Trace the Backbone of Protein and RNA with Known Key Atom Positions

Cryogenic electron microscopy (cryoEM) has revolutionized structural biology by allowing the visualization of complex molecular structures at near-atomic resolution. Skilled structural biologists often spend months, or even longer, constructing an atomic model from scratch based on these maps, and a reliable atomic model is crucial for understanding the molecule's functionality. To speed up the modeling process, AI in image segmentation is used to identify key atom positions in protein and RNA from the EM map. However, a significant challenge remains in the path to constructing an atomic model: **how to accurately trace the backbone using those key atoms?**

To address this main question, this project aims to develop an optimized algorithm to trace the protein and RNA backbone using the given key atom positions. The team will dedicate two semesters to this effort, focusing primarily on the following components:

1. **Generate the atomic model file (CIF/PDB)**
2. **Develop the backbone tracing algorithm and create a software tool for easier use**

Phase 1 Requirements

- *Study* the format of biological atomic models.
- *Generate* the atomic model file line by line, containing only the backbone.

The project mentors will provide instruction on the fundamental information about atomic model files.

Phase 2 Requirements

- *Learn* two algorithms for the traveling salesman problem (TSP) and vehicle routing problem (VRP), respectively
- *Use* the VRP solver in the OR-tools package[1] and *modify* it for backbone tracing
- *Test* the modified VRP solver with key atom positions in an existing atomic model and key atom positions predicted from an EM map
- *Create* an easy-to-use software tool with clear input and output

The project mentors will supply the team with materials on the two optimized algorithms and provide key atom positions data for testing.

Depending on the project's success, the results are likely to be published in a professional journal.

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[1] https://developers.google.com/optimization/