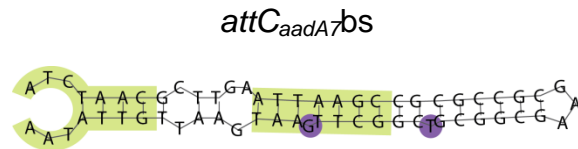


ΔG_{bs} value of the most stable structure without constraints= -15.5 kcal/mol

ΔG_{bs} value of the most stable structure with constraints (recombinogenic)= -15.5 kcal/mol

$attC_{bs}$ pfold value calculated with constrained vs. unconstrained folding= 0.30

The most stable structure is the recombinogenic one:



VCR₁₂₆

ts sequence: 5'- ATCTAACAAACGCCTCAAGAGGGACTGTCAACGCGTGGCGTTTCCAGTCCCATTGAGCCG
CGGTGGTTGCTGTTGTTGTGTTTGTGAGTTTAGTGGTAGTGCGTTGTCAGCCCCTTAGGCGGGCGTTATAC

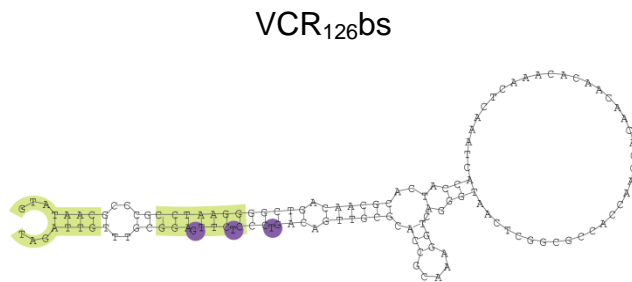
ΔG_{bs} value of the most stable structure without constraints= -24.1 kcal/mol

ΔG_{bs} value of the most stable structure with constraints (recombinogenic)= -16.7 kcal/mol

$attC_{bs}$ pfold value calculated with constrained vs. unconstrained folding= 1.04×10^{-5}

The most stable structure is a non-recombinogenic one (improperly folded).

The recombinogenic structure is:



VCR_{126*} - VCR_{126} synthetic cassettes**

VCR_{126*}

ts sequence: 5'- TTATAACAAACGCCTCAAGAGGGACTGTCAACGCGTGGCGTTTCCAGTCCCATTGGCCGC
GGTGGTTGCTGTTGTTGTGTTTGTGAGTTTAGTGGTAGTGCGTTGTCAGCCCCTTAGGCGGGCGTTAGAT

ΔG_{bs} value of the most stable structure without constraints= -20.4 kcal/mol

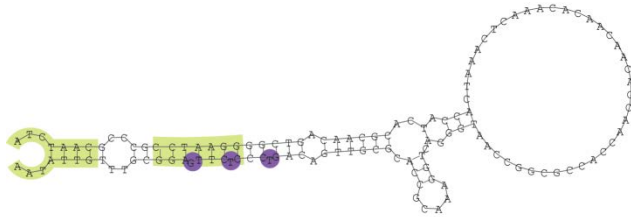
ΔG_{bs} value of the most stable structure with constraints (recombinogenic)= -16.7 kcal/mol

$attC_{bs}$ pfold value calculated with constrained vs. unconstrained folding= 3.09×10^{-3}

The most stable structure is a non-recombinogenic one (improperly folded).

The recombinogenic structure is:

VCR₁₂₆*bs



VCR₁₂₆**

ts sequence: 5'- ATCTAACAAACGCCTCAAGAGGGACTGTCAACGCGTGGCGTTTCCAGTCCCATTGAGCCG

CGGTGGTTGCTGTTGTTGTGTTTGAGTTTAGTGGTAGTGCGTTGTCAGCCCCTTAGGCGGGCGTTATTA

ΔG_{bs} value of the most stable structure without constraints= -24.1 kcal/mol

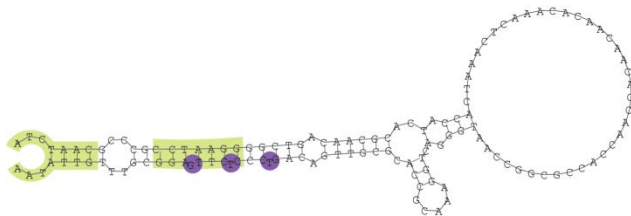
ΔG_{bs} value of the most stable structure with constraints (recombinogenic)= -16.7 kcal/mol

$attC_{bs}$ pfold value calculated with constrained vs. unconstrained folding= 7.86×10^{-6}

The most stable structure is a non-recombinogenic one (improperly folded).

The recombinogenic structure is:

VCR₁₂₆**bs



VCR₁₆*- VCR₆₄ synthetic cassettes

