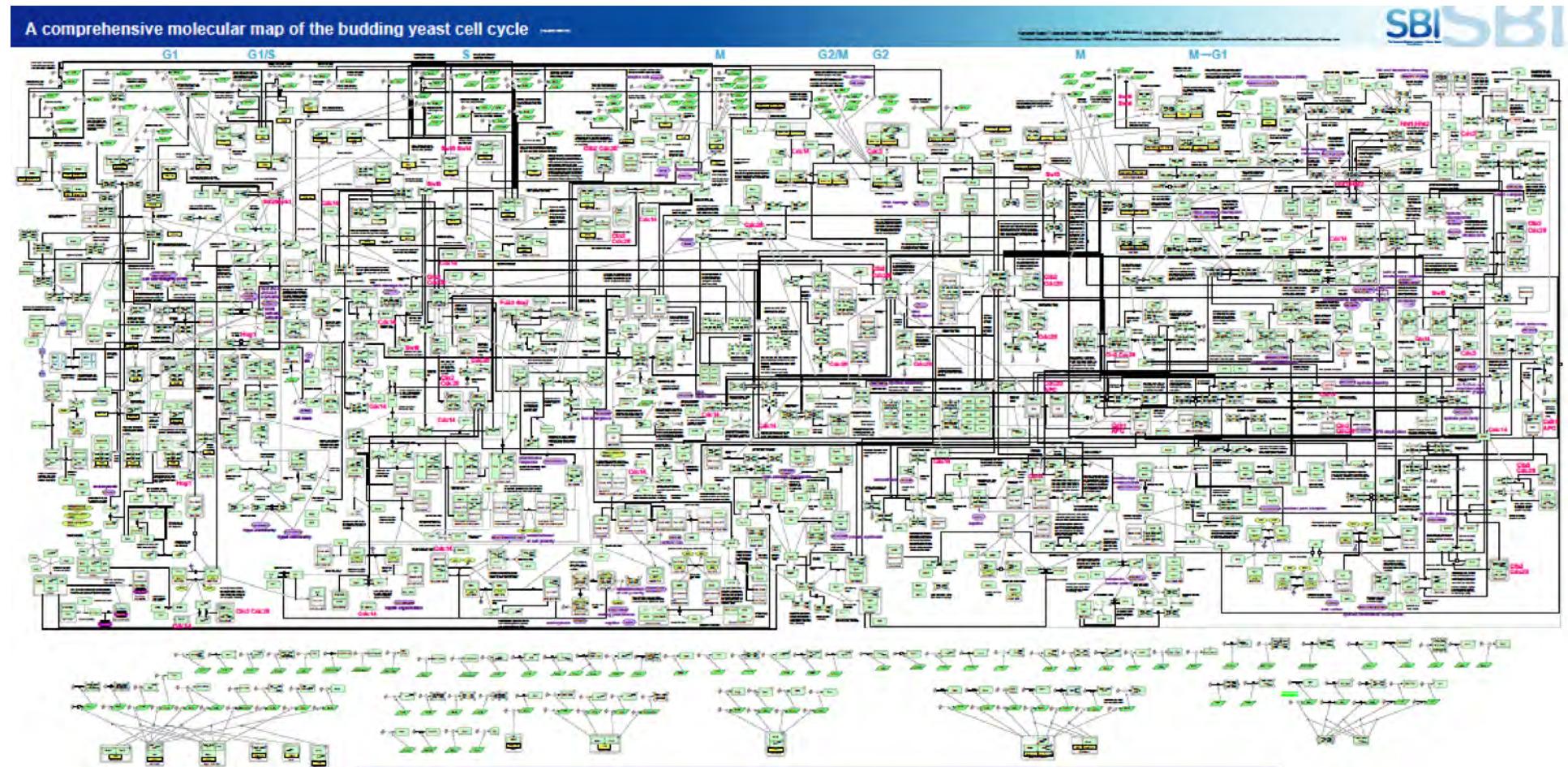


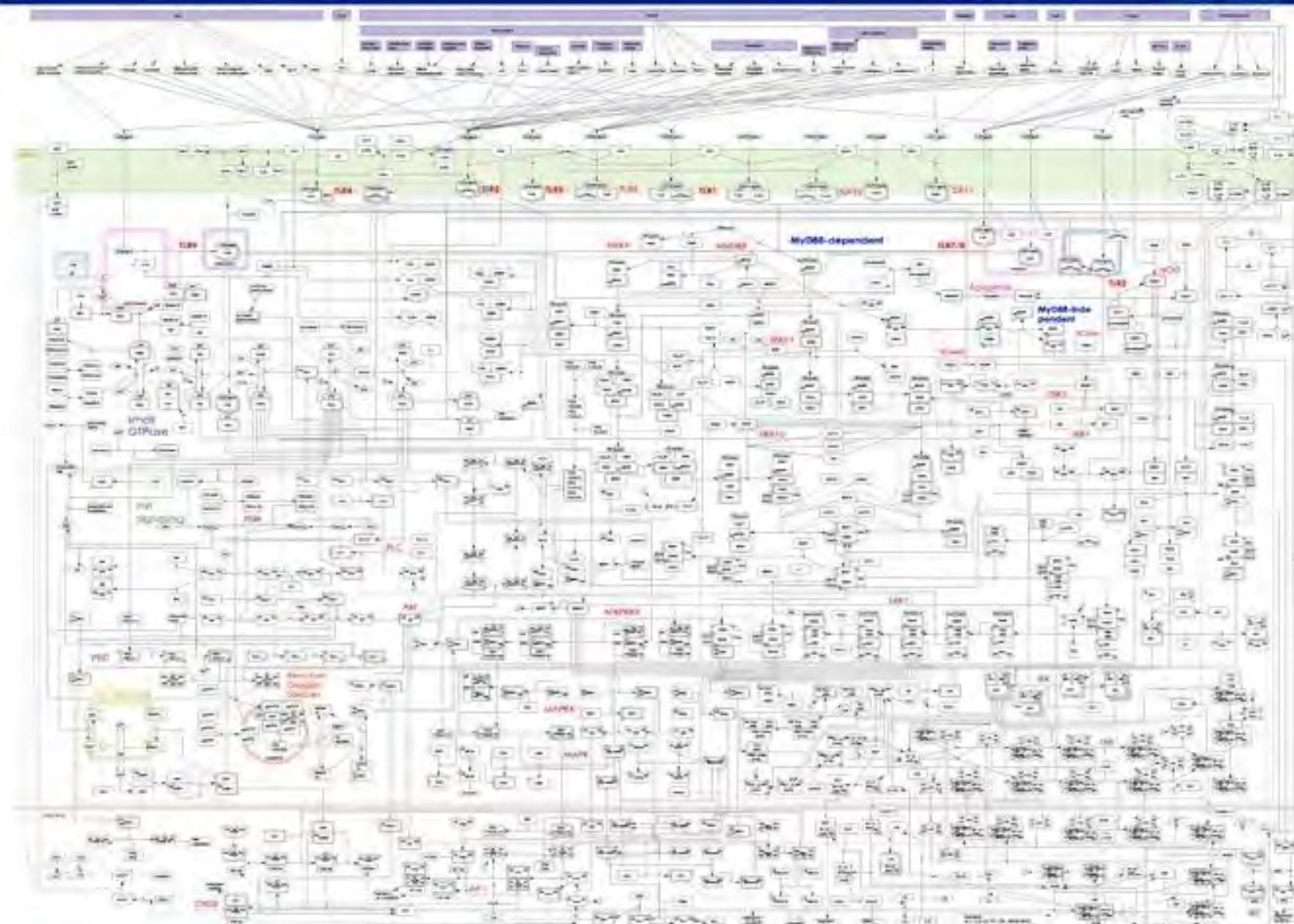
Alan Turing

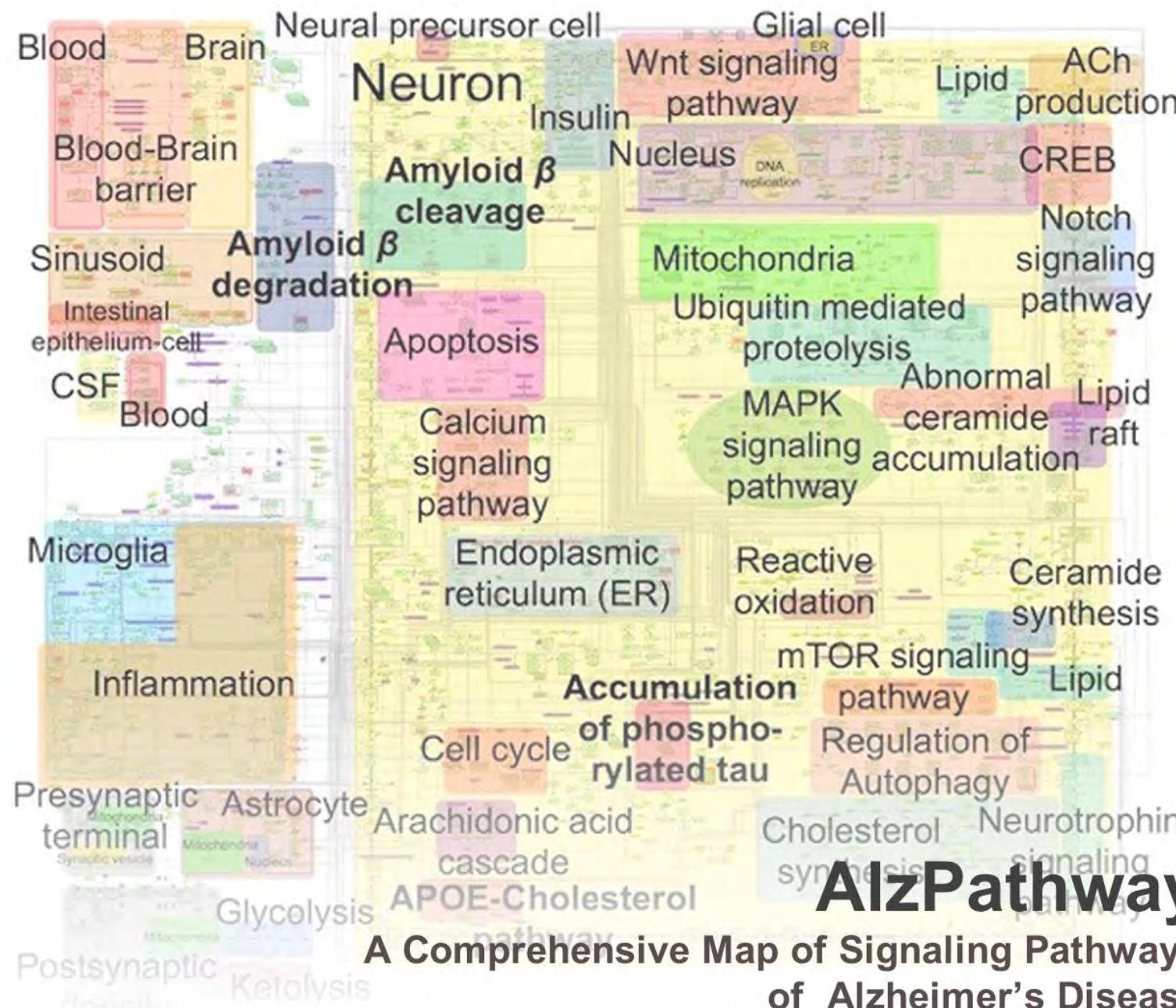
