# Akttyva Therapeutics Announces AIDE 2.0 Platform and Discovery of Novel Allosteric MK2 Modulator Classes

*Akttyva Therapeutics files of a patent application covering AIDE 2.0, an early stage next-generation high-performance computational drug discovery platform*

WATERTOWN, MA, UNITED STATES, December 19, 2025 /EINPresswire.com/ -- Akttyva Therapeutics, Inc. today announced the filing of a patent application covering AIDE 2.0, an early stage next-generation high-performance computational drug discovery platform, together with novel classes of allosteric MK2 modulators identified and experimentally validated using the platform.

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>
> *David Bowman*

AIDE 2.0 has been built from the ground up in 2025, developed to address one of the hardest problems in drug discovery: identifying and exploiting allosteric pockets, including flexible and transient binding sites that are inaccessible to conventional orthosteric approaches. While most discovery platforms focus on static active sites, AIDE 2.0 is designed to integrate large-scale computation with biological validation to target regulatory pockets across diverse protein families. HPC, Big Data, Advanced Primary Screening criteria including ADMET at the scale of billions of compounds and GenAI are at its foundation.

Using AIDE 2.0, Akttyva identified multiple previously unreported chemical scaffolds modulating MK2 via non-canonical binding modes. Initial in-vitro studies demonstrate direct binding, favorable dose-response behavior, and absence of cytotoxicity in early assays.

“What’s exciting here is the convergence of computation and biology,” “Allosteric drug discovery is exceptionally difficult because these pockets are transient, flexible, and often invisible to traditional screening approaches,” said Mario DiPaola, Ph.D., Principal Investigator at Akttyva. “Very few groups pursue allosteric modulation because it demands both precise computational hypotheses and careful experimental validation. Seeing direct binding signals and clean cytotoxicity at this stage is a strong indication that the approach is working.”

“This a totally new architecture designed to scale across proteins with complex allosteric regulation built this year. The discovery of multiple MK2 scaffold classes validates the platform’s broader applicability.” said David Bowman, CEO and CTO of Akttyva Therapeutics. “AIDE 2.0 was built specifically to explore this space at scale, integrating high-performance computing, AI, ML, adaptive screening, and biologically informed filtering. The discoveries we’re reporting could not have been made with conventional approaches.”

The company has filed a patent application covering:

The AIDE 2.0 computational architecture and discovery workflow

Classes of allosteric MK2 modulators, including structural families and analog series

Methods applicable to other proteins with regulatory or cryptic allosteric pockets

Akttyva is continuing biological validation and advancing lead optimization under its active NSF Phase II program. The early stage AIDE 2.0 is in continuing development.

MARIO DIPAOLA
Akttyva Therapeutics
+1 781-490-5757
mario@akttyva.com
Visit us on social media:
LinkedIn