



# Artificial Intelligence Molecular Screen (AIMS) Awards

## Request for proposals

Deadline: **29 March 2019**

*Please contact us for information on extensions and other accommodations.*

### **Why did Atomwise create this award?**

The goal of this program is to broaden the pool of scientists pursuing drug discovery. To advance this goal, Atomwise will award researchers with a customized virtual screen using cutting-edge Artificial Intelligence (AI) technology, free chemical compounds for physical screening, and technical support from medicinal chemists and computational biologists.

Researchers at universities and non-profit research institutes often have support for basic research and clinical research, but there is often little funding and many barriers for the intermediate stages of drug discovery and development. These barriers include a lack of knowledge of how to perform drug discovery and lead optimization, the cost of chemical compounds, the need to develop high throughput assays, and insufficient technical support.

Many scientists with the deepest knowledge of disease processes are therefore not engaged in the identification of chemical compounds that could lead to new insights into diseases, innovative diagnostic tools, and novel medicines. In response, the AIMS Awards were created to harness AI technology to facilitate and encourage drug discovery for all scientists.

Atomwise's technology uses deep learning neural networks to perform structure-based predictions (AtomNet™). This AI technology can virtually screen millions of chemical compounds to select those that are most likely to bind a target protein with high affinity and high specificity. AtomNet™ applications include discovering novel drugs, fast-tracking drug discovery, optimizing lead compounds, repurposing medicines, and

uncovering the mechanisms of action for drugs discovered in phenotypic screens. Atomwise can help researchers pursue projects at a fraction of the cost, time, and resources of traditional approaches.

### **What will awardees receive?**

AIMS Awards provide researchers with the following at no cost:

- customized virtual screen of chemical compounds\* using AtomNet™;
- 72 chemical compounds predicted to bind to their selected protein;
- chemical compounds that can serve as controls, if available;
- ordering of chemical compounds from suppliers, QC verification by mass spectrophotometry, resuspension and dilution to a convenient concentration, aliquoting into microtiter plates, and delivery to the researcher's lab;
- randomized "blinding" of molecules;
- support from Atomwise medicinal chemists and computational biologists; and
- additional chemical compounds and support if criteria are met.

\* Note: chemical compounds (or small molecules) will usually exclude molecules > 1000 Daltons, macrocycles, nucleic acids, peptides, polysaccharides, and lipids.

### **What types of projects are likely to win an award?**

Project topics can be in any area, including agriculture, animal health, biotechnology, human biology, medicine, microbiology, plant biology, and virology.

Highly suitable projects for the award will have both:

1. A target protein with:
  - an X-ray crystal structure or good homology model, AND
  - an identified site for the chemical compounds to bind.
2. An established assay(s) that can:
  - test at least 72 chemical compounds, AND
  - directly measure protein function or activity, AND
  - measure IC<sub>50</sub>, EC<sub>50</sub>, K<sub>i</sub>, K<sub>d</sub>, or equivalent.

## **Who is eligible?**

Applicants must be a Principal Investigator. Research scientists, graduate students, or postdoctoral researchers can apply for the AIMS Award on behalf of or with the approval and support of a Principal Investigator; in these cases, the Applicant with responsibility for the performance of the project must still be the Principal Investigator. The research must be performed at a non-profit university or research institute.

Grantees must agree to the Terms and Conditions of this RFP, and the Principal Investigator and their university or research institute must complete a research agreement with Atomwise (which is based on standard academic collaborative agreements).

## **How do I apply?**

Apply online at: <http://www.atomwise.com/aims>

Required to complete the application:

- Contact details so we can provide updates about your application.
- Information about your project to learn how we can help you improve the world:
  - research area, disease, or condition of interest;
  - protein of interest and its significance; and
  - purpose and potential impact of a chemical compound.
- Information about your protein:
  - UniProt ID, PDB code, and residues of target site; and
  - any relevant publications.
- Information about the type of chemical compounds you would prefer.
- Information about your assay.

## **What is the timeline?**

Application deadline: **29 March 2019**

Announcement of recipients: **May/June 2019**

## **Who can I contact for further information and assistance?**

Dr. Sara Omlid: [academics@atomwise.com](mailto:academics@atomwise.com)