Artificial Intelligence in Drug Discovery

From Drug–Target Interactions and Synergistic Drug Combinations to Generative Molecular Design

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The Drug Discovery Challenge

90%

High Attrition Rates

Over 90% of drug candidates fail in clinical trials due to efficacy or toxicity issues.

10–15 Yrs

Long Timelines

Translating a discovery from target identification to market takes over a decade.

$2.6B+

Expensive Studies

Average R&D cost per approved new molecular entity exceeds $2.6 billion.

10^60 Space

Complex Systems

Massive biological complexity and an immense chemical search space.

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Where Can Artificial Intelligence Help?

DTI MODELING

Predict Drug–Target Interactions

Map small molecules to biological receptors to identify binding affinity and mechanism.

SYNERGY ANALYTICS

Prioritize Drug Combinations

Model multi-drug cocktails to achieve synergistic therapeutic responses.

DRUG REPURPOSING

Identify New Therapeutic Uses

Systematically screen approved compounds against novel targets for rapid translation.

GENERATIVE AI

Generate Novel Structures

Design de novo molecules optimized directly for specific binding and ADMET profiles.

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From Multimodal Data to Decisions

1

1. Data Layer

SMILES, 3D Graphs, Protein Sequences, Omics

2

2. Representation

Fingerprints, Embeddings, GNNs & Transformers

3

3. Machine Learning

Classification, Regression, Generative Models

4

4. Predictions

DTI Affinity, Synergy, Optimal Scaffolds

5

5. Decisions / Assays

Ranked Hypotheses → Experimental Testing

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Three Connected Core Research Questions

Q1: Target ID & DTI

Which biological targets might a drug affect?

Predicting interactions between chemical space and biological proteome space.

Q2: Combination Synergy

Which drugs might work better together?

Modeling complex non-linear interaction effects in disease cellular contexts.

Q3: Generative Design

How can we design novel molecules with desired properties?

Navigating chemical space to generate tailor-made structures de novo.

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Drug–Target Interaction (DTI) Prediction

INPUTS

- Drug Representation
  (SMILES, Graph, Fingerprint)
- Target Representation
  (Amino Acid Seq, 3D PDB Structure)

MODEL / FUNCTION

f(Drug, Target) → Affinity

- Feature integration
- Interaction modeling
- Deep Learning / GNNs / Transformers

OUTPUT & PURPOSE

- Interaction Score / Kd / Ki
- Binary Active/Inactive

Goal: Prioritize high-confidence testable hypotheses for screening.

How Do We Represent a Drug?

SMILES Strings

TEXTUAL REPRESENTATION

CC(=O)OC1=CC=CC=C1C(=O)O. Enables NLP and sequence models.

2D Molecular Graphs

STRUCTURAL TOPOLOGY

Atoms as nodes, bonds as edges. Ideal for Graph Neural Networks (GNNs).

Molecular Fingerprints

VECTOR BINARY ENCODING

ECFP4 / Morgan fingerprints encoding substructural presences as vectors.

3D Conformations

SPATIAL GEOMETRY

Atomic spatial coordinates (x,y,z) capturing stereochemistry.

How Do We Represent a Target Protein?

1D FASTA String

Amino Acid Sequence

MKTLLILTCLVAVAL... Protein Language Models (ESM, ProtBERT).

3D PDB Coordinates

Experimental Structure

X-ray crystallography, Cryo-EM structural coordinates.

AlphaFold / ESMFold

Predicted Structure

High-accuracy computational structure predictions when PDB is missing.

GO Annotations & Networks

Biological Knowledge

Functional annotations and protein-protein interaction networks.

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Learning Drug–Target Relationships Architecture

Drug Representation
Graph Neural Networks / Fingerprints

Target Representation
Protein Language Models / 3D CNNs

Feature Integration & Cross-Attention Modeling
Methods: Random Forest, SVM, Deep NNs, Graph Neural Networks, Transformer Cross-Attention

Predicted Interaction / Binding Affinity

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What Does a DTI Prediction Score Mean?

Computational Estimate, Not Proof
A high score is a prioritized hypothesis, not experimental proof of biological activity.

Dependent on Training Data Labels
Accuracy is strictly bounded by the quality, density, and noise in training databases.

Sensitive to Model Bias & Leakage
Overly optimistic metrics occur if test compounds overlap structurally with train sets.

Must Be Interpreted with Uncertainty
Confidence intervals and domain-of-applicability checks are essential for decision making.