# Yeast Signaling



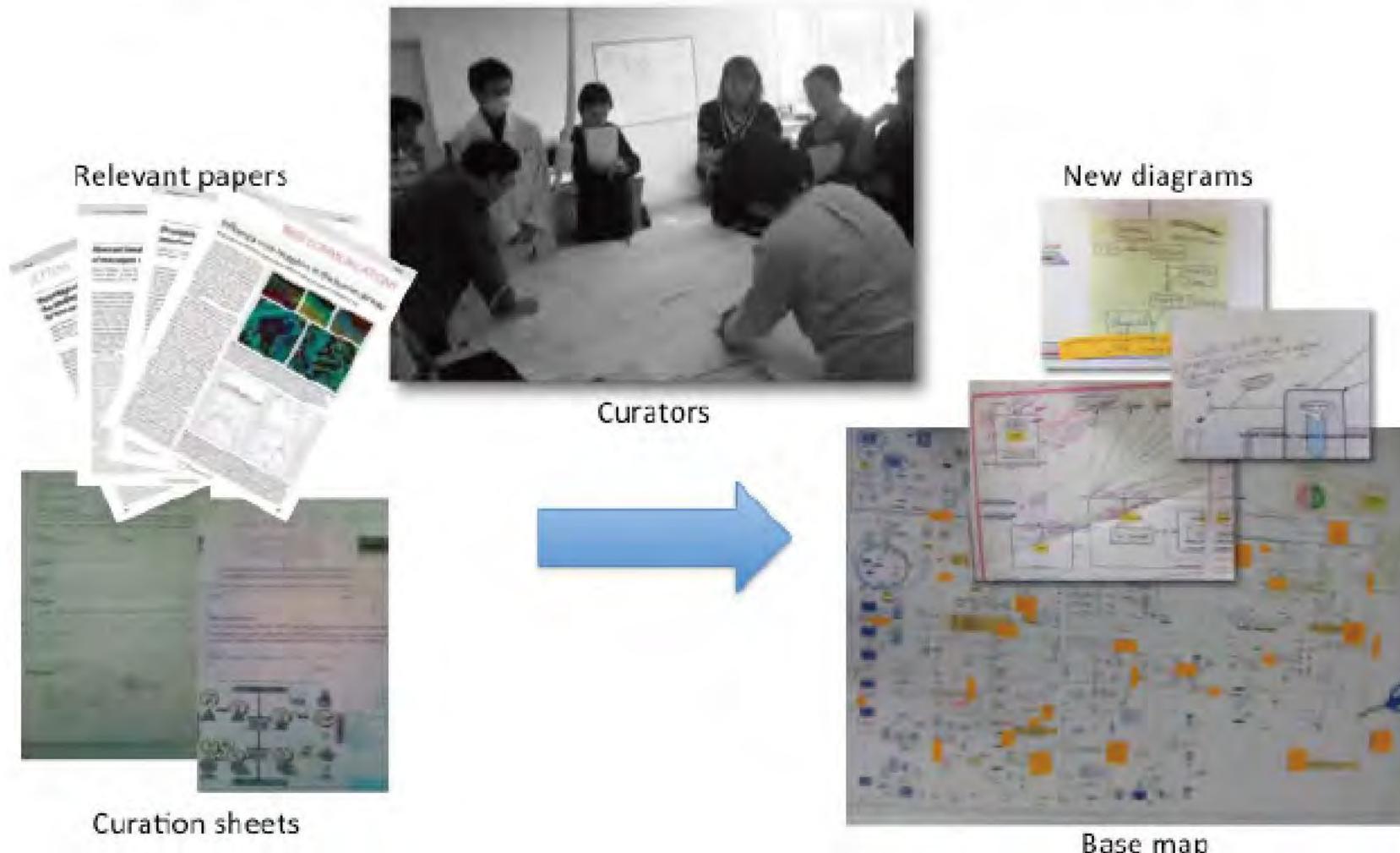
# Yeast Cell Cycle







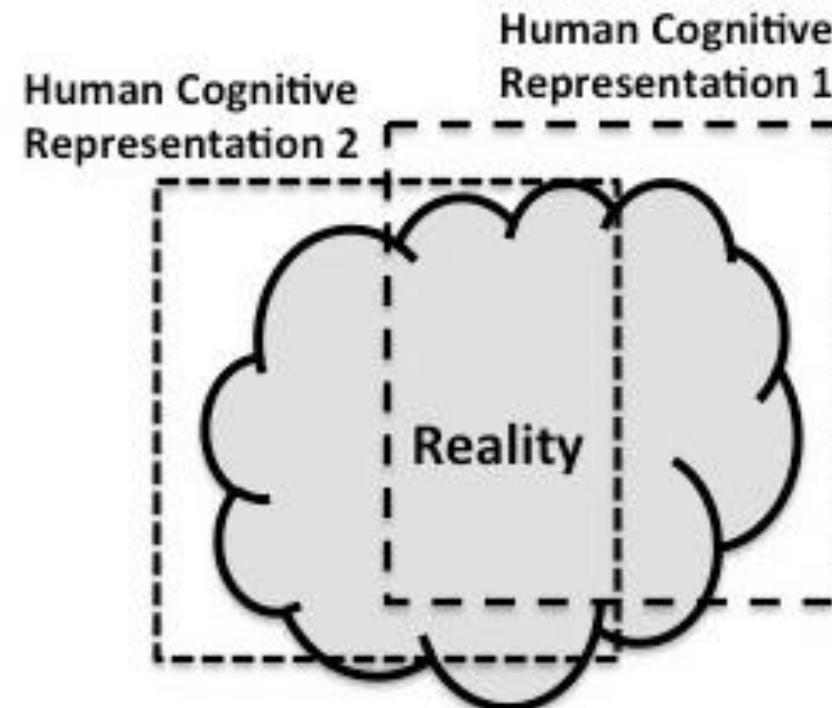
# “Mapathon” = Mapping Marathon



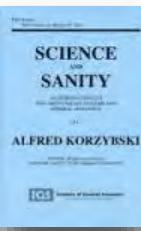
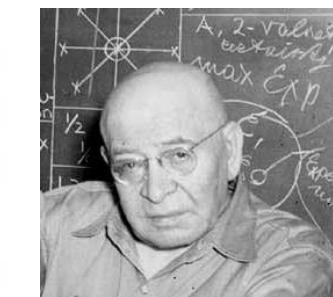
# Human Cognitive Bias and Limitations of Semantic Mapping

## Cognitive Bias in Clinical Reasoning

- Anchoring Bias
- Availability Bias
- Confirmation Bias
- Premature Closure
- Representativeness

