Supporting Information

Predicting ion-nucleic acid interactions by energy landscape-guided sampling

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In Fig. 1 we show the free energy landscape $\Delta G(N_b, \Delta G_M)$ for the BWYV structure immersed in a Mg^{2+}/Na^{+} mixture solution where [Na^{+}] is fixed at 0.054M. As [Mg2+] is increased from 1 mM to 10mM, the energy landscape shows two changes. First, the location of the free energy minimum shifts from $(N_b^*, \Delta G_M)$ = (3, 23.85 kcal/mol) to (8, 18.61 kcal/mol). Second, the width of the free energy basin is increased. Physically, the increase in the Mg^{2+} ion concentration causes more Mg^{2+} ions to bind to the RNA and hence a lowered electrostatic energy. In addition, a higher [Mg^{2+}] leads to stronger ion correlation and thus a larger TB region. For a given ion distribution mode, a larger TB region means a larger space for the TB ions to move around and hence a broader energy distribution. On the energy landscape, this is shown as the broader valley at the free energy minimum.

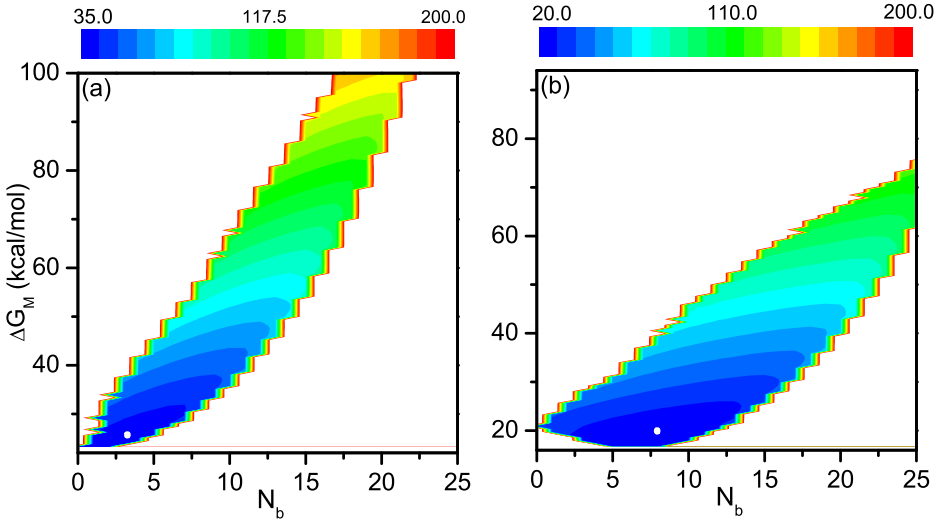

Figure 1: The electrostatic free energy landscape $\Delta G(N_b, \Delta G_M)$ for the BWYV pseudoknot in the 1mM (a) and 10mM (b) [Mg^{2+}] ion solutions with a fixed 0.054 [Na^{+}] background. The unit of the color bar is $kcal/mol$; The white solid circles denote the most stable states of the system. In order to eliminate any possible uncertainties caused by incomplete sampling of the modes, we have used the exact enumeration for all the modes, including the high energy modes.