Mechanism of pH influence on aptamer binding with Cd^{2+} revealed by molecular dynamics simulation

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Supplementary material

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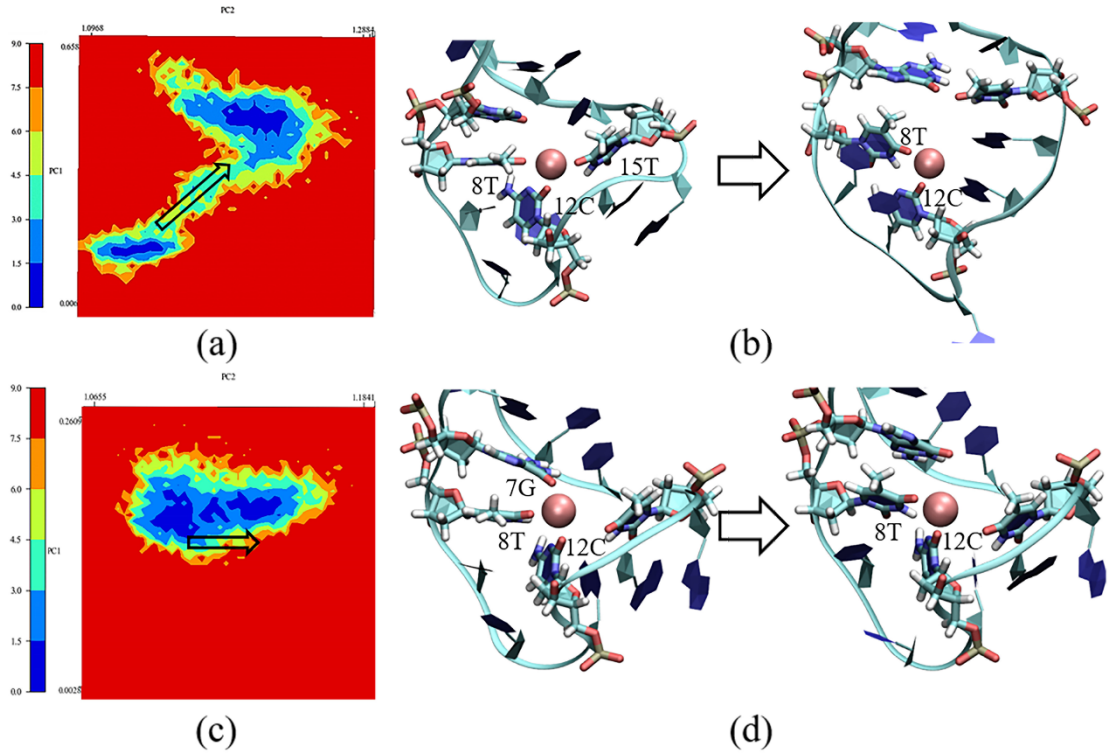

Fig. S1 The Free energy landscapes (FEL) plots of two parallel trajectories (a) and (c). (b) and (d) are snapshots of the structural transition of the Cd^{2+}-aptamer complexes at the two minimum positions in the FEL of (a) and (c), respectively. The arrow indicated the structural transformation trend obtained over time.