# Exscientia

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http://drug.design

# Re-energising Small Molecule Drug Discovery by Centaur Chemist

*Daisuke Tanaka, PhD*

The British Embassy Tokyo

25 July 2018

# Re-energising
## Small Molecule Discovery

90%

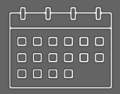
of all drugs are
small molecules

# Re-energising
## Small Molecule Discovery

50%

of clinical trials are for small molecules

# Re-energising
## Small Molecule Discovery



**5 yrs**

Typical time to identify a drug candidate

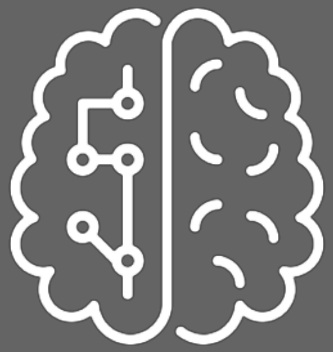
**2500**

Typical number of compounds to move from idea to candidate

Yet small molecule discovery remains inefficient and has not adopted the approaches advancing other fields

5 years; typical industry value
*Paul et al How to Improve R&D Productivity 2010 Nature Rev Drug Discovery*

# Re-energising
## Small Molecule Discovery



Exscientia's AI systems directly challenge pharma industry preconceptions of acceptable productivity

# Exscientia Objective

## Smart Candidate Discovery

~~2500~~ Compounds

500 Compounds

~~5~~ Years

1.5 Years

5 years and 2500 compounds are typical industry values

*Paul et al How to Improve R&D Productivity 2010 Nature Rev Drug Discovery*

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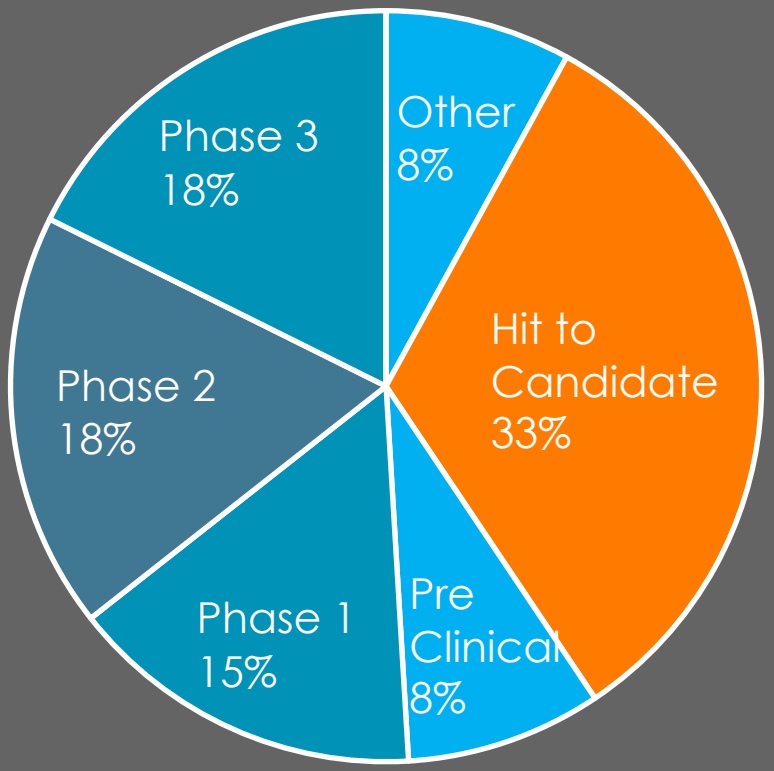



