

Project Overview

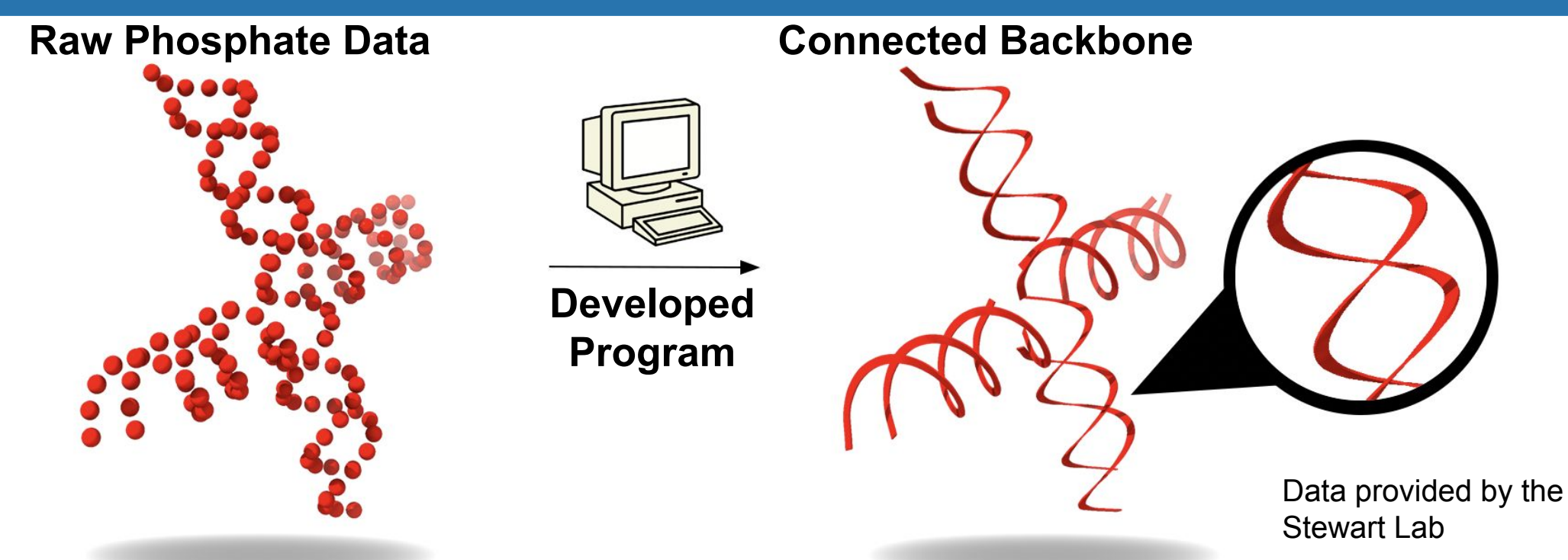


Figure 1: Overview visualization of the developed program's functionality

Background: CryoEM & RNA Backbone Tracing

- **Cryo-EM:** Converts 2D slices into 3D molecular structures
- **Challenge:** Resolution limits hinder RNA model accuracy
- **Bottleneck:** Manual backbone tracing is slow
- **Solution:** Automate tracing for faster, more reliable results

