Pfizer Logo

XtalPi Inc. Announces Strategic Research Collaboration with Pfizer Inc. to Develop Artificial Intelligence-Powered Molecular Modeling Technology for Drug Discovery

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CAMBRIDGE, Mass., May 8, 2018 –XtalPi Inc. (“XtalPi”), a computation-driven pharmaceutical technology company, announced today a strategic research collaboration with Pfizer Inc. (NYSE:PFE) (“Pfizer”) to develop a hybrid physics- and artificial intelligence (AI)-powered software platform for accurate molecular modeling of drug-like small molecules.

This state-of-the-art platform will combine quantum mechanics and machine learning algorithms with cloud computing architecture to improve the accuracy and chemical-space coverage of molecular mechanics modeling, and enable the prediction of pharmaceutical properties relevant for drug discovery and development. Building upon XtalPi’s existing relationship with Pfizer for crystal structure prediction (CSP), this research collaboration aims to help XtalPi and Pfizer further advance their capabilities in computation-based rational drug design and solid-form selection.

As part of the collaboration, a portion of the molecular mechanics parameters generated with publicdomain compounds will be made available to the academic community in hopes of fostering continuous improvement and scientific innovations in related fields.

“The XtalPi collaboration is an opportunity to enhance our computational modeling capabilities,” said Charlotte Allerton, Pfizer’s Head of Medicine Design. “We are looking forward to potentially utilizing new tools to increase our effectiveness in small molecule drug discovery and development.”

“We are excited to partner with Pfizer, a leading pharmaceutical innovator which shares our belief that algorithm-driven technologies with physics insight will give rise to a new generation of highly efficient and accurate drug research and development tools,” said Shuhao Wen, XtalPi's Co-founder and Chairman of the Board. "The collaboration allows us to apply our expertise in molecular modeling, AI, and cloud computing towards improving existing computational methods while exploring new algorithms to address a wide range of drug design challenges. We look forward to helping expedite research into novel therapeutics as our intelligent digital drug discovery and development platform continues to expand and succeed.

” About XtalPi Inc.
XtalPi is a pharmaceutical technology company that is reinventing the industry's approach to drug research and development with its Intelligent Digital Drug Discovery and Development (ID4) platform. With tightly interwoven quantum physics, artificial intelligence, and high-performance cloud computing algorithms, XtalPi’s ID4 platform provide accurate predictions on the physiochemical and pharmaceutical properties of small-molecule candidates for drug design, solid-form selection, and other critical aspects of drug development. XtalPi

is dedicated to improving the efficiency, accuracy, and success rate of drug research and development, and contributing to a healthier society worldwide.
Founded in 2014 by a group of quantum physicists at MIT, XtalPi has since built an elite team with multidisciplinary expertise in physics, chemistry, pharmaceutical R&D, and algorithm design. XtalPi's cuttingedge technologies, innovative solutions, and diverse applications across the pharmaceutical value chain have helped it gain industry approval and establish strategic partnerships with top international pharmaceutical companies.

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