# HIT TO CANDIDATE

**MOST EXPENSIVE PART OF DRUG DISCOVERY**

Largest opportunity to improve productivity

COSTS PER LAUNCHED DRUG

# AI platform at Exscientia

# AI-Design, Make, Test

## Proprietary system delivers novel patentable compounds for each design cycle

**Genome-scale Pharmacology Data**
Potency, selectivity, anti-targets, ADME

HTS / Fragment screens

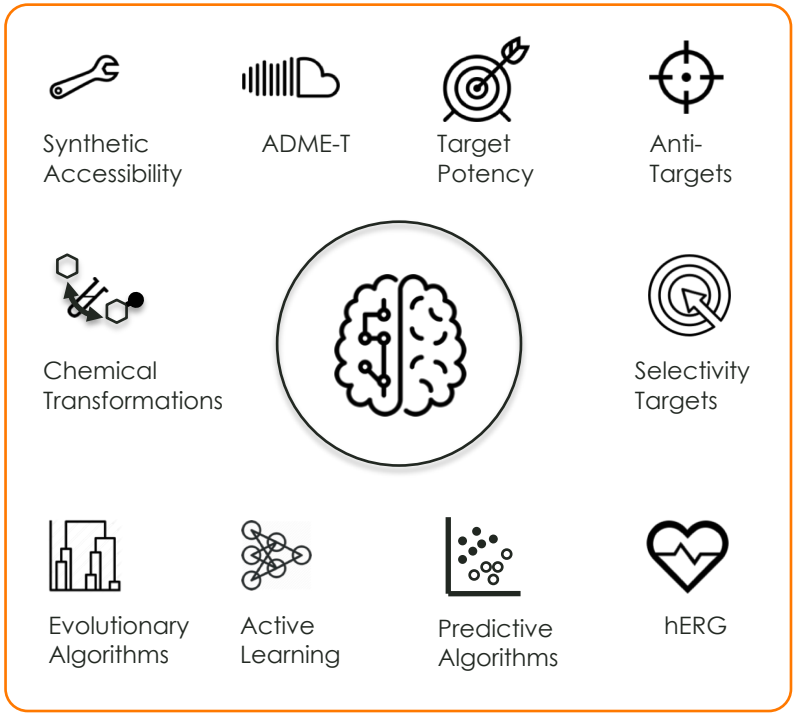
Literature SAR

Patent derived SAR

Competitor intel

Structural complexes

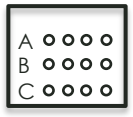
**AI-Design of novel compounds.**
System proposes next set of compounds to make against selection pressure for target, selectivity, anti-targets and ADMET predictions




