



Supplemental Material to:

**Senada Nozinovic, Anke Reining, Yong-Boum Kim,
Jonas Noeske, Kai, Schlepckow, Jens Wöhnert,
Harald Schwalbe**

**The importance of helix P1 stability for structural pre-
organization and ligand binding affinity of the adenine
riboswitch aptamer domain**

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Supporting Information

Aptamer Domain Of The Adenine-Sensing Riboswitch: Role Of Helix Stability In Structural Pre-Organization And Binding Affinity

Senada Nozinovic^{1,2}, Anke Reining^{1,2}, Yong-Boum Kim^{1,2}, Jonas Noeske³, Kai Schlepckow^{1,2}, Jens Wöhnert^{1,4}, Harald Schwalbe^{1,2*}

¹Johann Wolfgang Goethe-University Frankfurt, Center for Biomolecular Magnetic Resonance (BMRZ), Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

²Institute of Organic Chemistry and Chemical Biology

³Department of Molecular and Cell Biology, University of California at Berkeley, Berkeley, CA 94720, USA.

⁴Institute for Molecular Biosciences Max-von-Laue-Strasse 9, 60438 Frankfurt (Germany)

* To whom correspondence should be addressed.

Email: schwalbe@nmr.uni-frankfurt.de, Tel: (+49)69-798-29130, Fax: (+49) 6979829515

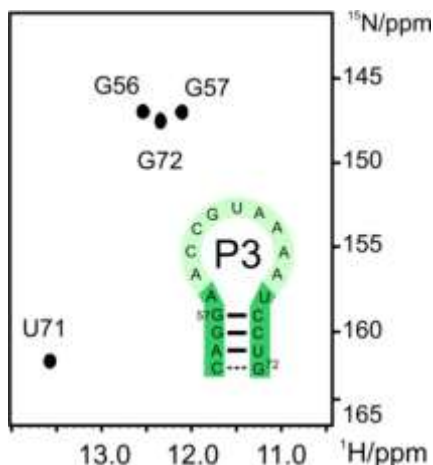


Figure S1: Secondary structure of isolated helix P3 ([RNA]=1 mM). Imino regions of the 2D- ^1H , ^{15}N -HSQC spectra at 283 K in the presence of Mg^{2+} .

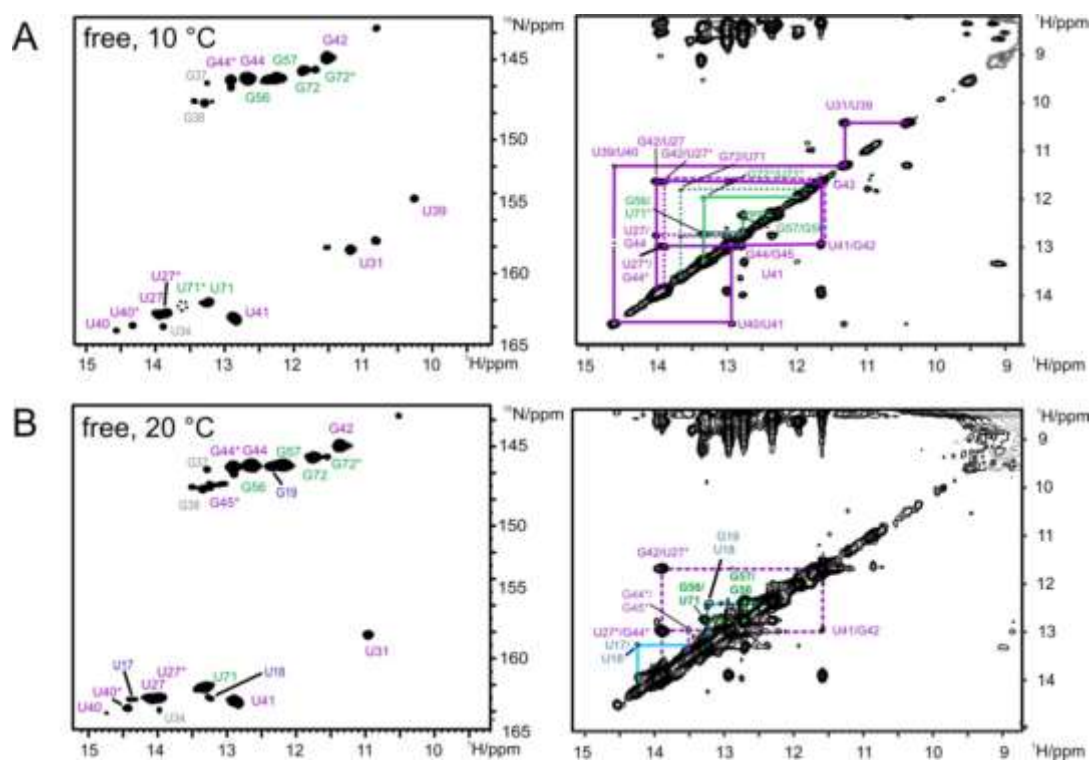


Figure S2: Temperature-induced changes in the wild-type aptamer domain ([RNA] = 0.5 mM). Imino regions of the 2D- ^1H , ^{15}N -HSQC spectra (left) and 2D- ^1H , ^1H -NOESY spectra with 200 ms mixing time (right) measured at 900 MHz and 10 °C (A) and 20 °C (B). NOE connectivities by solid lines and dashed lines (and *) indicate two different conformations. The color code for assignments is adapted to the presentation of the secondary structure in Figure 4D.

