XtalPi Holdings Limited
晶泰控股有限公司

(Incorporated in the Cayman Islands with limited liability)

(Stock Code: 2228)

VOLUNTARY ANNOUNCEMENT

STRATEGIC PARTNERSHIP WITH A LEADING BIOPHARMA COMPANY TO DEVELOP ORAL SMALL MOLECULE THERAPEUTICS FOR A GPCR TARGET, WITH A TOTAL POTENTIAL DEAL VALUE OF OVER US$400 MILLION

This announcement is made by XtalPi Holdings Limited (the "**Company**" or "**XtalPi**", together with its subsidiaries, the "**Group**") on a voluntary basis. The purpose of this announcement is to keep the shareholders and potential investors of the Company informed of the latest business development of the Group.

The board of directors of the Company (the "**Board**") is pleased to announce a strategic partnership with a prominent international biopharmaceutical company. The collaboration focuses on developing a best-in-class small molecule against a G protein-coupled receptor (GPCR). This agreement builds upon a rigorous and successful pilot phase, where XtalPi's integrated quantum physics and AI algorithms delivered breakthrough hit rates, confirming the platform's capacity to tackle this complex metabolic target.

Under the agreement, the partner will provide an upfront payment and fully fund XtalPi's early R&D efforts. In addition, XtalPi is also eligible to receive potential preclinical, clinical, and commercial milestones, along with potential future royalties, bringing the total potential deal value to over US$400 million. This partnership underscores the industry's strong confidence in XtalPi's scientific infrastructure and reinforces XtalPi's competitive edge and sustainable growth in conquering high-value targets.

Navigating Structural Blind Spots

The specific GPCR target receptor central to this collaboration exhibits extreme conformational plasticity, making its active pockets notoriously difficult for small molecules to selectively engage. Compounding this challenge is the absence of publicly reported high-resolution experimental structures bound to small-molecule ligands. Operating within this structural blind spot, traditional high-throughput screening (HTS) methods frequently fall short in delivering molecules that satisfy the stringent, multidimensional requirements for potency, subtype selectivity, and oral bioavailability.

To bypass the structural data void with this highly dynamic GPCR, XtalPi's R&D team deployed multiscale enhanced sampling simulations to rigorously map the receptor's functional conformational landscape and implemented a dynamic, multi-conformational screening strategy.

Elucidating Conformational Dynamics

Leveraging advanced quantum physics models and AI algorithms, XtalPi executed highly efficient virtual screening across hundreds of millions of commercial compounds. The company then applied its proprietary XFEP (Free Energy Perturbation) platform for precise binding affinity prediction.

Scaling R&D with a Closed-Loop AI and Robotics Engine

Entering the comprehensive collaboration phase, XtalPi will fully deploy its structure-based rational drug design platform. By seamlessly integrating quantum physics, generative AI, and large-scale automated chemical synthesis orchestrated by a Multi-AI-Agent system, XtalPi will drive rapid Design-Make-Test-Analyze (DMTA) cycles.

This automated laboratory infrastructure bridges the historical gap between computational design and wet-lab synthesis and validation, continuously generating novel drug candidates optimized for high potency and ideal ADMET (absorption, distribution, metabolism, excretion, and toxicity) profiles. Ultimately, this approach aims to significantly expand the druggable chemical space and shorten discovery timelines, accelerating the translation of cutting-edge computational breakthroughs into substantial clinical assets for patients worldwide.

Forward Looking Statement

There is no assurance that any forward-looking statements regarding the business development of the Group in this announcement or any of the matters set out herein are attainable, will actually occur or will be realized or are complete or accurate. Shareholders and/or potential investors of the Company are advised to exercise caution when dealing in the shares of the Company.

By Order of the Board
XtalPi Holdings Limited
Dr. Wen Shuhao
Chairman of the Board and Executive Director

Hong Kong, 9 June 2026

As at the date of this announcement, the Board comprises Dr. Wen Shuhao, Dr. Ma Jian, Dr. Lai Lipeng and Dr. Jiang Yide Alan as executive Directors, and Mr. Law Cheuk Kin Stephen, Ms. Chan Wing Ki and Mr. Chow Ming Sang as independent non-executive Directors.