Electronic Supplementary Information for PCCP


# Supplementary Information

# Conformational Selection or Induced Fit for Brinker and DNA Recognition

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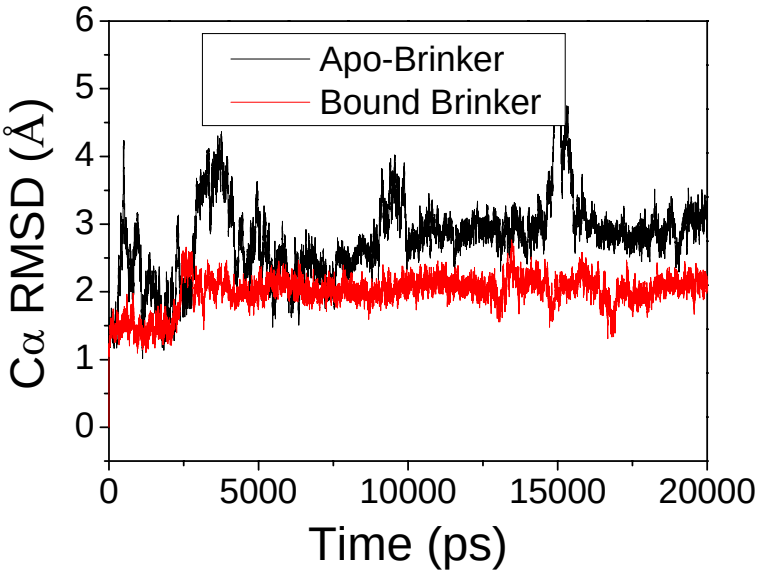


Figure 1S. Cα RMSD relative to initial NMR structure of bound and apo-Brinker.

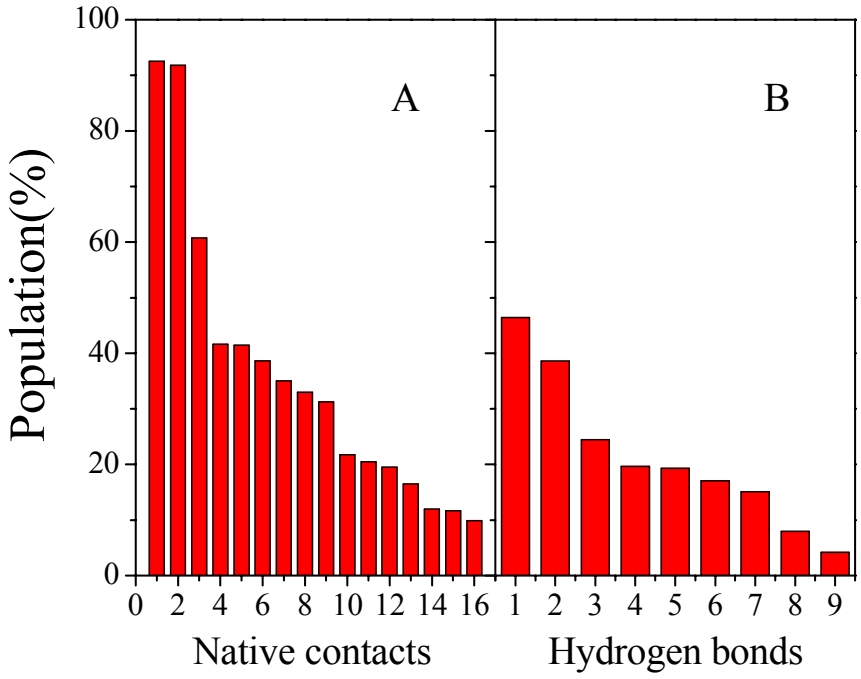


Figure 2S. Native contacts and hydrogen bonds between DNA and Brinker. A: native contacts. B: hydrogen bonds.