**Make and Test.**
Rapid synthesis and assay of prioritised compounds

Proprietary Balanced Compound Designs

Synthesis




Assays

**Learn**
Enhance project specific models with latest data

# AI Design

## Proprietary system delivers novel patentable compounds for each design cycle

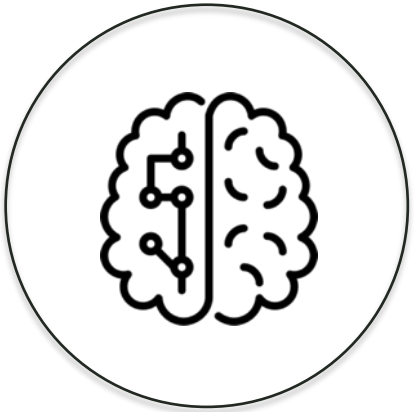
Synthetic Accessibility

ADME-T

Target Potency

Anti-Targets

Chemical Transformations



Selectivity Targets

Evolutionary Algorithms

Active Learning

Predictive Algorithms

hERG

# AI Design

## Proprietary system delivers novel patentable compounds for each design cycle

Evolutionary Algorithms

Chemical Transformations

Synthetic Accessibility

**AI Design**
Novel molecules evolved

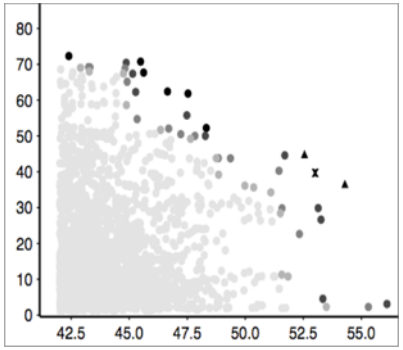
Target Potency

Selectivity Targets

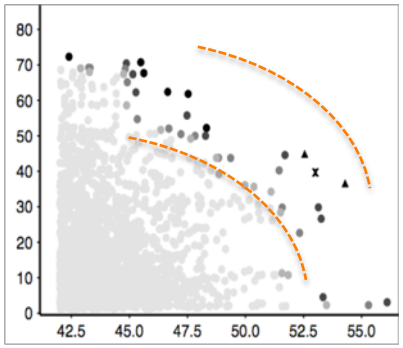
Anti-Targets

ADME-T

hERG




**Project specific Score**
Balanced properties for ideal molecules. Model scores




**Active Learning**
Select Compounds to Synthesize and Test

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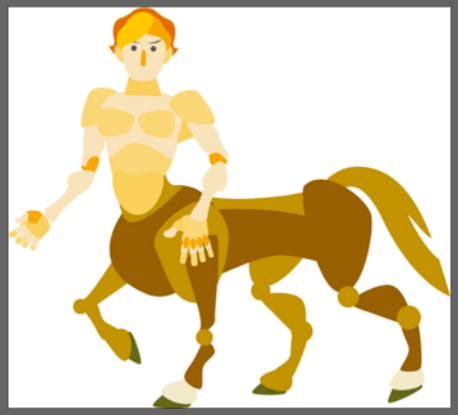