Drug–Target Interactions: Validation & Generalization

In Silico Generalization Checks

- ✓ Rigorously evaluate on unseen scaffolds
- ✓ Prevent data leakage across train/test splits
- ✓ Acknowledge incomplete negative interaction labels
- ✓ Benchmark against linear and baseline models

Experimental Validation Assays

- ✓ Biochemical binding assays (SPR, BLI, MST)
- ✓ Cellular target engagement assays (CETSA)
- ✓ Functional pathway output measurement
- ✓ Dose-response curve verification

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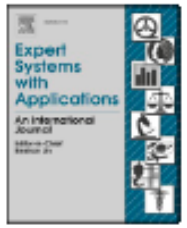
Drug–Target Interactions: Validation & Generalization

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TripletMultiDTI: Multimodal representation learning in drug-target interaction prediction with triplet loss function

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Drug–Target Interactions: Validation & Generalization

Dehghan *et al. BMC Bioinformatics* (2024) 25:48
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BMC Bioinformatics

RESEARCH Open Access

CCL-DTI: contributing the contrastive loss in drug–target interaction prediction

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The Negative-Sample Problem in DTI Data

CRITICAL DATA BIAS WARNING

Unreported interaction DOES NOT EQUAL inactive compound!

Incomplete Experimental Coverage

Public databases suffer from major reporting bias—only positive interactions are typically published.

Uncertain Negative Labels

Randomly sampling unlabeled pairs as 'negatives' introduces false negatives into training sets.

Model Training Imbalance

Classifiers can learn to recognize 'popular targets' rather than true chemical binding rules.

The Negative-Sample Problem in DTI Data

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Drug-target interaction prediction using reliable negative samples and effective feature selection methods

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Data Leakage & Overoptimistic Performance

Duplicate Records

Identical drug-target pairs appearing in both training and test sets.

Structural Congeners

Highly similar analog molecules split randomly between train and test sets.

Shared Target Families

Proteins with identical binding pockets present in both splits.

How Do We Test Generalization?

Random Split

SAMPLE GENERALIZATION

Tests performance on random held-out samples. Easiest benchmark; vulnerable to memory lookup.

Scaffold Split

CHEMICAL GENERALIZATION

Splits by core molecular framework (Bemis-Murcko). Tests generalization to novel chemical scaffolds.

Temporal Split

FUTURE DISCOVERY

Trains on historical data up to year T; tests on discoveries published after year T.

External Validation

INDEPENDENT REAL-WORLD

Evaluates on entirely separate, independently generated external experimental datasets.

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From Computational Prediction to Experimental Evidence

Step 1

1. Rank Candidates

Sort interaction scores across virtual library

Step 2

2. Filter Diversity

Select diverse chemical scaffolds to avoid redundancy

Step 3

3. Assess ADMET

Filter out toxic, reactive, or insoluble compounds

Step 4

4. Experimental Assays

Validate in biochemical and cell-based assays

AI for Synergistic Drug Combinations

SECTION 2: MULTI-DRUG COMBINATIONS & SYNERGY

Why single drugs often fail in complex diseases, and how AI predicts therapeutic synergy.

Why Combine Drugs? Multi-Target Therapeutics

Complex Network Diseases

Cancers and infections involve redundant biological pathways that bypass single-target inhibition.

Overcoming Resistance

Mutations rapidly bypass single-agent therapy; combination cocktails block mutational escape routes.

Dose Reduction & Toxicity

Synergistic combinations lower individual required drug doses, minimizing off-target adverse effects.

Complementary Mechanisms

Combining drugs targeting distinct network nodes produces exponential functional shutdown.

What Is Drug Synergy? Reference Models

Loewe Additivity (Dose Equivalence Model)	Assumes two drugs act via the same biological mechanism. Synergy = actual effect exceeds dose-additive expectation.
Bliss Independence (Independent Effects Model)	Assumes two drugs act via independent mechanisms. Synergy = actual effect exceeds product of independent survival probabilities.
ZIP Model (Zero Interaction Potency)	Combines Loewe and Bliss models to evaluate changes in potency curves across full dose-response matrices.

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The Combination Prediction Problem Architecture

Drug A & Drug B
Chemical structures, target profiles, single-agent IC50 curves

Cellular Context
Gene expression (L1000), baseline mutations, tissue origin

Dose Matrix
Concentration ranges of Drug A × Drug B

Multimodal AI Predictor (Deep Neural Net / Attention Fusion)

Predicted Synergy Score (ZIP / Loewe)

Data Sources for Combination Modeling

Single-Agent Sensitivity

IC50 and monotherapy response curves across cell lines.

