Creative Biolabs Expands Integrated AI-Driven Chemical Synthesis Platforms to Accelerate Next-Generation Drug Discovery

Creative Biolabs has expanded its end-to-end AI-driven synthesis solutions to address critical bottlenecks in modern medicinal chemistry.

SHIRLEY, NY, UNITED STATES, September 9, 2026 /EINPresswire.com/ -- The platform integrates AI-based molecular design, synthetic feasibility assessment, automated chemical synthesis, and experimental validation within a unified DMTA (design-make-test-analyze) workflow. By operating under this cohesive capability framework, the company delivers tailored discovery pipelines spanning small molecules, antibody-drug conjugates (ADCs), and targeted protein degraders (PROTACs). Offering comprehensive AI drug discovery services and medicinal chemistry services, Creative Biolabs bridges in silico predictions directly with automated wet-lab synthesis, allowing biopharmaceutical researchers to bypass traditional trial-and-error chemistry.

Unlocking Uncharted Chemical Space with Generative AI
Traditional lead generation often yields candidate compounds that are difficult or expensive to synthesize. Through its advanced AI chemical synthesis and de novo design services, Creative Biolabs navigates vast chemical space while embedding synthetic accessibility constraints directly into generative algorithms.

Multi-Parametric Lead Optimization: Simultaneously optimizes potency, selectivity, ADMET profiles, and production costs.
Integrated Retrosynthesis: Evaluates commercial building blocks and organic reaction pathways in silico to ensure proposed molecules have viable, high-yield synthetic routes.
Automated DMTA Cycles: Connects virtual screening results to high-purity automated synthesis

platforms for rapid hit-to-lead transitions.
Commercial Impact: This streamlined workflow significantly reduces synthesis failures, accelerates hit-to-lead timelines, and lowers the attrition rate of early-stage candidate compounds.

Engineering Next-Generation ADCs with Mathematical Precision
Developing stable, homogeneous antibody-drug conjugates requires overcoming payload aggregation, narrow therapeutic windows, and variable drug-to-antibody ratios (DAR). To de-risk ADC development and synthesis, the company utilizes geometric graph neural networks (GNNs) and structural deep learning to predict conjugation sites, paratope integrity, and linker cleavage kinetics prior to wet-lab bioconjugation.

Site-Specific Bioconjugation: Facilitates highly homogeneous DAR profiles via enzymatic, genetic, and Fc-affinity peptide-guided tagging.
Hydrophobicity Masking: Generates hydrophilic branched PEG spacers and XTEN polypeptide linkers designed to minimize aggregation and support circulatory half-life.
Predictive DMPK & Stability: Models systemic plasma stability to help prevent premature payload release and reduce off-target toxicity.
Commercial Impact: By resolving these conjugation challenges, developers obtain robust, structurally validated experimental materials that are immediately ready for downstream in vivo evaluation.

Overcoming Linker and Ternary Bottlenecks in Targeted Protein Degradation
Targeted protein degradation leverages cellular ubiquitin-proteasome systems to destroy previously "undruggable" proteins. However, empirical linker optimization and unstable ternary complex formation frequently stall discovery campaigns. Creative Biolabs addresses these hurdles through its specialized PROTAC design and synthesis services.

Ternary Complex Simulation: Overcomes limited crystal structure availability by predicting stable ternary interactions between the protein of interest (POI), E3 ligase, and bifunctional degrader.
Rational Linker Design: Computationally evaluates extensive libraries of linker geometries and attachment vectors to maximize degradation selectivity.
High-Purity Complex Synthesis: Employs multi-step organic synthesis protocols to deliver bifunctional degraders with industry-standard high purity (typically >95% as verified by LC-MS and HPLC).
Commercial Impact: This computational-to-synthetic pipeline solves the challenge of hard-to-synthesize molecules, keeping degradation campaigns on schedule and minimizing wasted experimental bandwidth.

About Creative Biolabs
Creative Biolabs is a global biotechnology partner specializing in computational drug discovery, recombinant antibody engineering, and custom chemical synthesis. Combining state-of-the-art AI algorithms with deep medicinal chemistry expertise, the company empowers

biopharmaceutical innovators to accelerate candidate developability and streamline translational pipelines.

Candy Swift
Creative Biolabs
+1 631-830-6441
marketing@creative-biolabs.com