# AI-DESIGN AND HUMAN

# CENTAUR DRUG DESIGN

# The Rise of Artificial Intelligence

## March 1997

Kasparov loses to IBM Deep Blue

## March 2016

Lee Se-dol loses to alphaGo

# The Rise of Centaur Intelligence

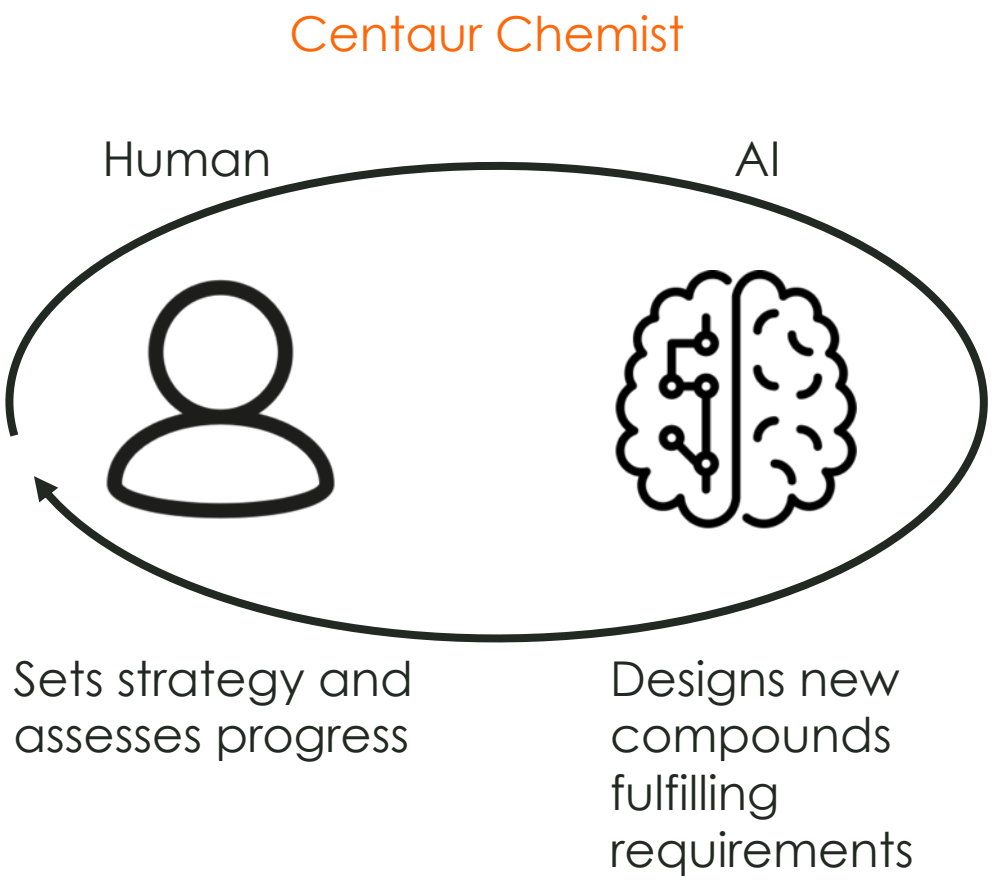
## Centaur: Human + Machine

2013

Olena Boytsun (ELO 2264) and Anna Ushenina (ELO 2477)