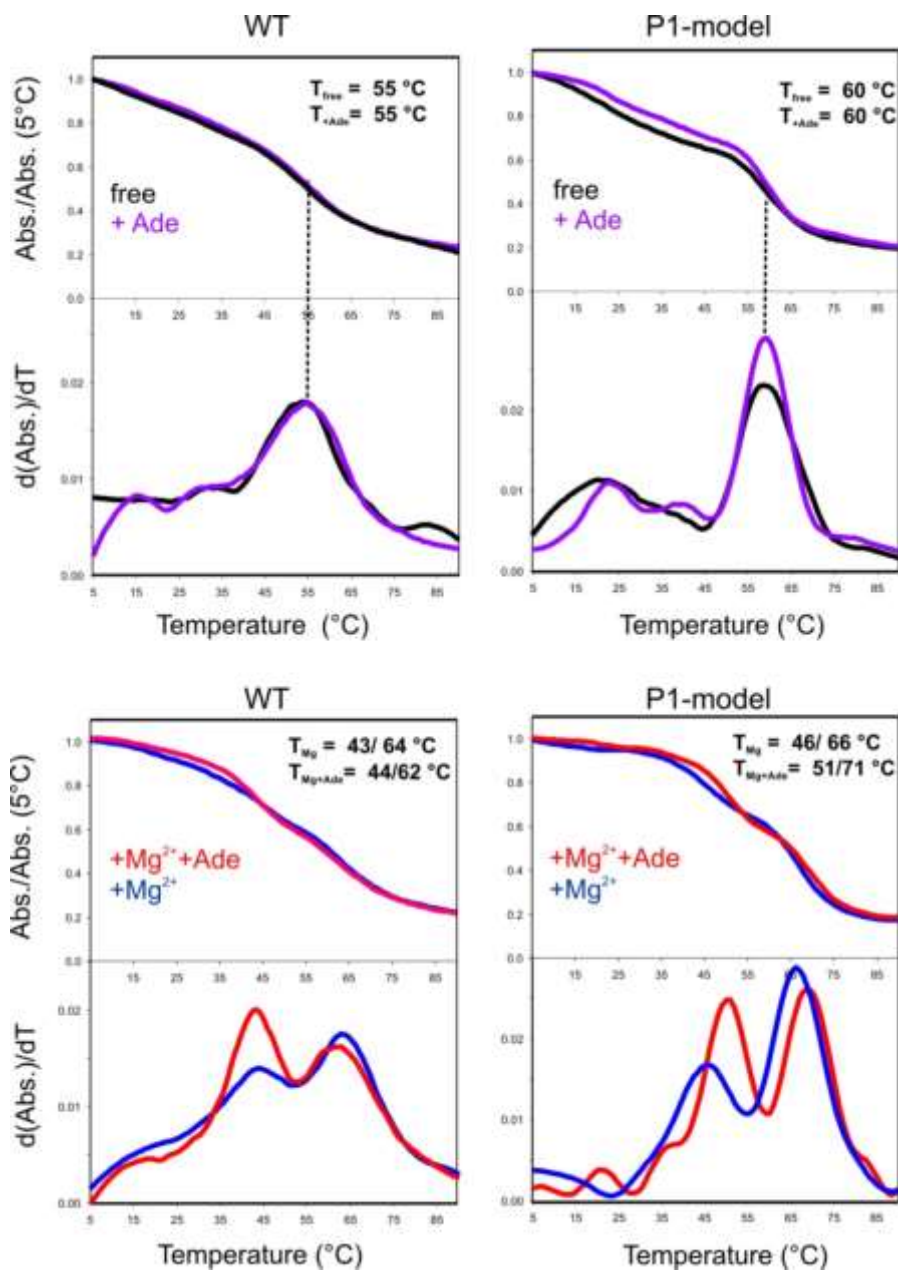


Figure S3: Thermal stability of aptamer domains. The CD melting curves of the wild-type and the P1-model aptamer domain under different conditions (free, with Mg²⁺ and/or adenine) are recorded at a wavelength of 258 nm. The first derivative of the CD melting curve is shown below.