Al to Improve Productivity in Drug Discovery

Atomwise's Technology & Academic Collaborations

Sara Omlid, PhD Partnering Executive



Cost of Drug Discovery



13 yr & \$1,778 million

873 million out-of-pocket

Paul, SM, et al. Nature Rev. 2010, 9, 203-214.

[†] Cycle time of the stage. [‡] Cost per launch (capitalized). [§] Probability of moving to the next stage.

Overview



Natural synergies with Foundational Support

Rapid Growth

Al in Healthcare

Al Healthcare Market Size (US)

Global AI in Healthcare Market Report for 2016-2027. Cision, PR Newswire. 2018 (link).

AI Healthcare Startups Growth

Kuo, E. Al in Healthcare: Industry Landscape. TechBurst.io 2017 (link).



2018 estimate







Kuo, E. Al in Healthcare: Industry Landscape. TechBurst.io 2017 (link).

Al's Impacts on Drug Discovery

Implications for Productivity

Machine learning is a method of data analysis that automates analytical model building - systems learn from data, identify patterns and make decisions with minimal human intervention.



Atomwise's Approach





Small Molecule-Proteins Binding Predictions

- Therapeutic advances are closely linked to protein structure and function structure based drug design (SBDD).
- Atomwise uses a *global AI model* for SBDD statistical top-down approach.
- US Patent #9,373,059

Applying Atomwise's Technology

Early Drug Discovery Stages







Highlights

Atomwise's Technology



TOUGH PROBLEMS

E.g. PPI, homology models, mutant stabilization

ANY CHEMICAL LIBRARY

E.g. standard, FDA approved drugs, custom/virtual

DISEASE & SPECIES AGNOSTIC



Drug Discovery in Academia

SHIFTING TRENDS

The pharmaceutical industry's investment in in-house early stage drug discovery programs has rapidly declined.

More and more, academic researchers are taking on drug discovery projects. Today, there are over 150 academic drug discovery programs.

Palmer, M; Chaguturu, R. *Expert Opinion of Drug Discovery* **2017**, 12(6), 537-540. Ellinger, B; Gribbon, P. *Expert Opinion of Drug Discovery* **2016**, 11(4), 333-336. Academic Drug Discovery Consortium (ADDC), 2018. (<u>link</u>). An Overview: Support for Hit Discovery Efforts **AIMS Awards Program**





Artificial Intelligence Molecular Screen (AIMS) Awards Program

What do awardees receive with an AIMS Award?

Virtual screening for their target protein with 10+ million commercially available small molecules 72+ small molecules, prepped, QC tested, and plated, ready for testing in their lab



AIMS Awards Program

Applicant Research Areas





Infectious Diseases

AIMS Awards Program **Highlights**



Started in 2017, closed our third round in late September

Accept applications twice a year

Exponential growth in application rate (over 200 in our last round)

~300 projects will be selected for awards next year

"

With this award I was able to pursue an exciting idea for targeting a highly pathogenic porcine virus and obtain additional funding support. I am hopeful that this research will lead to the discovery of a small molecule that can effectively block entry of this virus; this could have an enormous impact on animal well-being.



Professor Young Tang, PhD University of Connecticut Quote from our June 1, 2018 PR

>

Brand & Marketing

Relationship Building

Training Data

AIMS Awards Program

Academic-Industry Partnership

Build Trust

Academia is naturally skeptical of other scientists capabilities and the motives behind industry research.

Academic Mindset

Assume that the academic's reason for pursuing the project is purely academic. No other pursuits should be treated as a given unless clearly defined and adopted together.

Goal Alignment

The goals of the academic partners have to match or compliment the goals of the industry partner.



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Research Agreement & IP

Clearly define all aspects on the research and responsibilities in the agreement, as well as obligations.

Frye, SV, et al. *Nat Rev Drug Discov.* **2011**, 10(6), 409-410. Palmer, M; Chaguturu, R. *Expert Opinion of Drug Discovery* **2017**, 12(6), 537-540. Ellinger, B; Gribbon, P. *Expert Opinion of Drug Discovery* **2016**, 11(4), 333-336.



Our Standard Policies on IP

AIMS Awards Program

Commercial Compounds

No novel composition of matter.

No restrictions on publications.

Open Collaboration

Ownership follows inventorship according to US patent law.

No reach-through rights.

Summary & Next Steps

THE PROBLEM:

The a decline in R&D Productivity

Atomwise is tacking the problem in two ways:

- Increase Efficiency: A
- Increase Number of Researchers Involved in Drug Discovery: **AIMS Awards Program**

NEXT STEPS

Ways to collaborate with Foundations to:

- increase awareness of our AIMS Awards Program
- identify other ways to leverage synergistic alliances

REMEMBER

We try to remember that medicine is for the patient. We try never to forget that medicine is for the people. It is not for the profits. The profits follow, and if we have remembered that, they have never failed to appear. The better we have remembered it, the larger they have been.

– George W. Merck



About Atomwise

Brief History About Atomwise



Atomwise was founded in 2012 by Abraham Heifets

Atomwise was founded in 2012 by Abraham Heifets and Izhar Wallach, while they were PhD students at the University of Toronto. Moved to San Francisco and went through Y Combinator in 2015. Announced a \$45 million Series A funding raise in March 2018.



About Atomwise





For inquiries, please email Dr. Sara Omlid at partnering@atomwise.com.

