

AI Drug Discovery Is Broken

Not because of data — but because of how we test it

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THE DATA

Methods with data leakage

A recent study reveals that nearly all top-performing AI models for protein-ligand binding prediction suffer from data leakage in benchmarking.

This undermines their real-world utility, as models trained on hidden data cannot generalize to novel compounds.

Source: Nature Machine Intelligence · Published October 23, 2026
<https://www.nature.com/articles/s42256-026-01331-8>



01

Testing Is the Real Bottleneck

The study emphasizes that reproducibility and rigorous data splits — like scaffold or cluster-based splits — are not optional; they are essential for meaningful progress. Without them, AI remains a black box with no real predictive power beyond its training set.

02

Quantum-Ready AI Requires Integrity

The study's proposed guidelines — including mandatory code and data disclosure, run-to-run variability checks, and out-of-distribution testing — are not just academic hygiene. They are the minimum requirement for any AI system that will be paired with quantum computing in high-stakes domains like drug discovery.



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