A Deep Learning Approach for RNA-Compound Interaction Prediction with Binding Site Interpretability

Haelee Bae
AI Graduate School
Gwangju Institute of Science and Technology
123 Cheomdangwagi-ro, Buk-gu,Gwangju 61005, Republic of Korea
haeleeeeleah@gm.gist.ac.kr

Hojung Nam
School of Electrical Engineering and Computer Science
AI Graduate School
Gwangju Institute of Science and Technology
123 Cheomdangwagi-ro, Buk-gu,Gwangju 61005, Republic of Korea
hjnam@gist.ac.kr

Abstract

RNA-compound interaction prediction is crucial for expanding the therapeutic target space beyond proteins. However, existing models are limited by data scarcity and often lack interpretability. We present DeepRNA-DTI, the first sequence-based deep learning model for RNA-compound interaction prediction. Our model leverages pretrained embeddings from RNA-FM for RNA sequences and MoleBERT for compounds, capturing complex interaction patterns through attention mechanisms. DeepRNA-DTI jointly predicts drug-target interactions (DTI) and RNA binding sites, enhancing interpretability. Trained on datasets from the Protein Data Bank (PDB) and literature, DeepRNA-DTI demonstrates improved performance in RNA-compound interaction tasks compared to existing methods. Our approach offers valuable insights into binding sites and opens new avenues for RNA-targeted drug discovery.

Acknowledgments and Disclosure of Funding

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2023-00257479), supported by Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE) (No. P0024560), and supported by Institute of Information communications Technology Planning Evaluation (IITP) grant funded by the Korea government (MSIT) (No.2019-0-01842, Artificial Intelligence Graduate School Program (GIST)).

AI for New Drug Modalities at NeurIPS 2024.