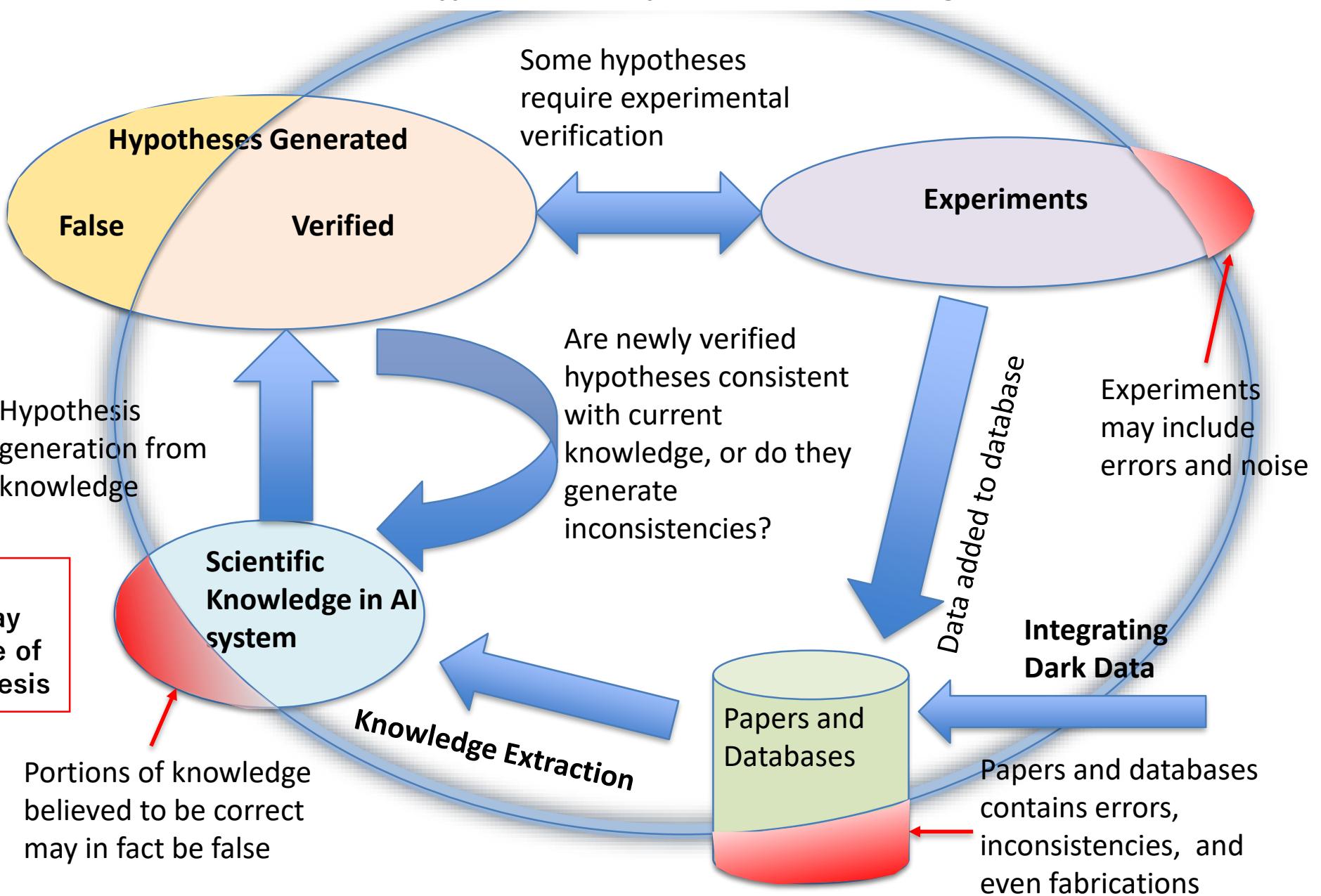


Map is not  
the territory



Alfred Korzybski

# Entire Hypothetical Body of Scientific Knowledge



# An Example of Knowledge Structure of Biological Discovery

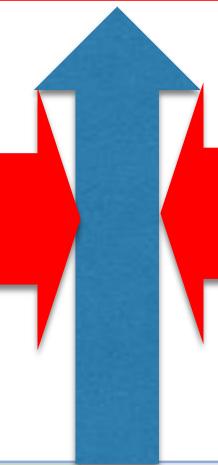
Explaining mechanisms of biological phenomena

