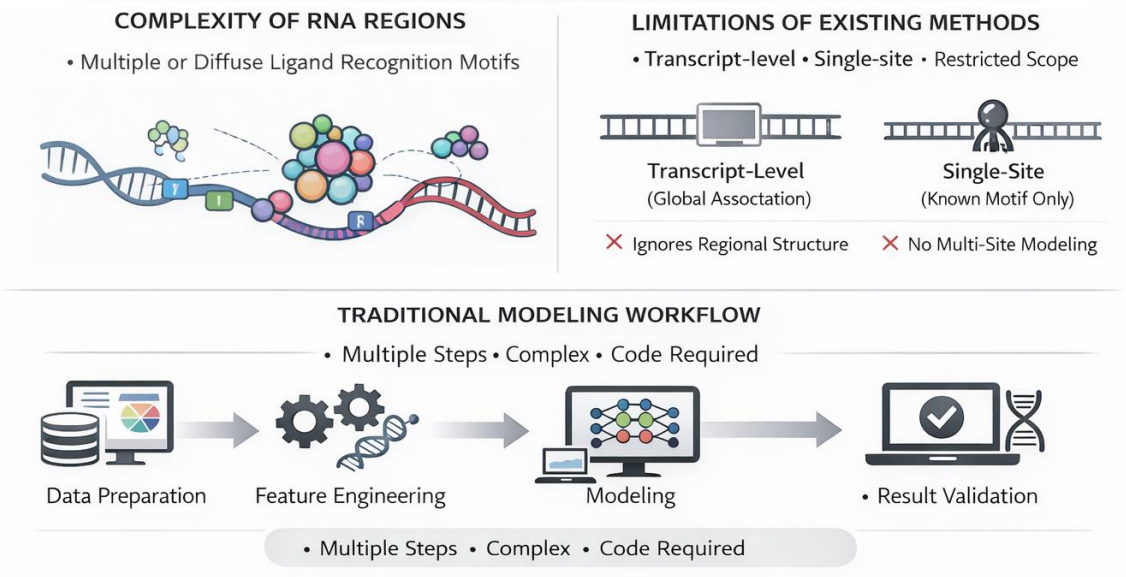
Dialogue-Guided Workflow for Automated RNA Region–Ligand Modeling

Zhejun Kuang, Yunkai Li, Yihang Bao, Weichen Song, Shengyang Zhou, Zeqi Dong, Weidi Wang, Guan Ning Lin, Han Wang, Zhe Liu

Frontiers of Computer Science, DOI: 10.1007/s11704-026-60013-1

Problems & Ideas

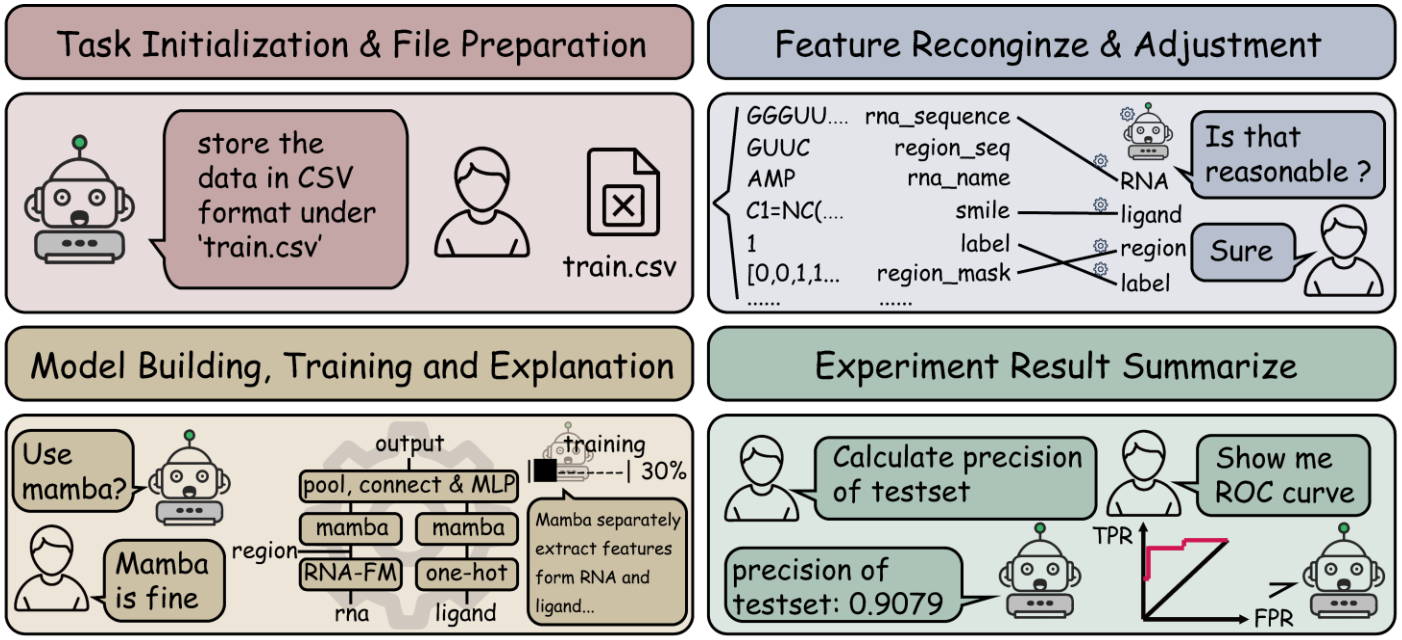
- Problems of RNA-ligand interaction prediction:
  - Predicting regions with multiple or diffuse ligand recognition motifs remains challenging.
  - The technical complexity of model development limits reproducibility and scalability.
- Ideas: A dialogue-guided LLM workflow to address region-level RNA–ligand modeling and reduce modeling complexity.



Full-length prediction cannot localize binding regions, while site-based methods fail to capture multiple or diffuse motifs in complex RNA segments. These limitations reduce flexibility for non-canonical regions. Both rely on code-intensive workflows, leading to high technical complexity and limited reproducibility.

Main Contributions

- **Contributions:**
  - **Dialogue-driven workflow**: Enables end-to-end RNA–ligand modeling through natural language, eliminating the need for manual coding
  - **Architecture-agnostic modeling**: Supports flexible integration of multiple backbones (e.g., Transformer, Mamba) for diverse scenarios
  - **Region-level interaction modeling**: Captures complex RNA regions with multiple or diffuse motifs beyond full-length or site-based methods



LargeR enables end-to-end, code-free RNA region–ligand modeling through a dialogue-guided workflow across task setup, feature recognition, model training, and result summarization.