



# Artificial Intelligence Molecular Screen (AIMS) Awards

## Request for Proposals

Deadline: **December 14, 2020**

*Please contact us for information on extensions and other accommodations at  
[academics@atomwise.com](mailto:academics@atomwise.com)*

### 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, approximately 72 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 and clinical research, but there is often little funding or support for the intermediate stages of drug discovery and development. Additional common barriers to pursuing drug development include a lack of knowledge about how to perform drug discovery, the cost of procuring diverse chemical compounds, the need to develop high throughput assays, and insufficient expertise in medicinal chemistry or computational biology.

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 neural networks to perform protein-structure-based binding predictions (AtomNet®). This AI technology can virtually screen billions of chemical compounds to select those that are most likely to bind a target protein with high affinity. Applications of the AtomNet® platform include discovering novel drugs, fast-tracking drug discovery, optimizing lead compounds, and repurposing medicines. 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:

- customized virtual screen of chemical compounds\* using the AtomNet® platform;
- approximately 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, purity verification by mass spectrophotometry, resuspension and dilution to a convenient concentration, aliquoting into screw cap tubes, 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 will usually exclude molecules > 1000 Daltons, macrocycles, nucleic acids, peptides, polysaccharides, and lipids.

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

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

Highly suitable projects for the award will have:

1. An unmet need that could be addressed via the development of a small molecule modulator for the protein target of interest.
2. A target protein with:
  - an X-ray crystal structure or good homology model template, AND
  - an identified site for the chemical compounds to bind.
3. An established assay(s) that can:
  - test at least 72 chemical compounds, AND
  - measure IC<sub>50</sub>, EC<sub>50</sub>, K<sub>i</sub>, K<sub>d</sub>, or equivalent.

Note: A structure or identified binding site is not required to receive the award. Our scientific team can often aid in the identification of appropriate structural data, homology model templates, and potential binding sites.

## **Who is eligible?**

Applicants must be a faculty or professional staff member. Research scientists, graduate students, or postdoctoral researchers can apply for the AIMS Award on behalf of or with the approval and support of a faculty or professional staff member. In these cases, the applicant with responsibility for the performance of the project must still be the faculty or

professional staff member. The research must be performed at a non-profit university or research institute.

Applicants must agree to the Terms and Conditions of this RFP, and the 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 such as:
  - 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 target of interest:
  - UniProt ID, PDB code, and/or 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: **December 14, 2020**

Announcement of recipients: **February 2021**

Time to receive compounds can vary but many projects have compounds in their lab for testing within 3-6 months of receiving notice of an award.

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

Reach out to the AIMS team at [academics@atomwise.com](mailto:academics@atomwise.com)