**Experimental Constraints**  
**Empirical Constraints**

**Biochemical Constraints**  
**Systems Constraints**

Possible combinations of  
molecular mechanisms

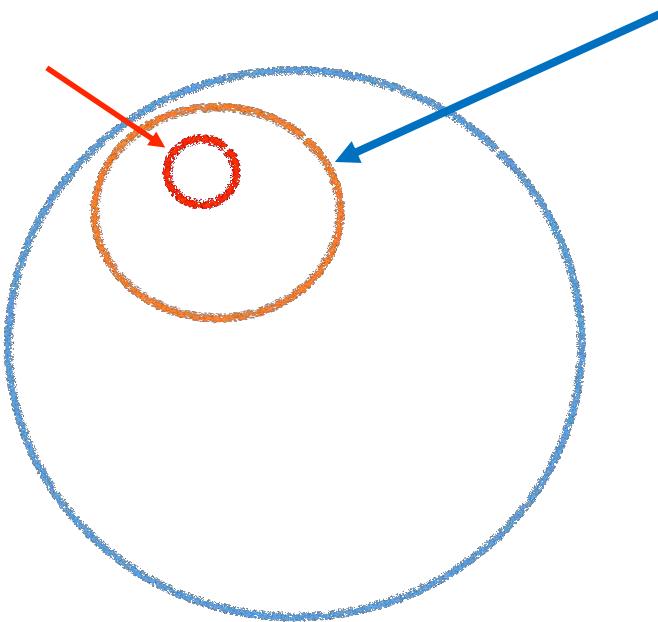
Molecules involved



# AlphaGo

*Human played games  
in the record*

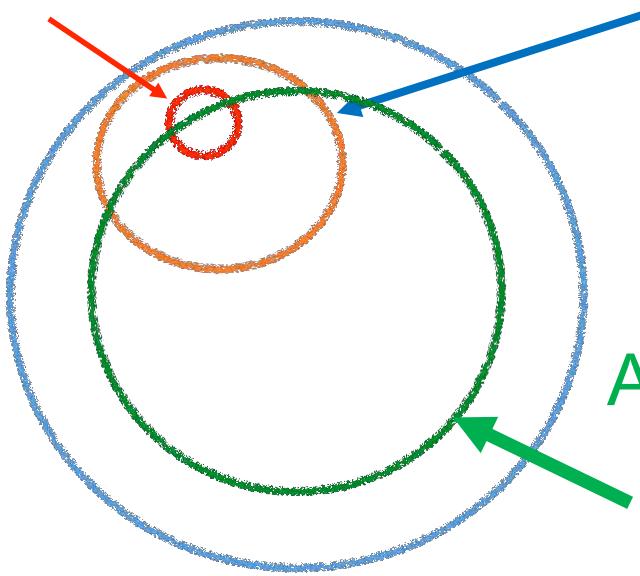
*Possible moves based  
on past human played  
games*



