Supporting Information

Unusually Strong Binding to the DNA Minor Groove by a Highly Twisted Benzimidazole-Diphenylether: Induced Fit and Bound Water[†]

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Figure S1. SPR sensorgrams for the kinetics interaction of RT29 with AATTAA hairpin DNA. The RT29 concentrations are from the lowest curve to highest curve 0, $1x10^{-9}$, $2.5x10^{-9}$, $3.5x10^{-9}$, $5.5x10^{-9}$, $2.5x10^{-8}$, $5x10^{-8}$, $7.5x10^{-8}$, and $1.0x10^{-7}$ M. The experiments were conducted at 25^{0}C in 10 mM Tris buffer, 1 mM EDTA, 1 M NaCl, pH 7.4 at a flow rate of 50μL/min.

Figure S2. ITC titration of RT29 into AATTAA hairpin DNA. The experiment were conducted in a Microcal VP ITC at 25°C in 10mM cacodylic buffer, 1mM EDTA, 200mM NaCl and pH 6.25. The experiments were conducted by injecting an initial 4 μl aliquot of the RT29 compound (35 μM) into DNA solution (10 μM in strand) in order to prime the syringe. This was followed by injection of a series of 10 μl aliquots of compound into DNA solution every 300 s.

Figure S3. Isothermal calorimetric titration curve of RT29 of 0.100mM into 0.0075mM 5'-CGATTCCGTCTCCGAATCG-3' sequence hairpin duplex in (CAC20 buffer with 200mM NaCl) at 25 ºC. The corrected heat was fitted to obtain ΔH.

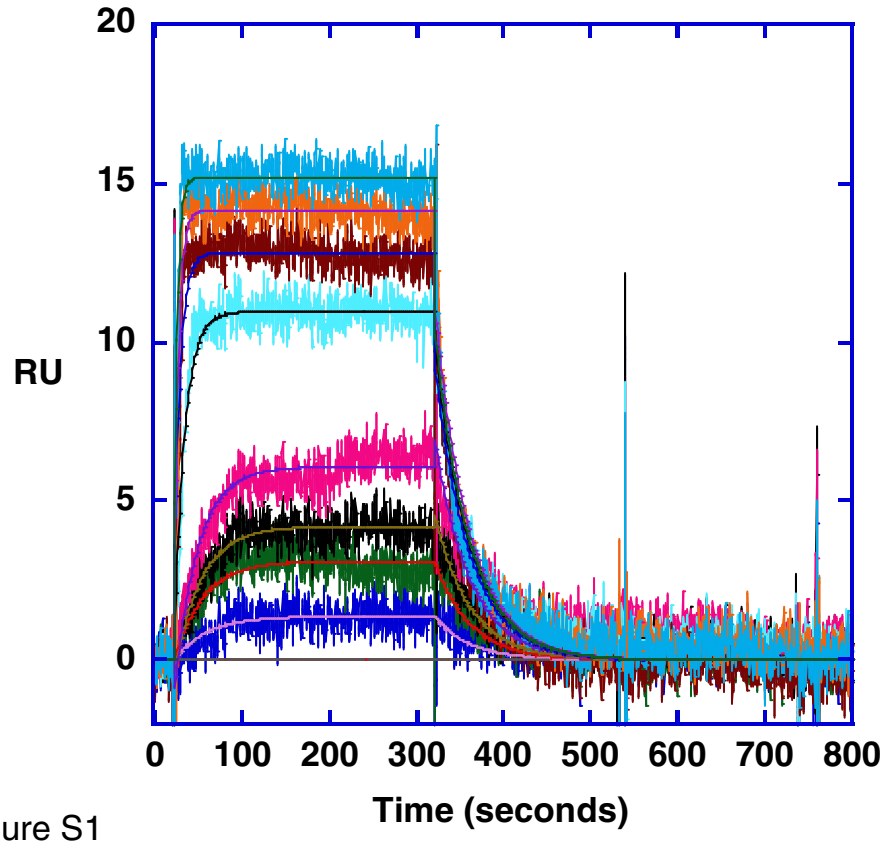
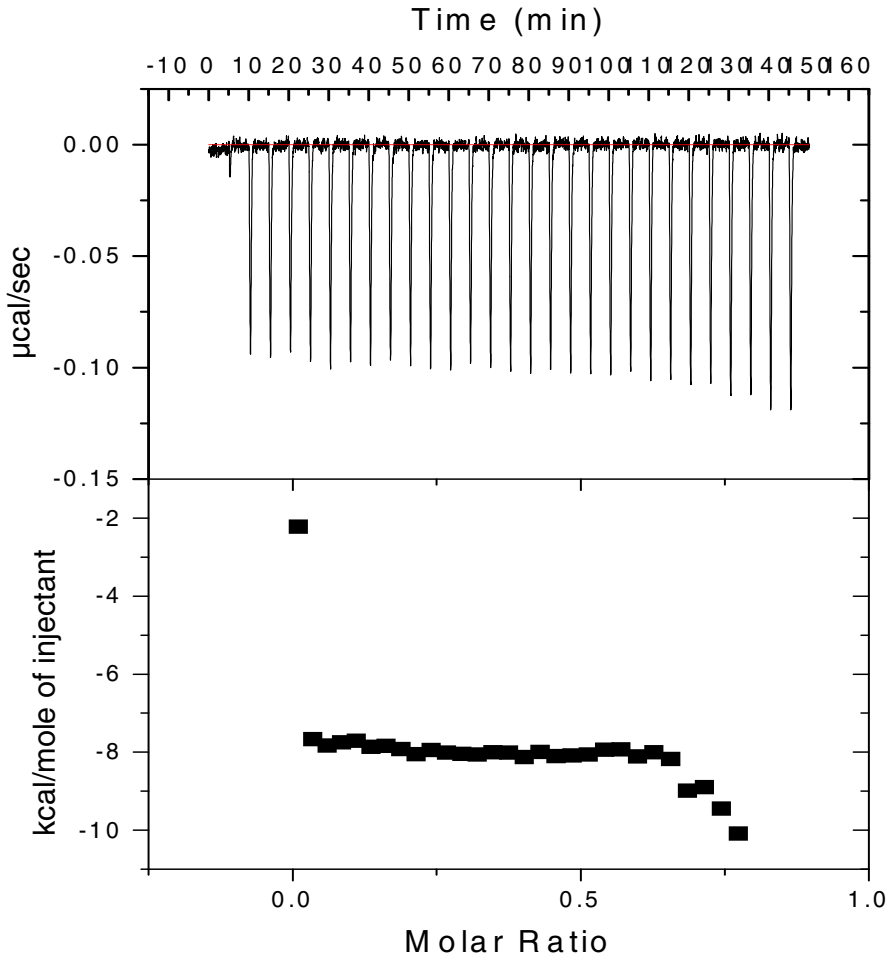