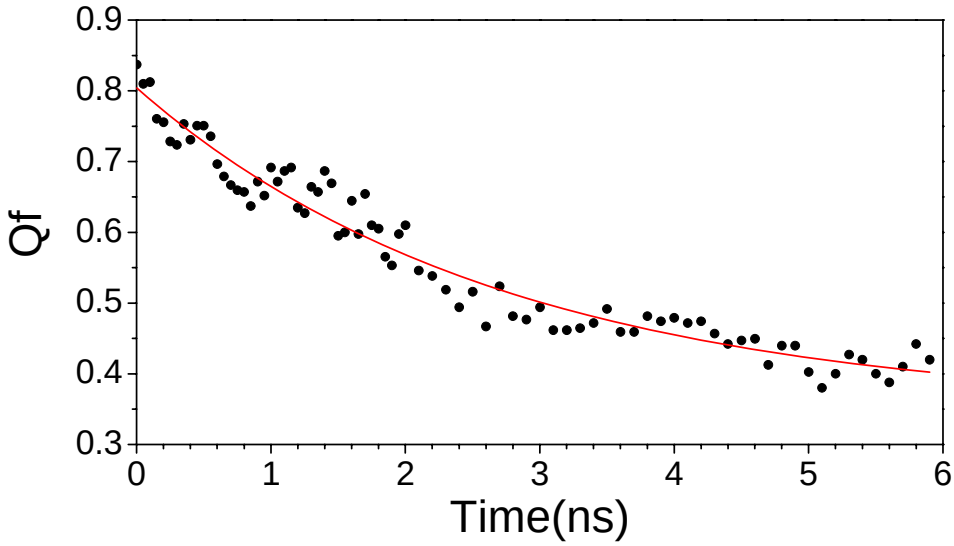


Figure 3S. Kinetics fitting for apo-Brinker.

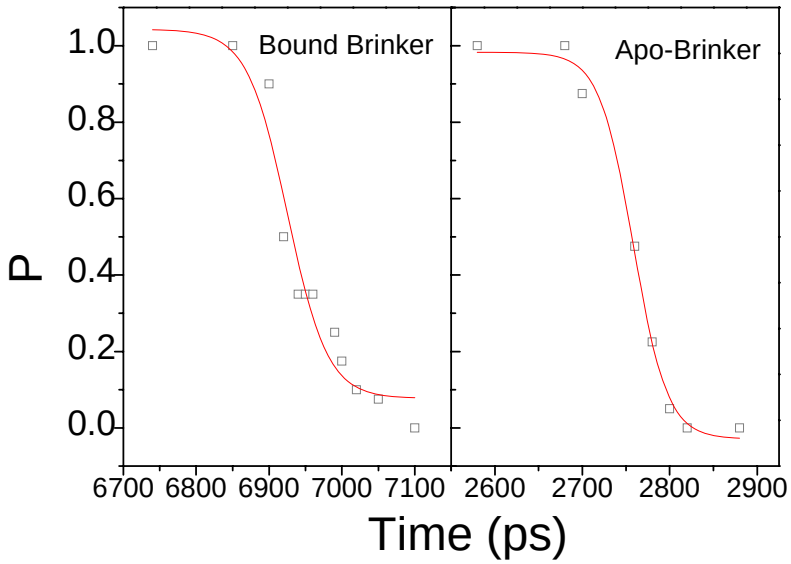


Figure 4S. A representative transition probability P calculated at 498K for the F⇔U transition for snapshot in the transition region for one of trajectories for bound and apo-Brinker, respectively. The red line is the fit to $P = 1/\{1+ \exp[(\tau-\tau_{TS})/\tau_{trans}]\}$.