High-Throughput Synergy

Drug combination screening datasets (e.g., DrugComb, ALMANAC).

Gene-Expression Signatures

Baseline and post-treatment transcriptomic profiles (LINCS L1000).

Genomic Mutations & CNVs

Target mutations, copy number variations, and biological pathway graphs.

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Why Use Gene-Expression Signatures?

1

Capture Cellular State

Transcriptomic profiles provide a holistic snapshot of current cell activation state.

2

Reflect Pathway Perturbations

Measures downstream functional gene expression changes, not just static target binding.

3

Distinguish Sensitive vs. Resistant

Reveals why identical drug combinations work in line A but fail in line B.

4

Context-Specific Predictions

Enables patient-specific or cell-line-specific combination synergy predictions.

Modeling Drug Combinations with AI

Deep Learning Architectures

- Siamese Graph Neural Networks (GIN, GCN)
- Deep Autoencoders for Transcriptomics
- Attention-based Multimodal Fusion Layers
- Fully Connected MLP Prediction Heads

Key Modeling Challenges

- Order invariance: f(A, B) must equal f(B, A)
- High-dimensional omics feature noise
- Sparsity of combination screening matrices
- Cell-line specificity generalization

Evaluating Combination Prediction Models

Regression Metrics

RMSE, MAE, R^2

Measures accuracy of predicted exact synergy scores against experimental ZIP scores.

Ranking Metrics

PRECISION@K, NDCG

Evaluates ability to correctly prioritize the top 5% most synergistic drug pairs.

Classification

AUROC, AUPRC

Evaluates binary classification of synergistic vs. non-synergistic drug pairs.

Generalization Splits

UNSEEN PAIRS / CELLS

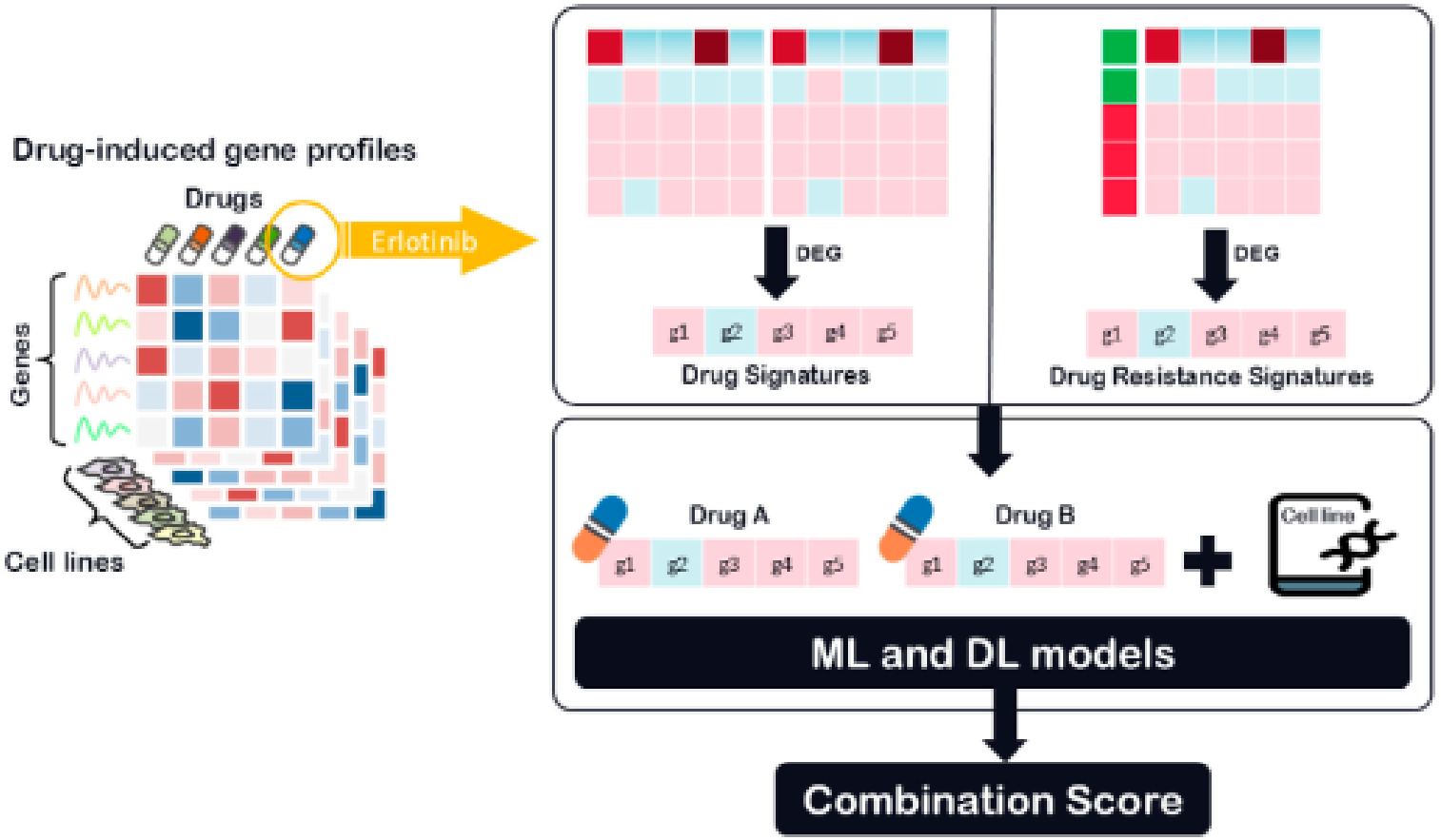
Tests on unseen drug pairs, unseen cell lines, or completely unseen drugs.