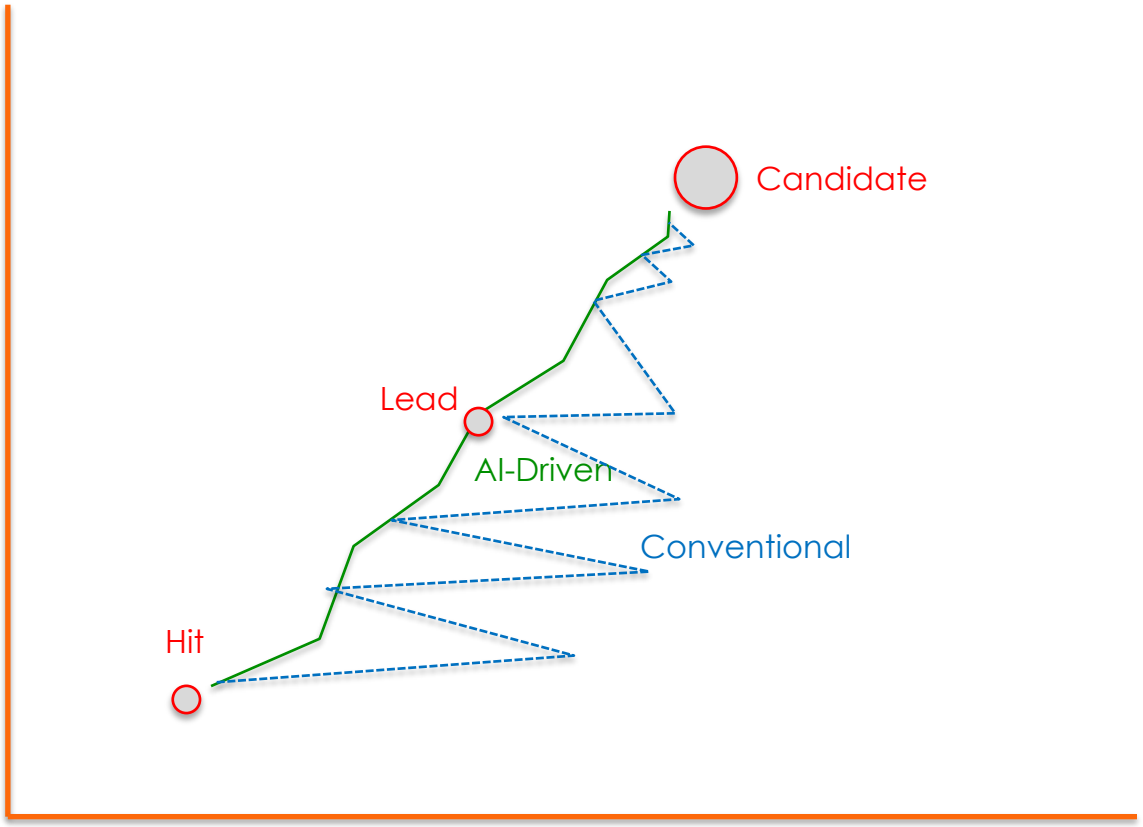
# The Centaur Chemist

## To Transform Drug Discovery Productivity



# Efficient Drug Discovery

## Combining ‘Man, Machine and Process’



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## PSYCHIATRIC DRUG DESIGN

- FIRST IN CLASS DUAL AGONIST

**COLLABORATION WITH SUMITOMO DAINIPPON**

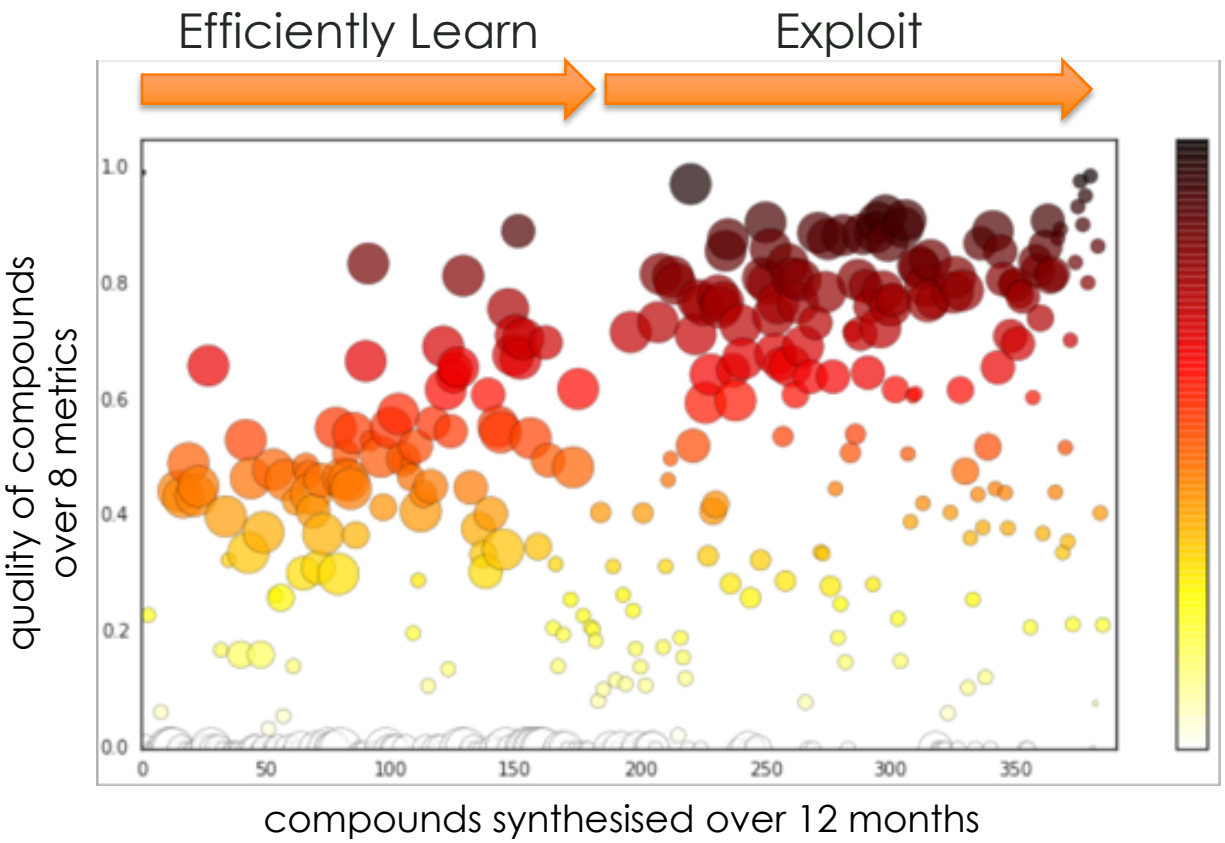
## ADENOSINERGIC IMMUNO-ONCOLOGY

- A2A SELECTIVE ANTAGONIST

**COLLABORATION WITH EVOTEC**

# Rapid pre-clinical candidate discovery

- Bispecific project with Sumitomo Dainippon Pharma
- <400 compounds synthesized and assayed
- 12 month discovery project, concept to candidate