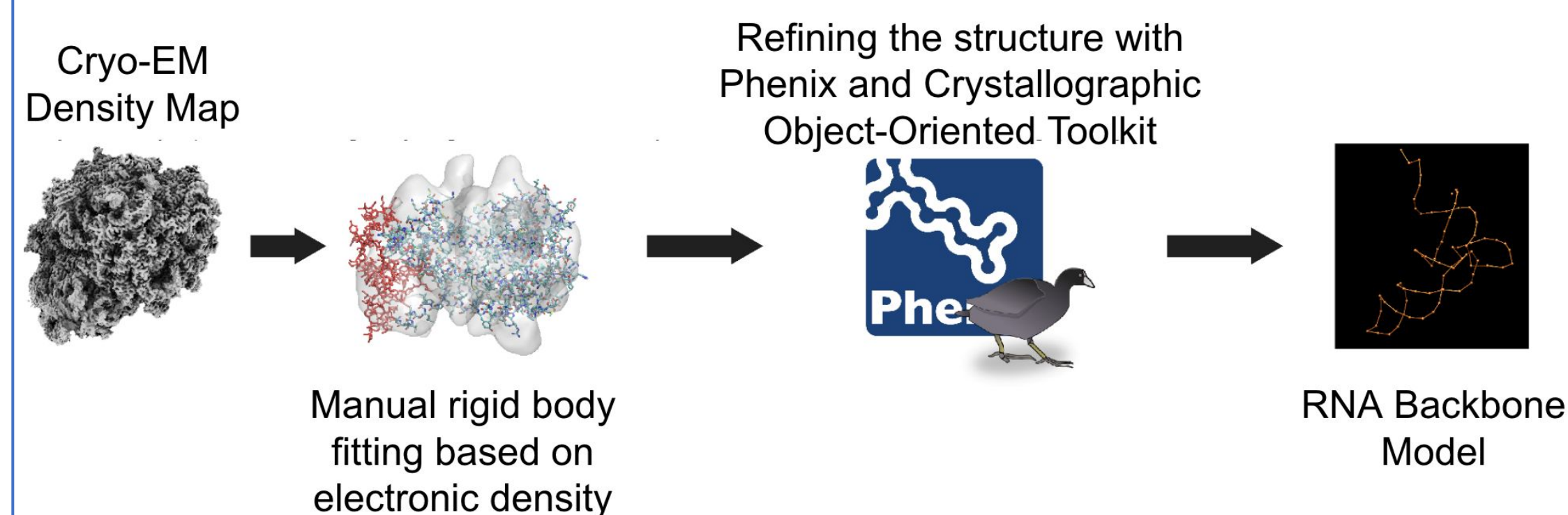


Figure 2: Cryo-EM RNA Reconstruction - convert density maps into refined backbone models

Methodology

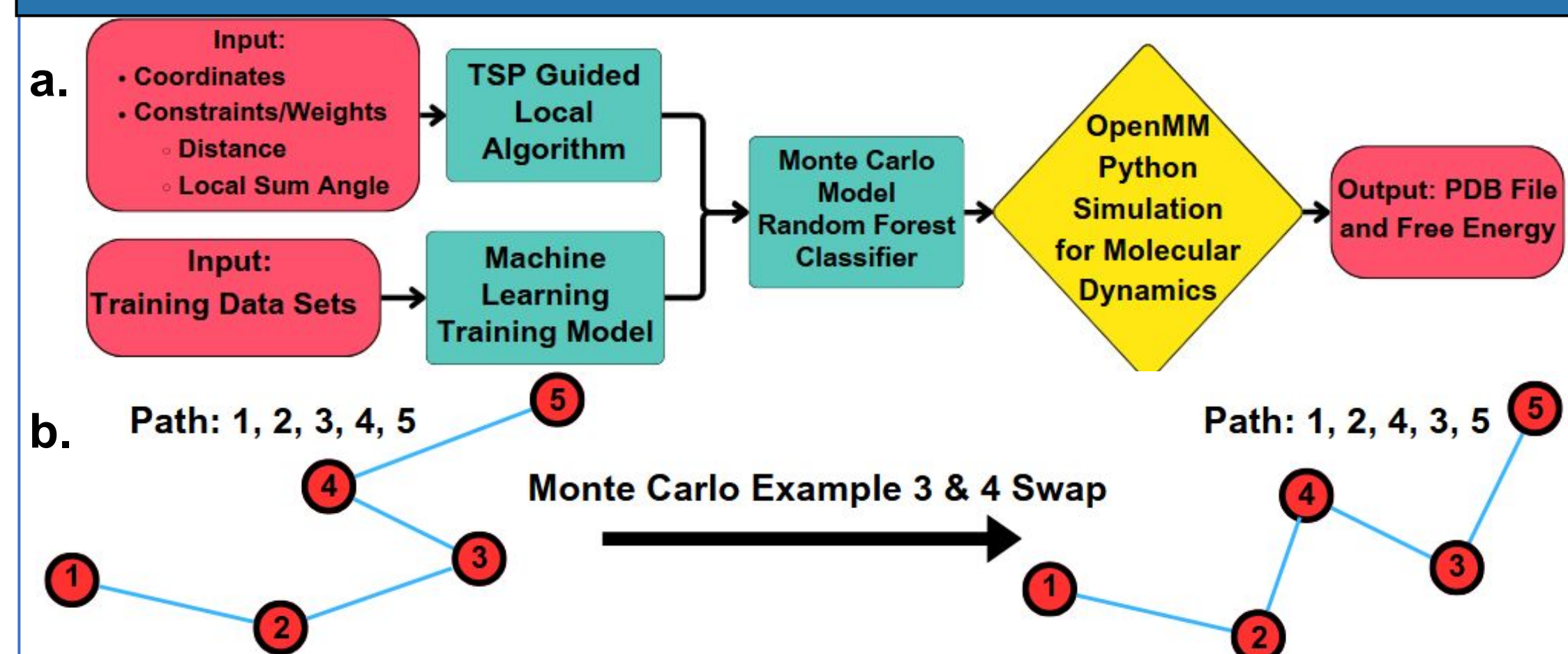


Figure 3a-b.) a. Implementation workflow of our prediction program constructing a refined molecular path with phosphate coordinates, b. Monte Carlo Visualization