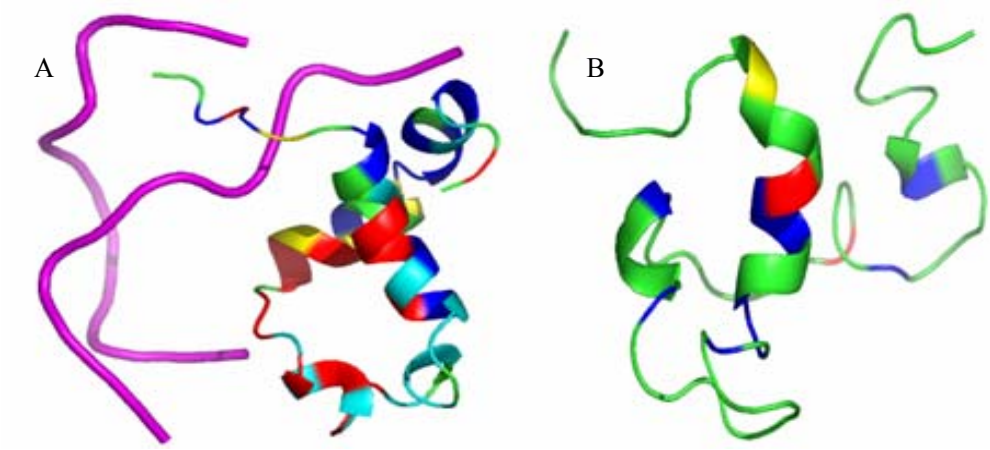


Figure 5S. Average structures of TSE for bound (A) and apo-Brinker (B). The Φ-value of red is equal to 1, blue equal to -1, and green between -1 and 1.

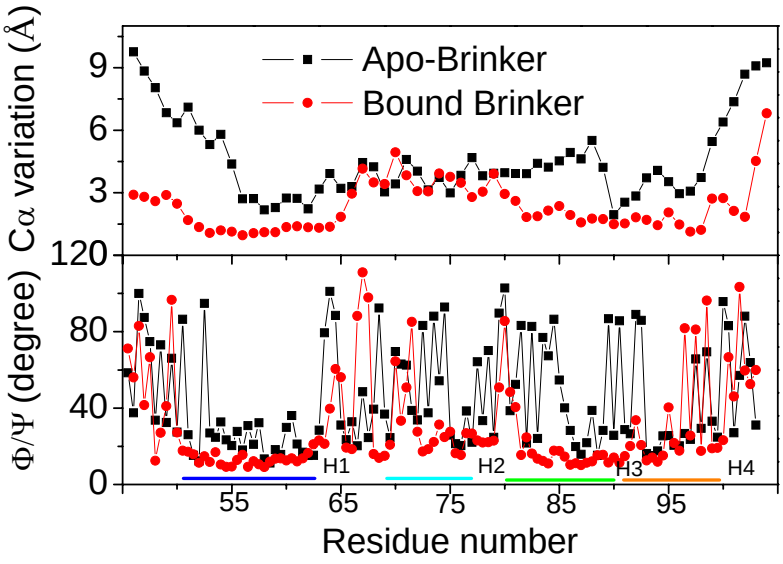


Figure 6S. Cα and Ψ/Φ variations relative to initial NMR structure at transition state for bound and apo-Brinker, respectively.

