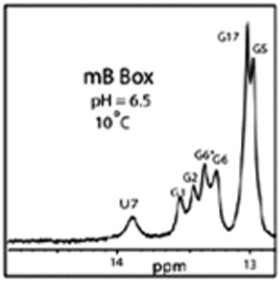
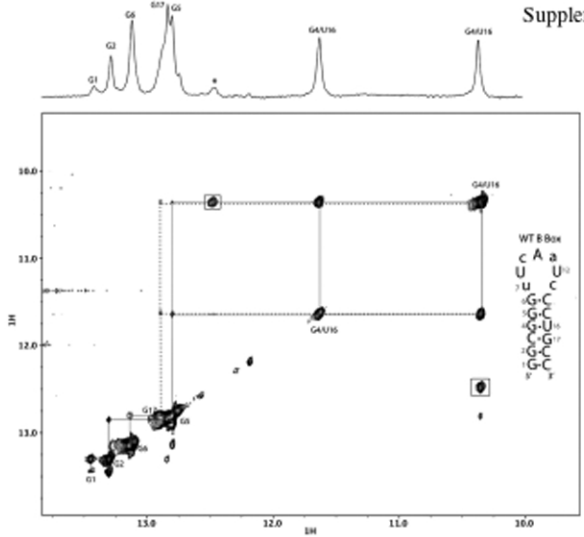
Supplemental Fig. 2



sFig. 2. The imino spectrum of the mBbox shows one additional broad peak which falls to the chemical shift range of a U imino proton in the UA or AU base pairs, which suggests the formation of AU base pair in its loop region. This peak was relatively broad at pH 6.5, and became even broader at pH 5.7, suggesting that the AU base pair is quite flexible. This is consistent with the existence of another peak right next to G6 peak (G6*), which might be the outcome of a slow exchange of the G6 imino proton between two different conformations. The suspected conformational exchange is further supported by the existence of a cross peak between the G6 and G6* peaks in water NOESY experiment (data not shown) and by the increased intensity of both U7 and G6* peak at pH 6.5 compared to the spectrum at pH 5.7.

Supplemental Fig. 3


G1
G2
G6
G17
G5
G4U16
G4U16
G4U16
WT B Box
C A a
U U
U C
G C
G C
G