Shuttle to Enter $3.24 Billion AI Pharmaceutical Market

GAITHERSBURG, Md., Oct. 09, 2025 (GLOBE NEWSWIRE) — Shuttle Pharmaceuticals Holdings, Inc. (Nasdaq: SHPH) (“Shuttle Pharma” or the “Company”), a discovery and development stage specialty pharmaceutical company, today announced the execution of a non-binding letter of Intent with Molecule.ai.

Molecule.ai, a pioneering artificial intelligence company founded by AI scientist and researcher **Dr. ZT Zhang, PhD**, today announced the execution of a letter of Intent to acquire Molecule.ai and its state-of-the-art platform designed to transform the way pharmaceutical and biotech companies discover and develop new therapeutics.

By leveraging advanced machine learning models, including large language models (LLMs), Molecule.ai delivers **industry-leading accuracy and efficiency** in evaluating novel molecules. The platform enables researchers to shorten development timelines, reduce costs, and increase the likelihood of identifying successful therapeutic candidates.

“Our vision is to empower scientists with the most advanced AI-driven tools to push the boundaries of drug discovery,” said **Dr. ZT Zhang, Founder and CEO of Molecule.ai**. “With Molecule.ai, we are not just accelerating the process – we are fundamentally changing what’s possible in the search for new therapies.”

The Molecule.ai platform introduces several groundbreaking capabilities:

1. **Molecule Property Prediction and Reasoning** – Rapid and large-scale evaluation of chemical and biological properties across massive compound libraries, including novel and previously uncharacterized molecules.
2. **Drug-Target Interaction Modeling** – A powerful new feature that identifies and optimizes molecule-target interactions, paving the way for more precise therapeutic design.
3. **Agentic AI Mode** – An autonomous framework that enables AI agents to perform multi-step drug discovery workflows, from compound screening through optimization, significantly reducing manual effort.

With these innovations, Molecule.ai positions itself as a trusted partner for pharmaceutical and biotechnology organizations aiming to accelerate discovery and bring life-saving treatments to market faster.

Terms of the non-binding letter of Intent are as follows:

Shuttle will acquire all of the rights, title and interests Molecule.ai has free and clear of all liens.

Shuttle will assume all liabilities in respect of Molecule.ai and at Closing (as defined below), Molecule.ai shall have no further obligations or liabilities thereunder.

Molecule.ai will extend the current AI model and platform to support Drug-Target Interaction.

Molecule.ai will add first version of Agentic AI mode that enables an automatic workflow for drug discovery.

Molecule.ai will serve as lead liaison and headhunter, leveraging its relationships in the artificial intelligence community to recruit additional employees and strengthen the team.

Consideration:

As consideration for the purchase and the Transaction, and Shuttle's assumption of its obligations and liabilities, Shuttle shall pay to Molecule.ai, at closing, a purchase price of $10 million payable, subject to the completion of the milestones, in a combination of cash and common shares of Shuttle. Consideration will be paid to Molecule.ai based upon certain milestones to be determined by both parties.

About Molecule.ai

Molecule.ai is an advanced artificial intelligence company focused on revolutionizing drug discovery and development. Founded by **Dr. ZT Zhang, PhD**, the company applies cutting-edge machine learning models and large language models (LLMs) to molecular evaluation, drug-target interaction modeling, and autonomous drug discovery workflows. Molecule.ai's mission is to empower researchers with next-generation tools that reduce costs, improve efficiency, and unlock new possibilities in therapeutic development.

About Shuttle Pharmaceuticals

Shuttle Pharma is a discovery and development stage specialty pharmaceutical company focused on improving the outcomes for cancer patients treated with radiation therapy (RT). Our mission is to improve the lives of cancer patients by developing therapies that are designed to maximize the effectiveness of RT while limiting the side effects of radiation in cancer treatment. Although RT is a proven modality for treating cancers, by developing radiation sensitizers, we aim to increase cancer cure rates, prolong patient survival and improve quality of life when used as a primary treatment or in combination with surgery, chemotherapy and immunotherapy. For more information, please visit our website at www.shuttlepharma.com.

Safe Harbor Statement

Statements in this press release about future expectations, plans and prospects, as well as any other statements regarding matters that are not historical facts, may constitute

“forward-looking statements.” These statements include, but are not limited to, statements concerning the development of our company. The words “anticipate,” “believe,” “continue,” “could,” “estimate,” “expect,” “intend,” “may,” “plan,” “potential,” “predict,” “project,” “should,” “target,” “will,” “would” and similar expressions are intended to identify forward-looking statements, although not all forward-looking statements contain these identifying words. Actual results may differ materially from those indicated by such forward-looking statements as a result of various important factors, including factors discussed in the “Risk Factors” section of Shuttle Pharma’s Annual Report on Form 10-K for the year ended December 31, 2024, filed with the SEC on February 26, 2025, as well other SEC filings. Any forward-looking statements contained in this press release speak only as of the date hereof and, except as required by federal securities laws, Shuttle Pharmaceuticals specifically disclaims any obligation to update any forward-looking statement, whether as a result of new information, future events or otherwise.

Shuttle Pharmaceuticals
Chris Cooper
Chief Executive Officer
info@shuttlepharma.com

Headline Reference – Artificial Intelligence In Pharmaceutical Industry Research Report 2025-2033: Merging AI Technologies to Revolutionize Drug Discovery, Improve Patient Outcomes, and Drive Operations Efficiency