Fragment-based modeling of protein-bound ssRNA
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The structure of an RNA-protein complex is a key to (i) understand its function or malfunction (ii) modulate or create it, for medicine or biotechnology Experimental methods to obtain such structure (X-ray, NMR) are costly, time-consuming and applied to some complexes. Therefore, it often requires computational modeling methods. Such methods exist for RNA-protein complexes, but fail at modeling single-stranded RNA because of their flexibility.

We blind-tested this approach on 8 complexes of known structure in [3]. We predicted the position and orientation of nucleotides with an experimentally measured contact, within 0.8 – 3.2 Å RMSD from the real structure, for 7 out of 8 complexes, among 130 to 270 proposed models.

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