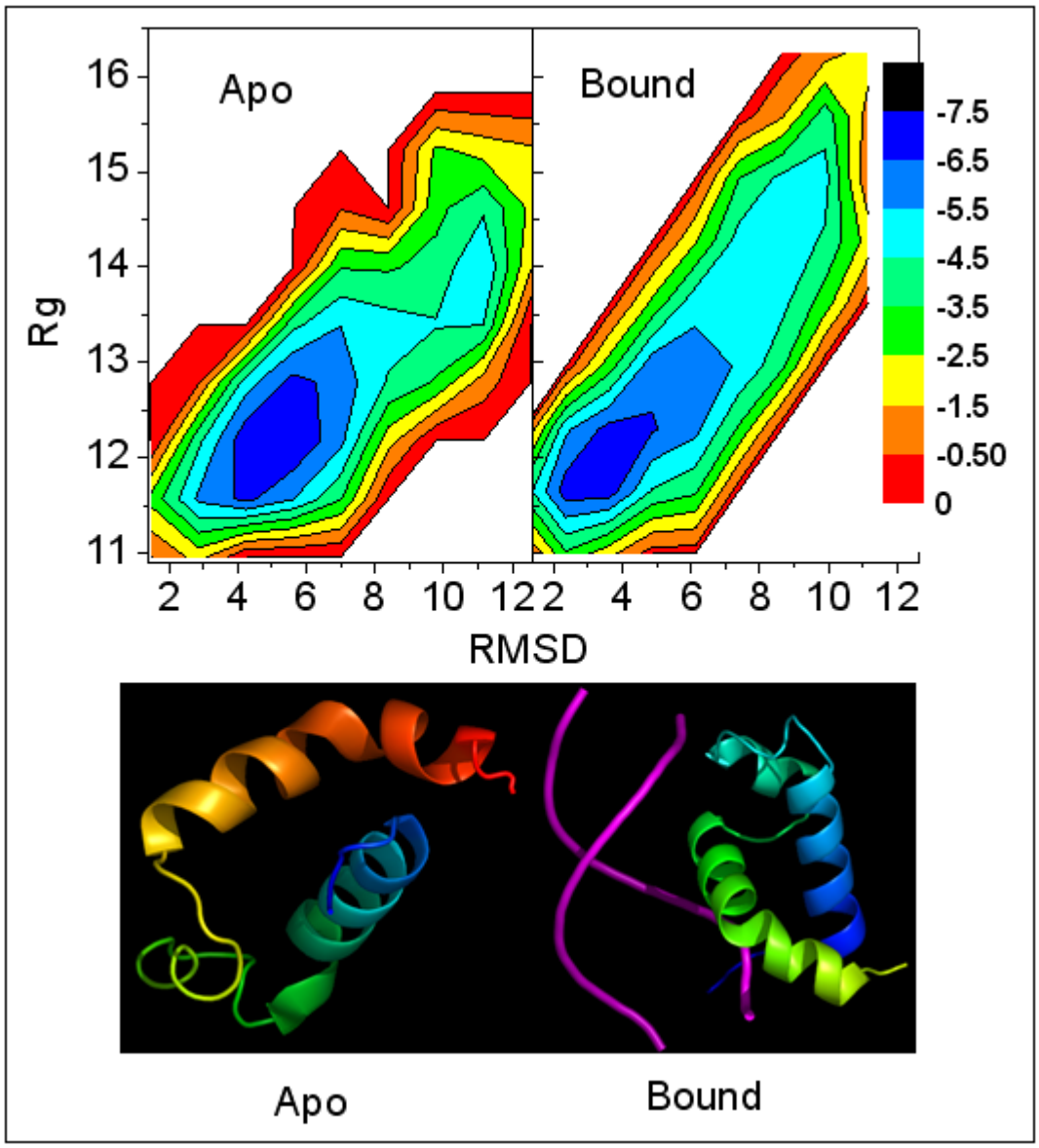


Figure 7S. The energy landscape with the variables of RMSD and Rg for bound and apo states at 498K.

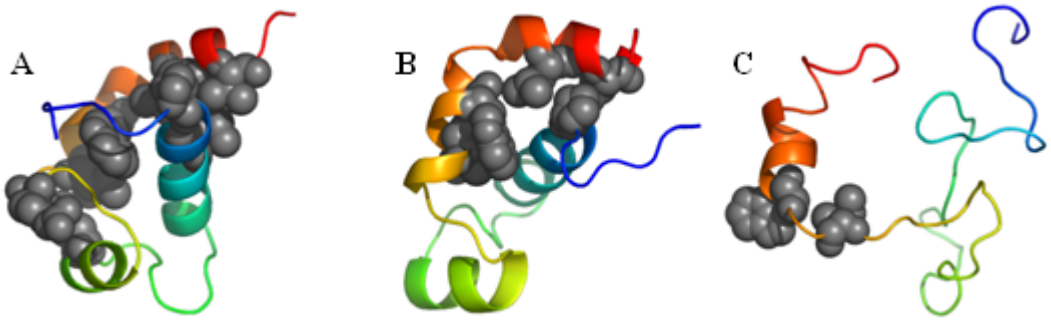


Figure 8S. Unfolding pathway of apo-Brinker. A: <0ns (F), B : 2.73ns ($\tau_{Qf}$), C: > 6ns (U).