Performance with Standard and Improper Data

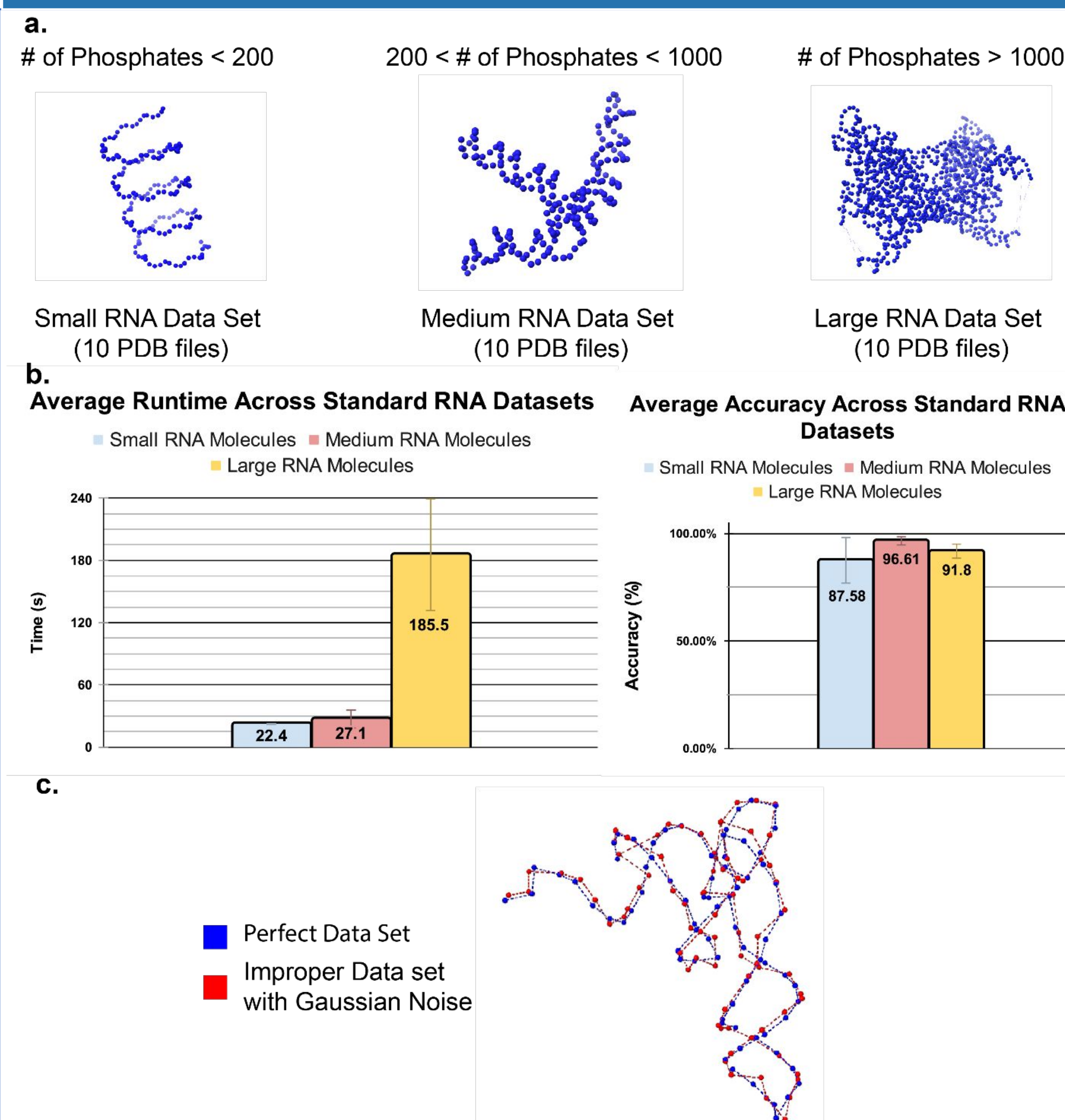


Figure 4 a-d.) a. To properly test our program, we utilized three datasets of varying sizes b. Our algorithm yielded high accuracies and short runtimes for all three RNA sizes c. To generate improper data sets we implemented gaussian error to all of the RNA molecules of 1 Å, 1.5 Å and 2 Å d. Our accuracy decrease as the amount of gaussian noise introduced increases across all three RNA sizes

