Supplementary Material for "Predicting structures and stabilities for H-type pseudoknots with inter-helix junctions"

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An internal/bulge loop in the stem can cause bending of the stem. To investigate the effect of bending stem on the conformational entropy, we performed a series of tests for the error caused by replacing a bent helix with an effective straight helix. The results are presented in the figure below.

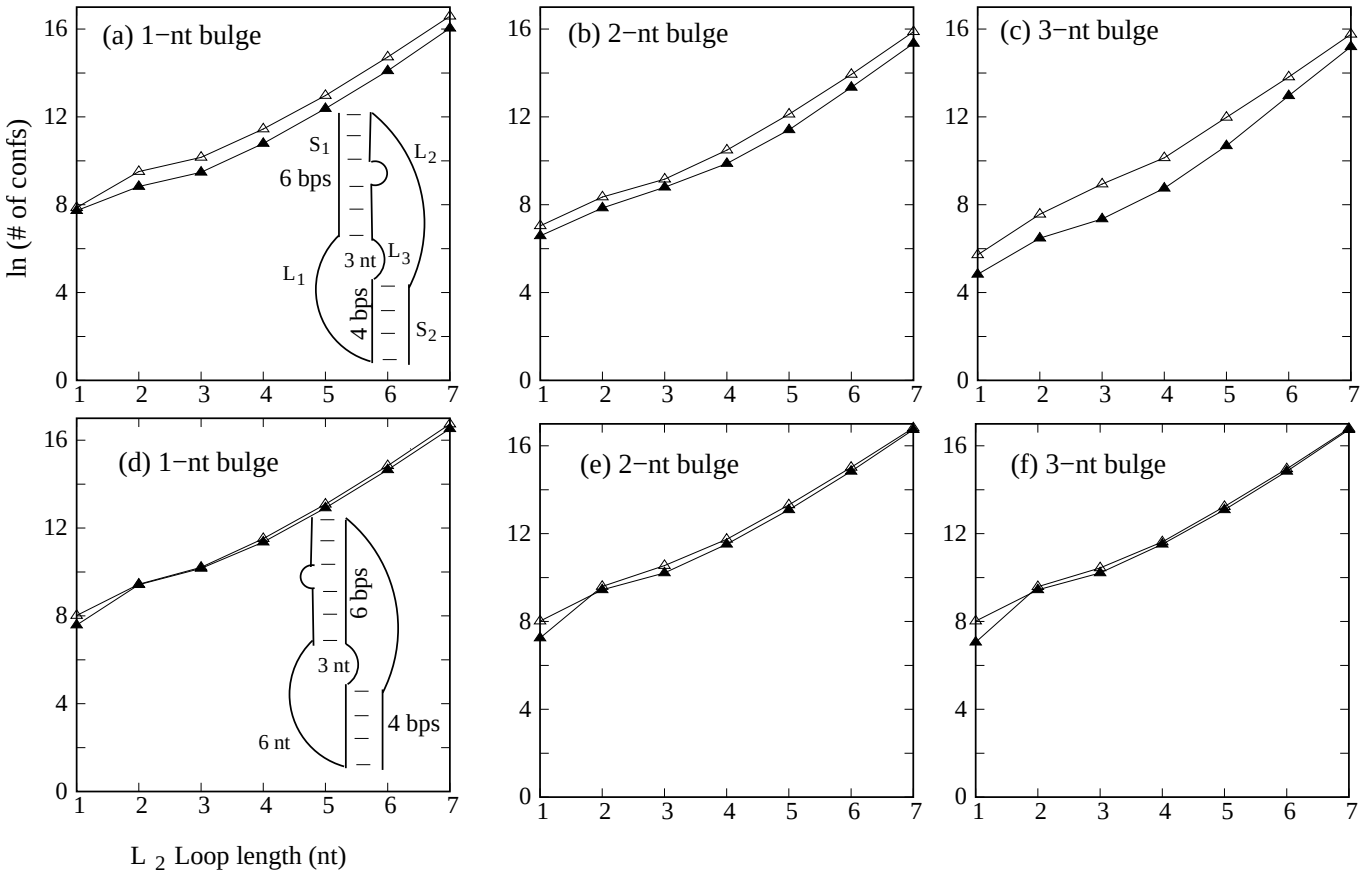

Figure 1: Comparison between the conformational entropies from the exact computer enumeration (filled triangle) and the approximation in Eq. 2 (i.e., replacing the bent helix by an effective straight helix) (empty triangle). In the upper and lower panels, a bulge is formed in the different strands of the stem S_1. For all the figures, we fix (S_1, S_2, L_1, L_3) = (6 bps, 4 bps, 6 nts, 3 nts) and vary L_2 from 1 nt to 7 nts and the bulge loop size from 1 nt to 3 nts. The largest error for the test cases here comes from (c), which has an error of 15%.

In the calculation of loop entropies, we use exact computer enumeration for the chain conformations:

1. For a pseudoknot with an enter-helix loop, there are three flexible loops L_1, L_2 and L_3. For example, we enumerate the conformations for loop L_3 from nucleotides c_1 to c_2 (Fig. 1a). The loop conformations are enumerated in a diamond lattice where a lattice bond represents a virtual bond of the nucleotide. The helix structure is represented as an off-lattice rigid A-form RNA helix. Helix and loop conformations are connected through minimum RMSD overlap between the on- and off-lattice coordinates for the terminal nucleotides a_1, a_2, b_1, b_2, c_1 and c_2 in Fig. 1a.

2. We count the total number of viable conformation for loop L_1, L_2 and L_3 through the exact enumeration. In the exact enumeration, we explicitly consider all the excluded volume interactions by disallowing any two atoms to bump into each other.