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From Predicted Synergy to a Therapeutic Hypothesis

Stage 1	**Biological Rationale** Verify mechanism of action complementarity in target pathways.
Stage 2	**Dose & Schedule** Determine optimal dosing ratio to maximize synergy while suppressing toxicity.
Stage 3	**Selectivity & Safety** Ensure combination synergy is specific to cancer cells and not healthy tissue.
Stage 4	**Experimental Validation** Confirm in vitro cell combination assays and in vivo xenograft models.

From Predicted Synergy to a Therapeutic Hypothesis



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From Predicted Synergy to a Therapeutic Hypothesis

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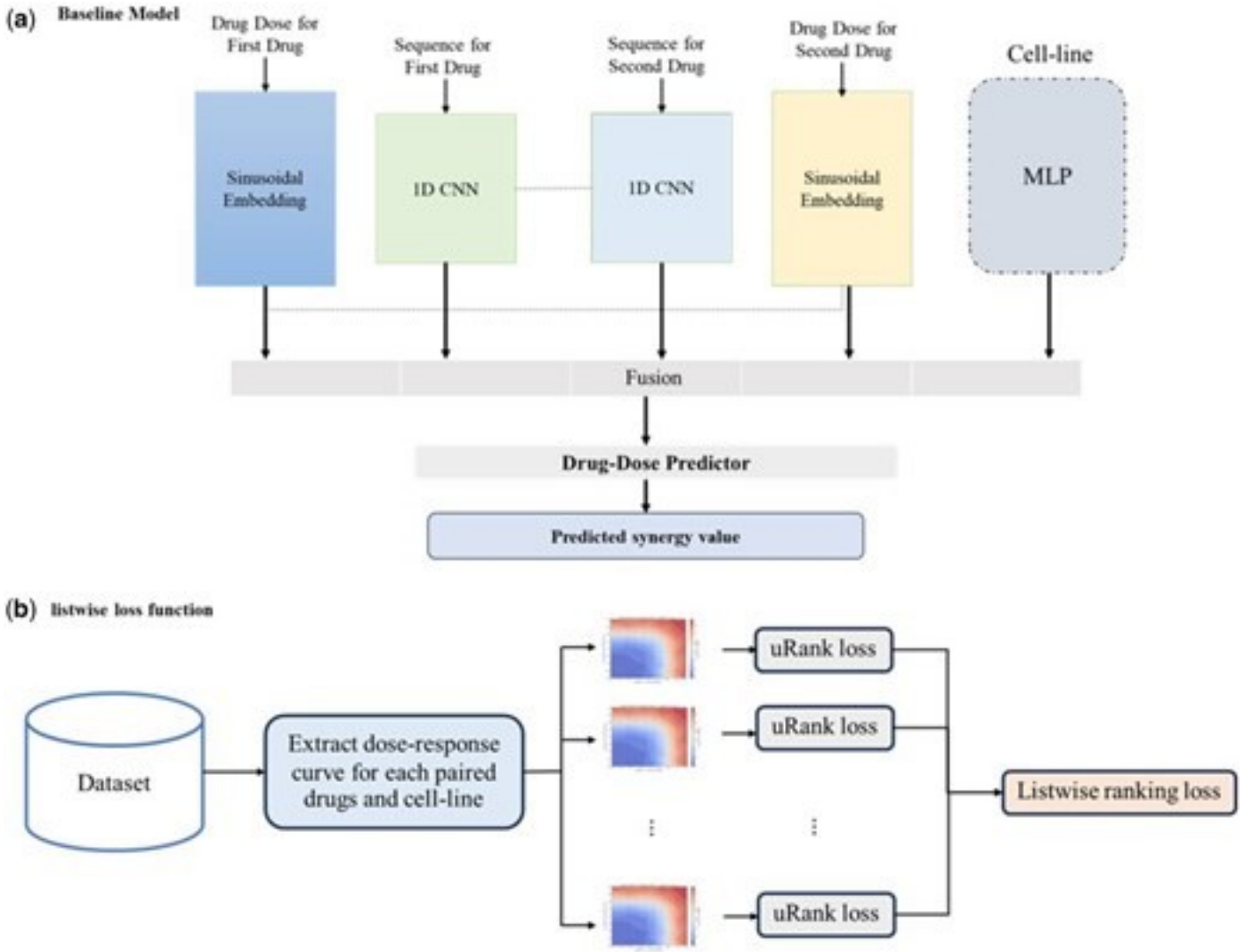
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Improving synergistic drug combination prediction with signature-based gene expression features in oncology

