IDEAYA Biosciences Announces Collaboration with ATTMOS to Accelerate AI/ML-Enabled Drug Discovery for Unprecedented First-in-Class Oncology Targets

SOUTH SAN FRANCISCO, Calif., March 3, 2025 /PRNewswire/ -- IDEAYA Biosciences, Inc. (Nasdaq: IDYA), a precision medicine oncology company committed to the discovery and development of targeted therapeutics, today announced a research collaboration with ATTMOS as part of its efforts to build a physics-based computational small molecule discovery platform that rapidly unlocks what are currently perceived as undruggable oncology targets.

The collaboration will integrate IDEAYA's differentiated and proven capabilities in structural biology and pharmaceutical drug discovery across multiple first-in-class oncology targets with ATTMOS's capabilities in computational chemistry method development, high performance computing, and software development. The focus of the partnership will be to engineer and optimize a workflow solution for high-throughput absolute binding free energy perturbation predictions (ABFEP) of first-in-class drug candidate molecules. This approach enables application of gold-standard physics-based statistical mechanics calculations of protein-ligand affinities at the scale required for virtual screens and represents what could become the industry's go-to standard for high-speed and high probability-of-success drug hit-finding against structurally-enabled novel biological targets.

"Current AI/ML-enabled drug discovery approaches have been largely applied to either already drugged targets or well-understood biological target classes and often fail when applied to first-in-class target opportunities. IDEAYA continues to enhance its computational drug discovery capabilities to pursue first-in-class oncology targets that are perceived as undruggable," said Michael White, Ph.D., Chief Scientific Officer, IDEAYA Biosciences. "Our partnership with ATTMOS will enable us to apply the principles of engineering to the field of drug discovery, at scale, for efficient prosecution of unprecedented oncology targets," said Paul Barsanti, Ph.D., Chief Technology Officer, IDEAYA Biosciences.

The collaboration will leverage the Amber molecular dynamics suite as the GPU-accelerated back-end free energy simulation engine. IDEAYA will train and evaluate ABFEP-based active learning cycles based on extensive ground-truth data sets derived from its successful wet-lab drug discovery campaigns against novel targets. These models will be used to screen enormous libraries of synthetically tractable chemical space for accurate and efficient de novo discovery of small molecule ligands for new targets. The work aims to overcome the limitations of current virtual screening approaches and accelerate the discovery of novel small molecule oncology therapeutics that address unmet clinical need.

About IDEAYA Biosciences

IDEAYA is a precision medicine oncology company committed to the discovery and development of targeted therapeutics for patient populations selected using molecular diagnostics. IDEAYA's approach integrates capabilities in identifying and validating translational biomarkers with drug discovery to select patient populations most likely to benefit from its targeted therapies. IDEAYA is applying its research and drug discovery capabilities to synthetic lethality – which represents an emerging class of precision medicine targets.

About ATTMOS

ATTMOS was founded in early 2022 by a diverse team of academics from Michigan State, Rutgers and UC San Diego. ATTMOS's mission is to bring novel technologies into the drug discovery process through a synergy between industry and academia and make this technology affordable and available to everybody.

Forward-Looking Statements

This press release contains forward-looking statements, including, but not limited to, statements related to the timing of ability to discover novel and potentially first-in-class small molecule oncology therapeutics. Such forward-looking statements involve substantial risks and uncertainties that could cause IDEAYA's preclinical and clinical development programs, future results, performance or achievements to differ significantly from those expressed or implied by the forward-looking statements. Such risks and uncertainties include, among others, the uncertainties inherent in the drug development process, including IDEAYA's programs' early stage of development, the process of designing and conducting preclinical and clinical trials, the regulatory approval processes, the timing of regulatory filings, the challenges associated with manufacturing drug products, IDEAYA's ability to successfully establish, protect and defend its intellectual property, and other matters that could affect the sufficiency of existing cash to fund operations. IDEAYA undertakes no obligation to update or revise any forward-looking statements. For a further description of the risks and uncertainties that could cause actual results to differ from those expressed in these forward-looking statements, as well as risks relating to the business of IDEAYA in general, see IDEAYA's Annual Report on Form 10-K dated February 18, 2025 and any current and periodic reports filed with the U.S. Securities and Exchange Commission.

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