All possible moves on GO

# AlphaGo ZERO

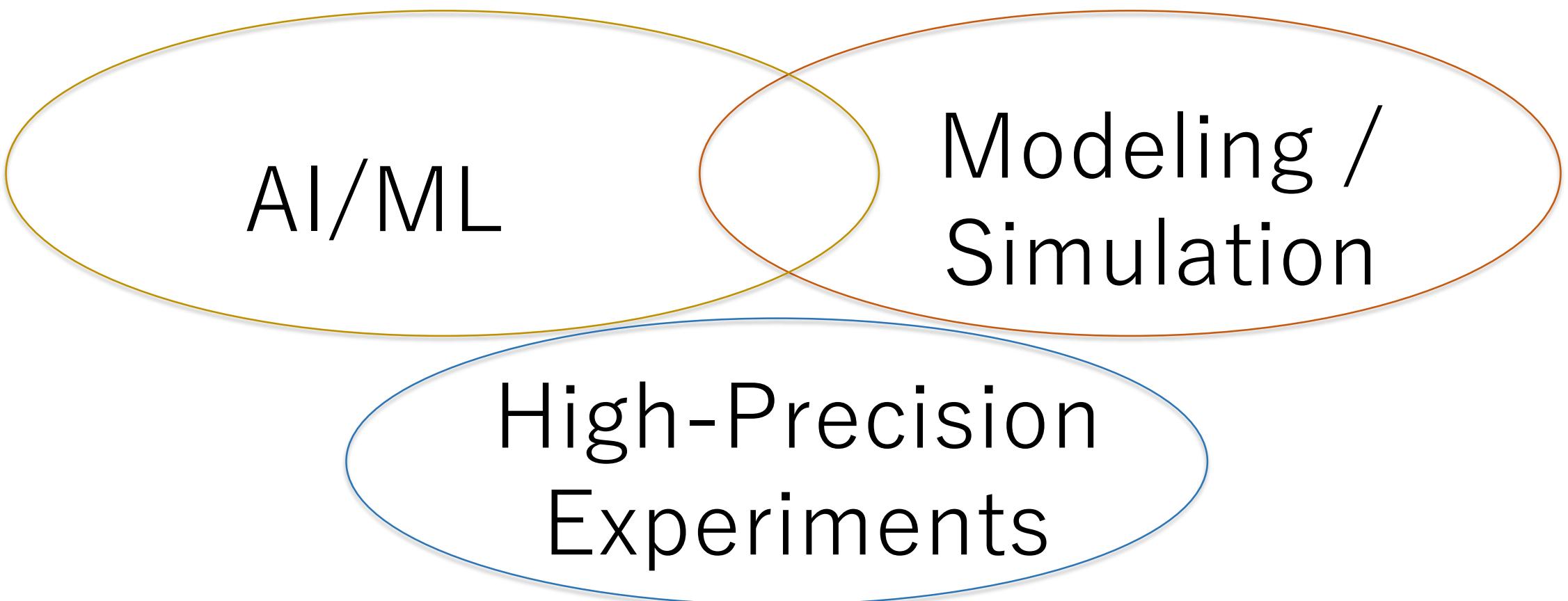
*Human played games  
in the record*



*AlphaGo*  
*Possible moves  
based on past  
human played  
games*

*AlphaGo Zero*  
*Tabula rasa based  
generation of games*

*All possible moves on GO*



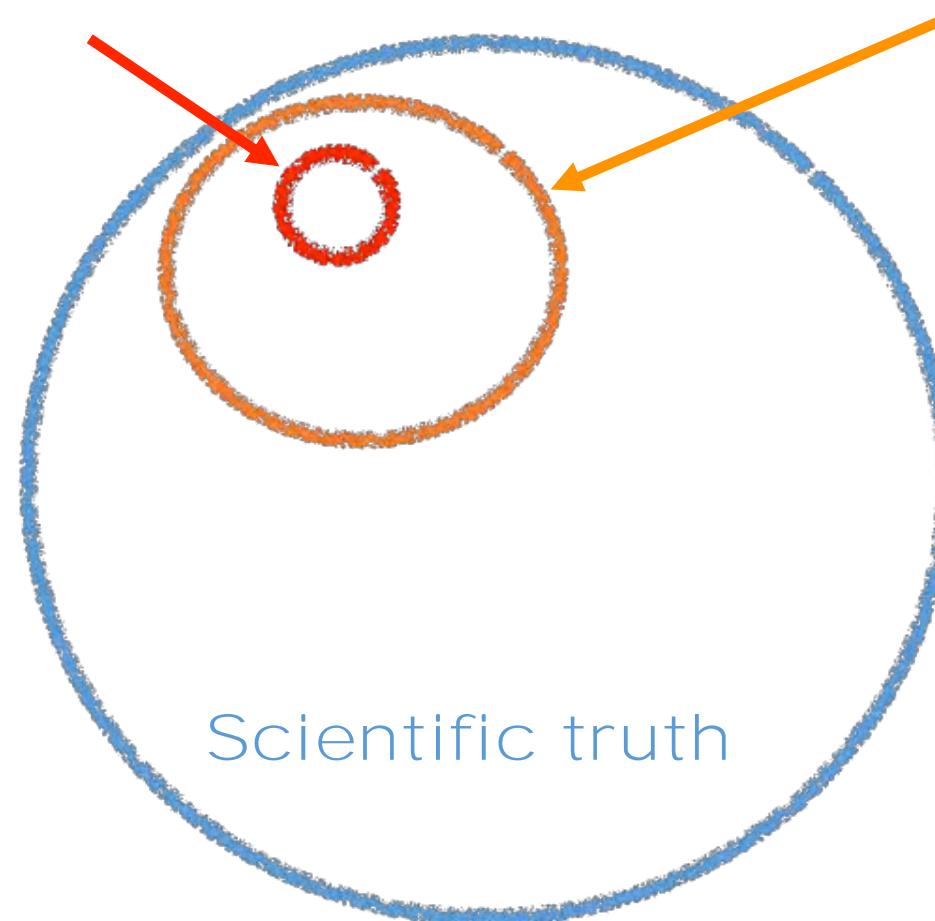
AI/ML

Modeling /  
Simulation