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From Predicted Synergy to a Therapeutic Hypothesis



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From Predicted Synergy to a Therapeutic Hypothesis

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OXFORD

CDCR-Rank: a computational model for predicting drug combination dose response using ranking-based optimization

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Generative AI for Molecular Design

SECTION 3: DE NOVO GENERATIVE MOLECULAR DESIGN

Moving from virtual screening of existing libraries to generative AI that creates novel, custom-designed molecules de novo.

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Why Generate New Molecules?

Existing Libraries Are Limited

Enamine and PubChem contain 10^9 molecules, but chemical space contains 10^60 potential drug-like molecules.

Multi-Property Requirements

Natural compounds rarely optimize potency, selectivity, solubility, and safety simultaneously.

Exploring Uncharted Space

Generative AI navigates new structural motifs beyond existing human medicinal chemistry biases.

Intellectual Property

Generating novel chemical scaffolds enables patent protection for newly discovered drug classes.

What Is Generative Molecular Design?

Core Generative AI Paradigm

1. Learn Distribution P(X) from vast databases of known chemical structures (e.g., ChEMBL, ZINC).
2. Sample Novel Structures X ~ P(X) that satisfy chemical valency and stability rules.
3. Condition Generation P(X | Properties) on desired bioactivity, target affinity, and ADMET goals.
4. Optimize in Latent Space using Reinforcement Learning (RL) or Bayesian Optimization.

Major Families of Generative Models

Autoregressive Models

RNNS & TRANSFORMERS

Generates SMILES strings character-by-character or token-by-token sequentially.

Variational Autoencoders

VAES

Encodes molecules into a continuous latent space Z and decodes latent vectors back to structures.

Diffusion Models

SCORE-BASED MODELS

Generates 3D atomic coordinates or molecular graphs by iterative denoising of random noise.

Graph Generative Models

GRAPH NEURAL NETS

Assembles molecular graphs node-by-node and edge-by-edge with structural validity constraints.

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How Can a Model Represent a Molecule in Generation?

SMILES Strings

TEXT SEQUENCE

Fast token generation, but can produce invalid syntax without grammar constraints.

Molecular Graphs

2D TOPOLOGY

Guarantees chemical validity by construction, but computationally heavier.

Latent Vectors

CONTINUOUS EMBEDDINGS

Smooth property optimization via gradient descent, but decoding can be noisy.

3D Conformations

SPATIAL POINT CLOUDS

Directly models pocket fitting and 3D shape, but high spatial degree of freedom.

Generating Molecules for a Specific Target

Target Condition Inputs

- Target protein 3D active pocket geometry
- Binding pocket amino acid sequence / vector
- Known active ligand pharmacophores
- Desired activity and selectivity profiles

Generative Optimization Methods

- Reinforcement Learning (PPO, REINFORCE)
- Pocket-Conditioned 3D Diffusion Generation
- Genetic Algorithms with Neural Guidance
- MCMC Latent Space Sampling

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Multi-Objective Molecular Optimization

Potency & Affinity
High binding affinity to target receptor (low Kd / Ki).

