SUPPLEMENTARY DATA

ZIP archive (IntaRNA_Supp.zip) containing the calculations performed on the web server version of IntaRNA (`http://bit.ly/IntaRNA`) at the temperatures: 10 °C, 25 °C and 45 °C (see Materials and Methods for the other parameters).

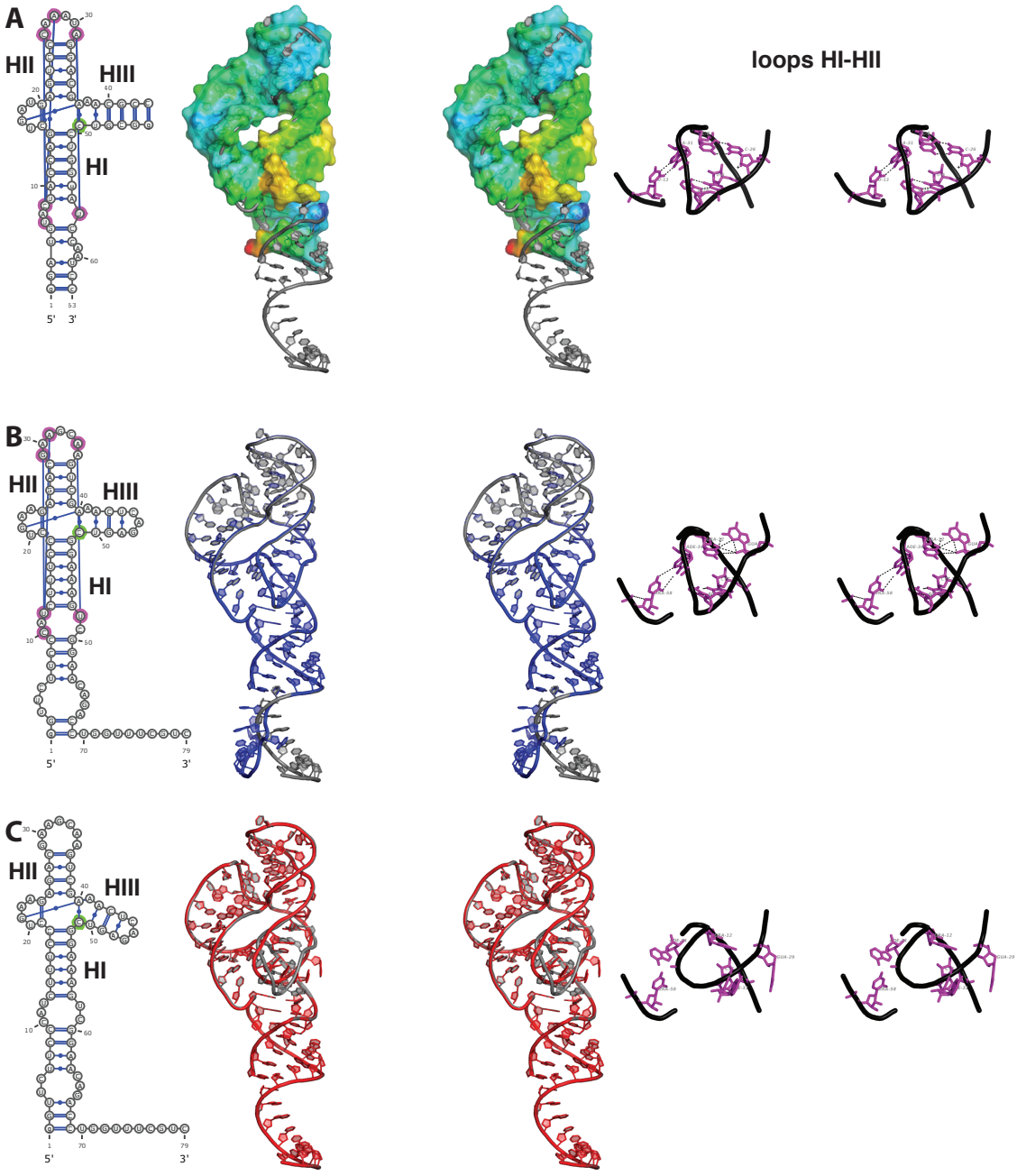

Figure S1: Comparisons of RNA 3D Structures from X-ray crystallography and RNA Modeling. (Legend on the following page).

Figure S1: Comparisons of RNA 3D Structures from X-ray crystallography and RNA Modeling.(A) 2D and 3D structures of the template and modeled ribozymes.Left: 2D structure of the template corresponding to the X-ray 3D structure of a minimal HHR ribozyme (PDB ID: 2OEU). Middle: stereo-view of the superposition between the 3D model of HHR (-) (79-mer) and the X-ray 3D structure of the template (PDB ID: 2OEU). The X-ray structure is represented by a solvent accessible surface using a color code corresponding to the B factors. The 3D model (grey) in cartoon representation shows slight structural differences: the presence of a triloop closing the HIII domain, the presence of bulge nucleotides in the HI domain which is also significantly extended in ASBVd. Right: stereo-view of the intramolecular tertiary contacts between the domains HI and HII in the template (PDB ID: 2OEU).(B) 2D and 3D structures of the foldedmonomer preserving tertiary contacts. Left: 2D structure with indication of the homologous 3D tertiary contacts. Middle: stereo-view of the superposition between the 3D model of HHR (-) in its unbound (grey)/bound (blue) conformations for the first monomer. Right: stereo-view of the intramolecular tertiary contacts between the domains HI and HII in the folded monomer.(C) 2D and 3D structures of the unfoldedmonomer in the HII terminal loop. Left:2D structure of the unfolded monomer.Middle: stereo-view of the superposition between the 3D model of HHR (-) in its unbound (grey)/bound (red) conformations for the unfolded monomer.Right: stereo-view of the lost intramolecular tertiary contacts between the domains HI and HII in the unfolded monomer.