High-Precision  
Experiments

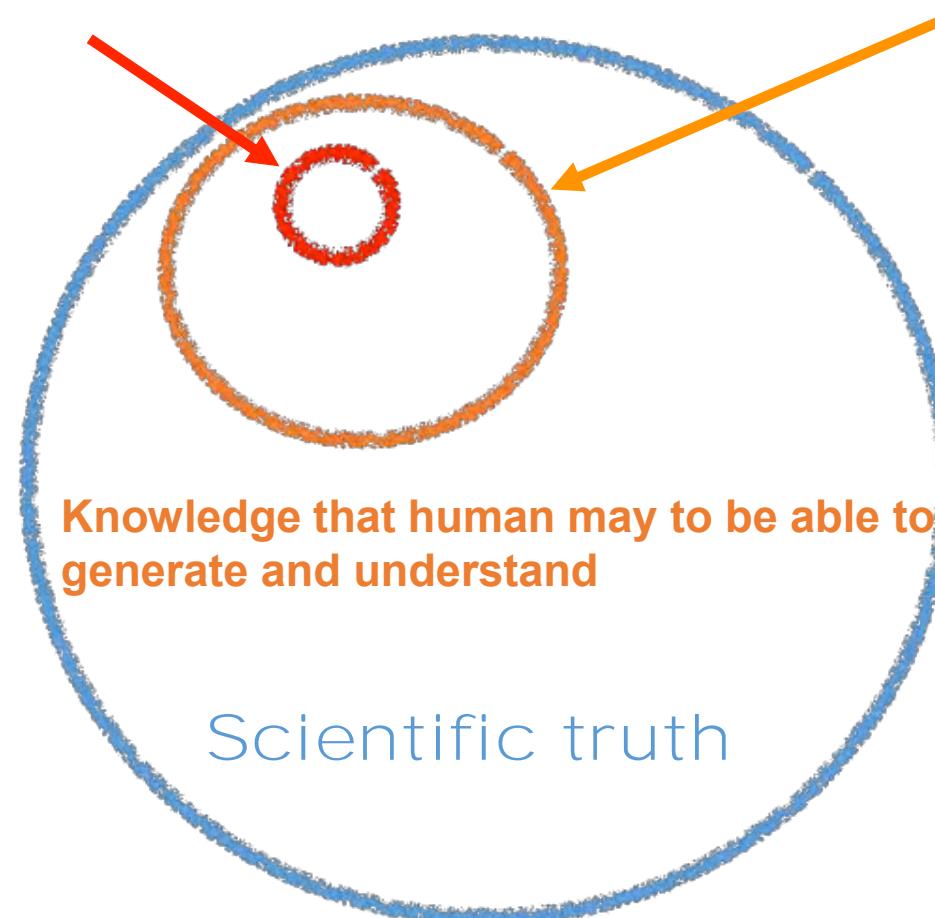
*Discovered knowledge*

*Human discoverable knowledge*



*Discovered knowledge*

*Human discoverable knowledge*



# Implications

- Alternative forms of scientific discovery
- Alternative forms of intelligence
- Accelerating sciences at unprecedented speed
- Machines to evolve by itself?