User Interface

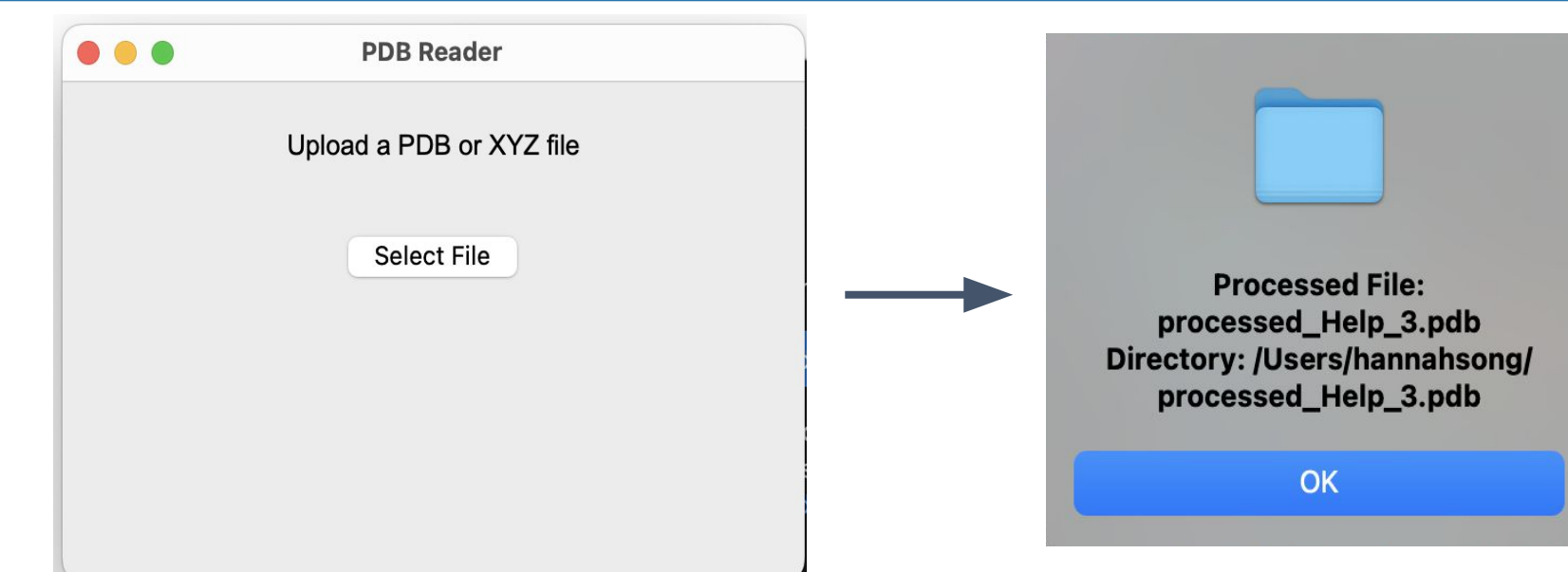


Figure 5. Pop-up windows appearing at the beginning and end of our program, prompting file drop and new document name with address, respectively.

Comparison to Competitors

| | Our Program | COOT & Phenix | CryoREAD | EM2NA |
|--------------------------------|---------------------------------------|--------------------------------------------------------------------------------------------------------|------------------------------------------------------|----------------------------------------------------------------------------------|
| Average time for a medium file | ~27 seconds | File and skill dependent – each bond is placed independently and depends exclusively on user expertise | ~3 hours | ~3.5 days |
| Average Accuracy | ~92% | | ~85% | ~85% |
| Required Atoms/Motifs | Phosphate | | Ribose | Phosphate, Ribose Carbon (C4') |
| Steps Required | 1 (Just upload the .pdb or .xyz file) | | 2 (Upload the .pdb or .xyz file and manually export) | 4 (Upload the .pdb or .xyz file, run software, post-refinement, manually export) |

Figure 6. Comparison of key variables of competitive methods for backbone tracing

Conclusions & Future Work

- New algorithm provides a software that is **accurate with minimal runtime** to quickly trace the backbone of RNA across various sizes with only the atomic position of phosphates
- The algorithm **significantly decreases the development time** needed for RNA based therapies like vaccines, RNA nanotechnology and medications that utilize RNA motifs
- Provides researchers the opportunity to **utilize non-perfect data sets** to help move RNA based research forward
- For the future it is necessary to train the machine learning model further with more RNA backbones with more unique structures for increased accuracy

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