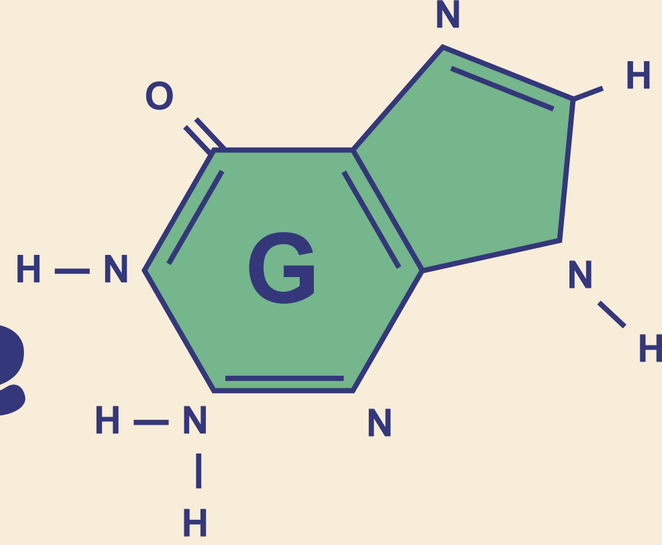
Optimizing Sequence Alignment with Machine Learning for Improved Protein-Compound Interactions



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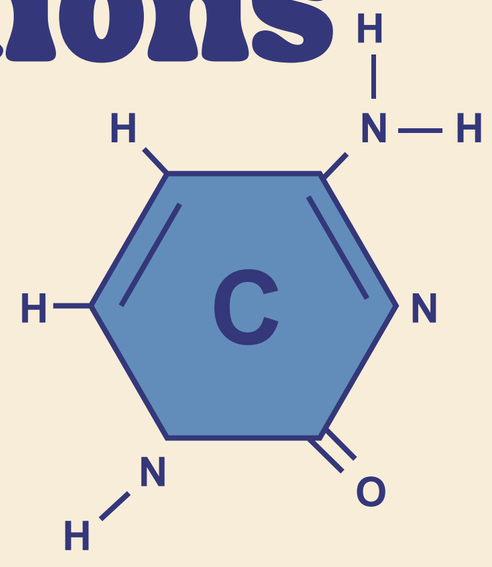
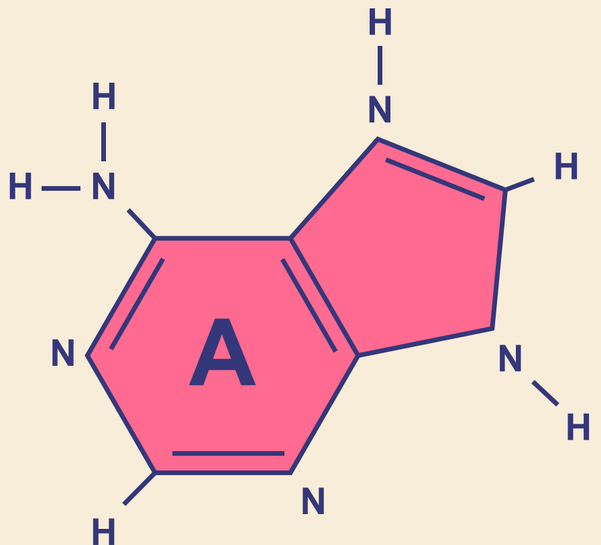
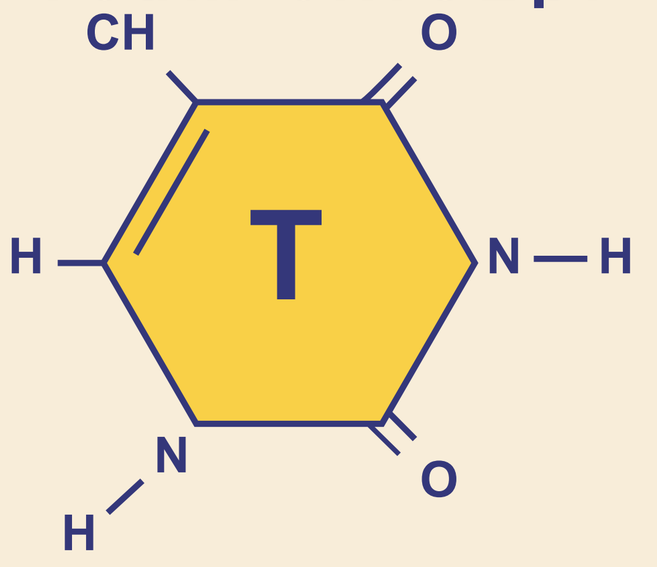






Multiple Sequence Alignment for Antimicrobial Resistance

AMR occurs when microorganisms become resistant to drugs.

