AI-driven peptide drug discovery enables sub-6-month identification of clinically validated binders

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Peptide drug discovery is typically constrained by iterative design and screening cycles requiring 12–24 months to identify functional binders with therapeutic relevance. Computational approaches have yet to consistently deliver candidates that translate into in vivo efficacy within clinically actionable timelines.

We present an integrated artificial intelligence and molecular modelling platform that reduces the design-to-validation cycle to under 6 months by combining data-driven sequence generation, structure-based modelling, and rapid experimental iteration.

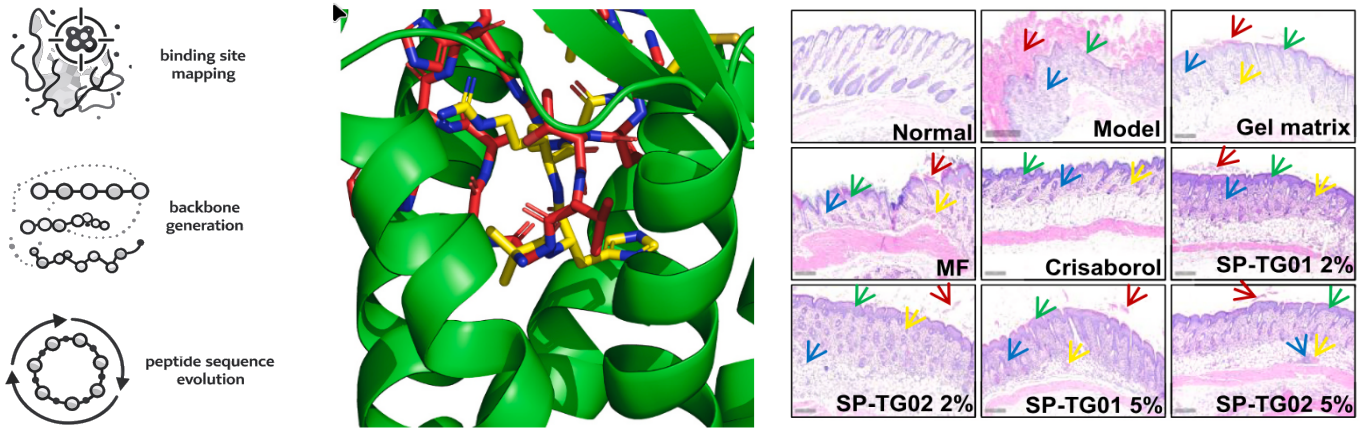

Figure 1. AI-driven peptide design and validation. Left: workflow schematic. Middle: structural model of peptide–CCR8 interaction. Right: histological sections of atopic dermatitis models showing reduced epidermal thickening and inflammation following peptide treatment.

We demonstrate this approach through the discovery of CCR8-targeting[1] peptide inhibitors for atopic dermatitis. AI-guided design[2] yielded nanomolar-affinity binders (K_D ≈ 8–17 nM) that showed robust *in vivo* efficacy across two independent models, significantly reducing disease severity, epidermal thickening, and inflammatory burden following topical administration. One lead candidate from this program has advanced to Phase 1 clinical evaluation.

These results show that integrated AI and modelling can deliver clinically relevant peptide therapeutics within substantially compressed timelines.

[1] S. Hao, J. Zhou, T. Siriwardena, S. Javor, B. Gan, R. He, Y. Song, Z. Wang, W. Xiao, Int. Immunopharmacol., 2026, 170, 116051.

[2] (a) E. Zakharova, M. Orsi, A. Capecchi, J.-L. Reymond, ChemMedChem, 2022, e202200291. (b) J. Arús-Pous, S. V. Johansson, O. Prykhodko, E. J. Bjerrum, C. Tyrchan, J.-L. Reymond, H. Chen, O. Engkvist, J. Cheminform., 2019, 11, 71.