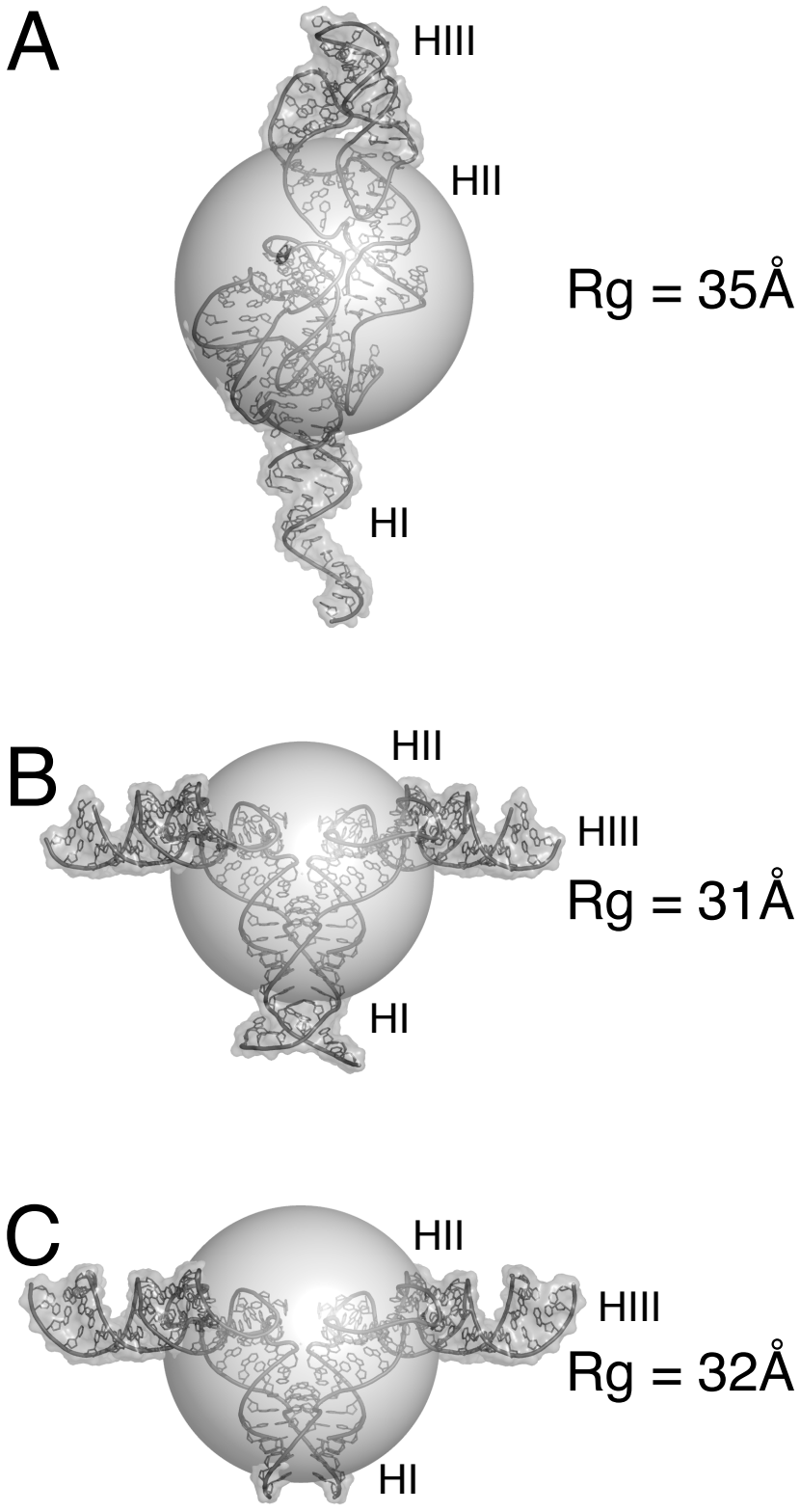

Figure S2: Relationship between the mode of association and the radius of gyration of HHR dimers. (A) 3D model of the HHR (-) dimer from ASBVd (Fig. 5C). (B) 3D structure of an artificial HHR dimer with an extended HI domain (PDB ID: 5DI2, 68 nt + 11 nt). (C) 3D structure of an artificial HHR dimer with an extended HIII domain (PDB ID: 5DI2, 68 nt + 11 nt). The 3D structures were extended by 11 nt in the HI or HIII domains to match the 79 nt length of HHR (-) and optimized using the same minimization protocol (see Methods). Using a scaling factor of 1.4 to account for the dynamics of the HHR RNA (see Results), the corrected radii of gyration are the following: 49Å (A), 43Å (B) and 45Å (C) versus 50Å as calculated from SANS data.