Drug development is expensive and time-consuming.

MSA helps identify resistance patterns in microbial genomes.

Our Approach

- Sequence alignment optimization is crucial for tasks like antimicrobial resistance detection.
- Challenges: Structural similarity among sequences during primary screening.
- Approach: Used Optimized Gearbox Score with LSTM and RL models.
- Improved alignment with higher scores using Reinforcement Learning and sequence modeling.
- Result: Decreased testing cost and faster screening.

Inspiration

Content:

- Problem: Traditional sequence alignment methods are time-consuming and costly.
- Goal: Speed up the alignment process in drug discovery and biological research.
- Impact: More efficient pipelines for biological studies and better drug-target interactions.
- Vision: Accelerate medical advancements and improve quality of life using optimized computational models.

What it Does / How We Built It

What is does?

- Predicts the optimal sequence alignment moves to maximize alignment scores.
- Focus on protein-compound interactions using the Optimized Gearbox Score.
- Features:Sequence position / Gap density / Mutation rate
- Goal: Accurate sequence alignment predictions to minimize experimental testing.

How we built it?

- Data: Used bioassay data from PubChem for training.
- Model: Combined LSTM-based sequence prediction with Reinforcement Learning (RL).
- Scoring: Optimized Gearbox Score to measure sequence alignments.
- Outcome: Model predicts the best alignment moves and provides a higher final score.

Overcoming Challenges

Feature Selection:

Difficult to identify which features (mutation rate, gap density) would significantly improve predictions.

Model Overfitting:

Ensuring the model doesn't overfit to small sample sizes was a challenge.

What's Next for Challenge

Feature Expansion:

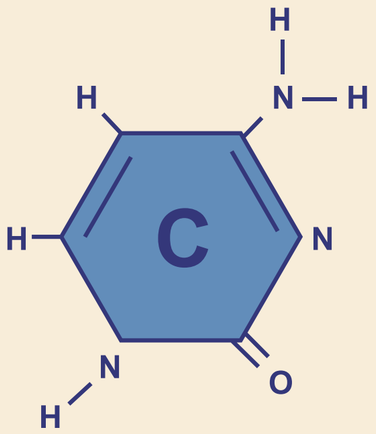
Use evolutionary motifs and substitution matrices to improve model performance.

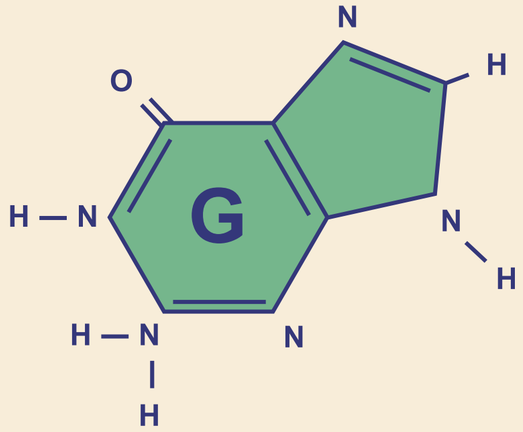
Model Tuning:

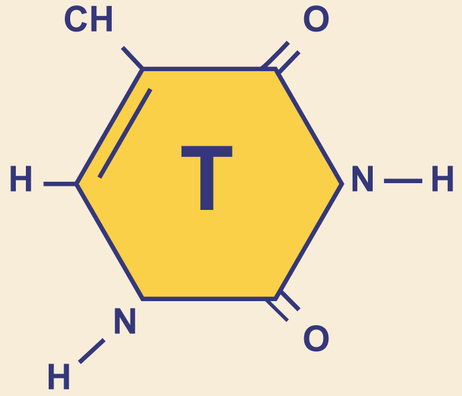
Explore genetic algorithms and reinforcement learning improvements for better convergence.

Scalability:

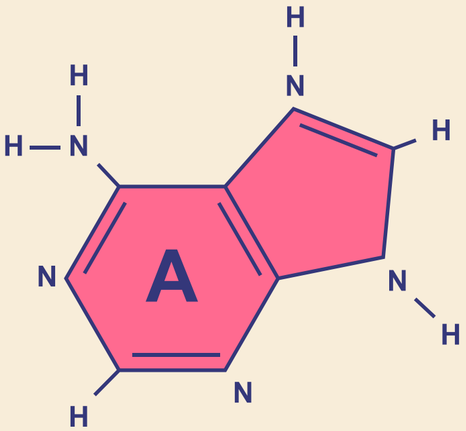
Test on larger real-world datasets to optimize model for production use.







Thanks!



Do you have any questions?