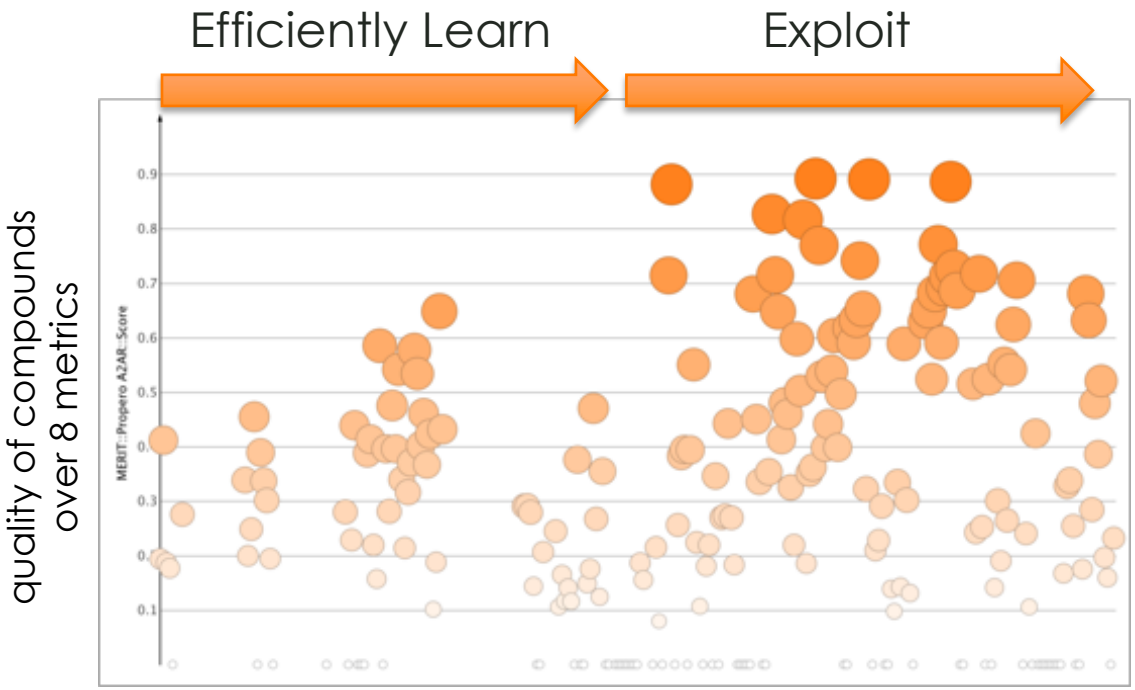



**circle size**
number of assays performed for each compound

**circle colour**
compound quality/proximity to objectives

# Another rapid discovery example

- 50:50 joint ownership with Evotec
- Best-in-class A2a selective antagonist for immuno-oncology
- Novel IP in crowded space
- Fragments to pre-clinical candidate; 225 compounds



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# DESIGNING DRUGS WITH AI

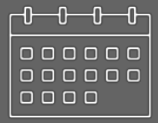
## SUMMARY

# Exscientia Productivity

## Metrics

**~500**

Consistent project delivery with Exscientia AI platform



**<1.5 yrs**

Rapid discovery reduces Cost of Capital and accelerates molecules to the clinic


**~$2.5M**

Cost of compound synthesis and assay per Exscientia project

**5x**

Capital Efficient delivery of concept to candidate chemistry

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*Artificial Intelligence will not replace chemists.*

*But chemists who don't use AI will be replaced by those who do.*

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