

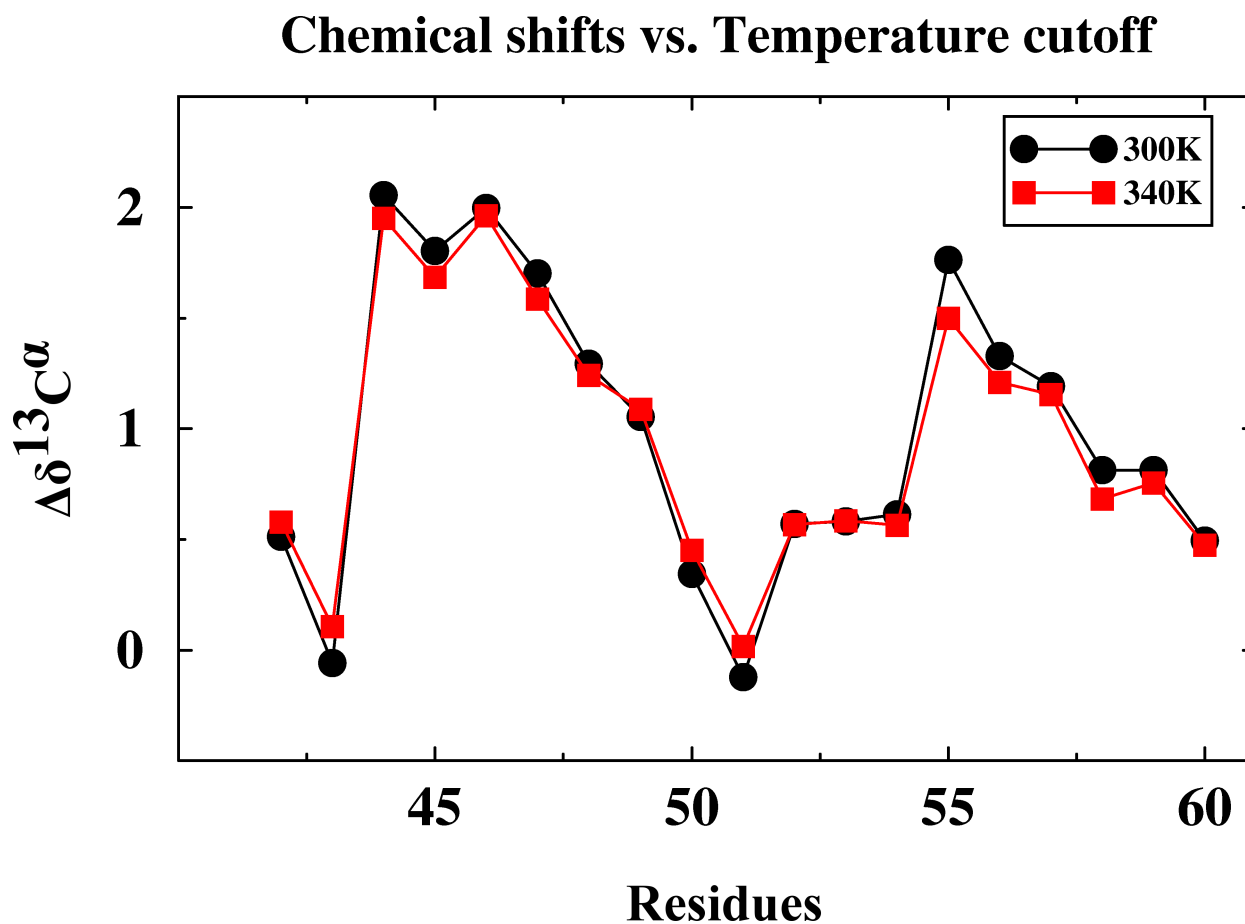
# **Supplementary material for**

**Characterizing a partially ordered miniprotein through  
folding molecular dynamics simulations : Comparison with  
the experimental data.**

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**Figure S1**



**Figure S1** : Comparison between the  $\text{C}^\alpha$  secondary chemical shifts (in ppm) obtained from the simulation using two different temperature ranges. The first (black curve) ranges from the lowest recorded temperature up to 300K, the second (red curve) from the lowest recorded temperature up to 340K.