Fragment-based modeling of protein-bound ssRNA
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## Fragment-based modeling of protein-bound ssRNA

**Biological Context**
- Biological function: Transport of nucleotides
- Biological function: Stabilization of methods
- Biological function: Regulation of transcription

**Methods**

**Docking**
- ATTRACT docking engine [1, 2]
  1. Random starting states (position + orientation + conformation)
  2. Energy minimization of bead-bead interactions in an empirical force field
  3. Elimination of redundant poses (performed on some local minima)
  4. Ranking of poses by score (pseudo-energy)
- For each fragment: best pose at 1-2 Å from X-ray structure

**Assembling**
- Up to $10^3$ poses per fragment
- Probabilistic
- Systematic
- Scoring
  - Chains are scored by the geometric mean of the ranking of the poses
  - 25% or more of poses have low score (good chance)

**Hierarchical clustering for efficient pruning**
- By distance
- By ranks

**Results**

**Without predicted contacts**
- We blind-tested this approach on 2 complexes of known structure [1]
- We predicted the position and orientation of nucleotides in the protein's consensus, as determined by the best possible score.

**With predicted contacts**
- We blind-tested this approach on 8 complexes of known structure [1]
- We predicted the position and orientation of nucleotides in the protein's consensus, as determined by the best possible score.

**Conclusions**
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