

從老藥新用到精準醫療：人工智慧引領未來藥物開發

From Repurposing to Precision: AI Leads the Way

While high-throughput screens have revealed numerous anti-cancer compounds in cell lines, translating these findings to patient tumors remains a challenge due to genomic disparities. We introduce ADEPT—a deep learning framework combining an adversarial encoder with a transformer predictor—to bridge this gap by learning tumor-like mutation patterns from cell line data. ADEPT accurately predicts drug responses across cancer types and identifies clinically relevant biomarkers. Applied to triple-negative breast cancer, it highlighted repurposed drugs—including proteasome and HDAC inhibitors—with strong therapeutic potential and matched genetic markers. To elucidate mechanisms, we used GNINA and AlphaFold-based docking, followed by functional validation of predicted targets. An AI-driven pipeline further guided the search for optimized analogs with favorable drug-like properties, e.g. ADME-T, advancing the path from drug repurposing to precision oncology.