Deep Learning-Based Algorithm for AI-Powered Drug Discovery and Development

Author: Your Name

Date: Submission Date

## Paper #3: AI-powered drug discovery for neglected diseases: accelerating public health solutions in the developing world

**📊 Dataset Used:**

* ChEMBL – Bioactivity data for compound–target interactions
* DrugBank – FDA-approved drug data
* ZINC – Commercially available compounds
* PDBbind – Structural data with binding affinities
* QM9 – Quantum chemical properties for small molecules

**🧠 Model/Methodology Used:**

* Graph Neural Networks (GNNs) for molecule representation
* Transformer-based architectures for protein and SMILES modeling

**✨ Novelty:**

* Emphasizes the use of AI specifically in neglected disease domains, where traditional R&D is underfunded
* Focuses on low-cost, end-to-end AI pipelines tailored to the developing world, enabling faster hit-to-lead transitions with fewer lab resources

**🎯 Accuracy (%):** N/A

**📏 Evaluation Metrics:** QED (Quantitative Estimate of Drug-likeness), SA Score (Synthetic Accessibility), Docking Scores, Binding Affinity, RMSE, MAE