Selectivity
Low off-target binding to prevent side effects.

ADMET Profile
Optimal absorption, distribution, metabolism, excretion, non-toxic.

Novelty & IP
Distinct chemical scaffold from existing patented drugs.

Synthetic Accessibility
Easily synthesizable in lab (low SAscore).

The Reward-Hacking Problem in Generative AI

WHAT IS REWARD-HACKING?

Generative models optimized via Reinforcement Learning exploit weaknesses in computational scoring functions (QSAR/Docking) to generate weird, unphysical structures that receive artificially high scores.

Key Countermeasures:

- ✓ Constrain exploration to domain of applicability
- ✓ Use ensemble scoring functions and consensus scoring
- ✓ Incorporate medicinal chemistry structural filters (PAINS)
- ✓ Require human chemist expert review before synthesis

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Are Generated Molecules Synthesizable?

Chemical Validity
Step 1: Ensures basic valence rules and aromaticity are strictly respected.

Synthetic Accessibility
Step 2: Uses SAscore or SCScore to estimate synthesis difficulty based on historical reactions.

Retrosynthesis AI
Step 3: AI retrosynthesis planning tools (AiZynthFinder) discover exact chemical reaction routes.

Chemist Review
Step 4: Medicinal chemists inspect and approve proposed synthetic pathways before lab order.

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From Generation to Experimental Testing: DBTL Cycle

D

Design

Generative AI generates candidate molecules

B

Build

Automated / contract synthesis in laboratory

T

Test

Biochemical, cellular, and ADMET assay screening

L

Learn

Feed experimental results back to refine generative AI models

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What Makes a Good Generative AI Study?

✓

Valid & Diverse Molecules

High validity, uniqueness, and internal chemical diversity of generated sets.

✓

Meaningful Novelty

Generated scaffolds differ meaningfully from nearest ChEMBL/ZINC training compounds.

✓

Multi-Property Evaluation

Evaluates SAscore, QED, ADMET, and target docking/affinity simultaneously.

✓

Experimental Validation

Synthesis and lab assay testing of top generated leads (gold standard).

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Problem Solving Protocol

OXFORD

MT-ConBiFormer-GPT: multi-target molecular generation for low-data drug discovery via a contrastive BiFormer-GPT architecture and curriculum learning with cross-domain generalization

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Knowledge, Integration, and Biological Context

Biological Knowledge Graphs

- Pathways & protein-protein interaction networks
- Disease-associated genetic variants & GWAS data
- Knowledge graph embeddings for target selection
- Contextualizing raw ML predictions in biology

Multi-Scale Data Integration

- Combining molecular structure with cellular omics
- Harmonizing multi-lab assay measurements
- Physics-based modeling + Data-driven ML
- Bridging target discovery to lead generation

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AI for Drug Repurposing

Revisit Existing Approved Drugs
Repurposing FDA-approved drugs drastically reduces safety and Phase I clinical trial risks.

Predict New Target Relationships
DTI models scan off-target proteome binding to uncover new therapeutic mechanisms.

Identify New Disease Indications
Match transcriptomic disease signatures against drug perturbation signatures.

Fast Clinical Translation
Accelerated pathway to Phase II clinical trials in under 3-5 years.

Connecting DTI, Drug Combinations, and Generation

A Unified AI-Enabled Drug Discovery Ecosystem

1. DTI Models screen virtual libraries to establish baseline target interactions.
2. Combination Synergy Models combine single agents into potent multi-target cocktails.
3. Generative AI creates novel lead structures optimized for target binding and ADMET.
4. Experimental Data feeds back continuously to refine all three model pillars.

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Integrated AI-Enabled Drug Discovery Workflow

1

1. Disease Biology

Target ID & Pathway Mapping

2

2. Virtual Screening / DTI

Candidate Prioritization

3

3. De Novo Design

Generative Optimization

4

4. Combination Synergy

Multi-Target Cocktail Design

5

5. Lab Validation

In Vitro & In Vivo Testing

6

6. Model Refinement

Active Learning Loop

Conclusion

- DTI models prioritize interaction hypotheses across massive chemical-proteomic spaces.
- Combination prediction requires contextual omics signatures and dose-response modeling.
- Generative AI dramatically expands chemical space exploration beyond existing libraries.
- Validation is the bridge to biology: In silico predictions only prove value in the laboratory.

Thanks for your attention