Figure S1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0.00
-0.05
-0.10
-0.15
µcal/sec
-2
-4
-6
-8
-10
kcal/mole of injectant
0.0
0.5
1.0
Molar Ratio

Figure S2

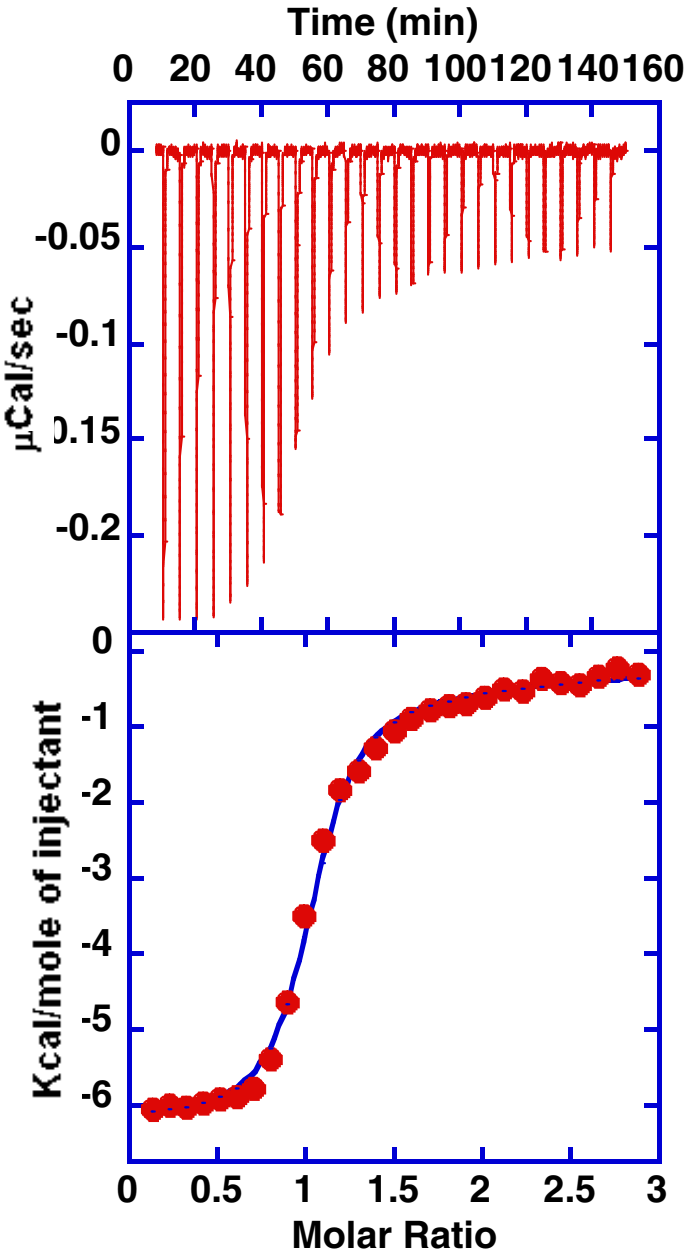
Time (min)
0 20 40 60 80 100120140160
0
-0.05
-0.1
0.15
-0.2
µCal/sec
0
-1
-2
-3
-4
-5
-6
Kcal/mole of injectant
0 0.5 1 1.5 2 2.5 3
Molar Ratio

Figure S3