Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Information

Entropy and metal ions control ligand affinity and specificity in the malachite green binding RNA aptamer †

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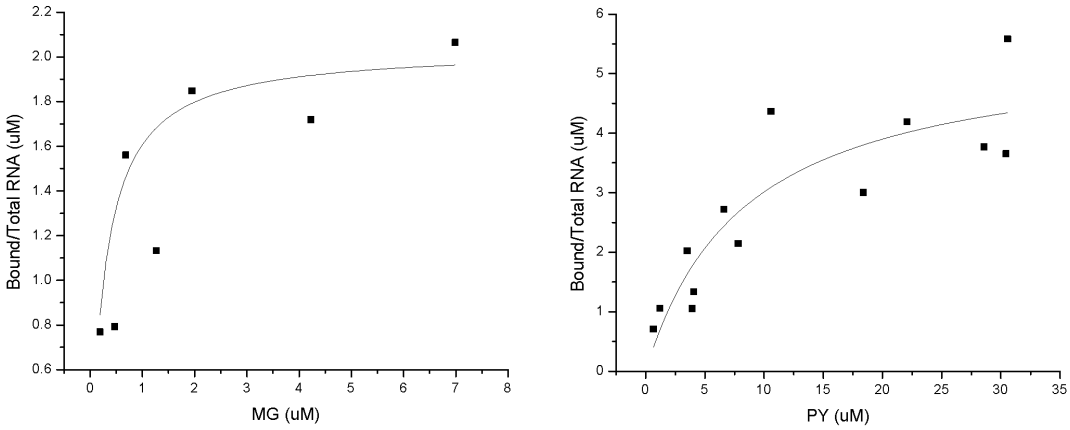
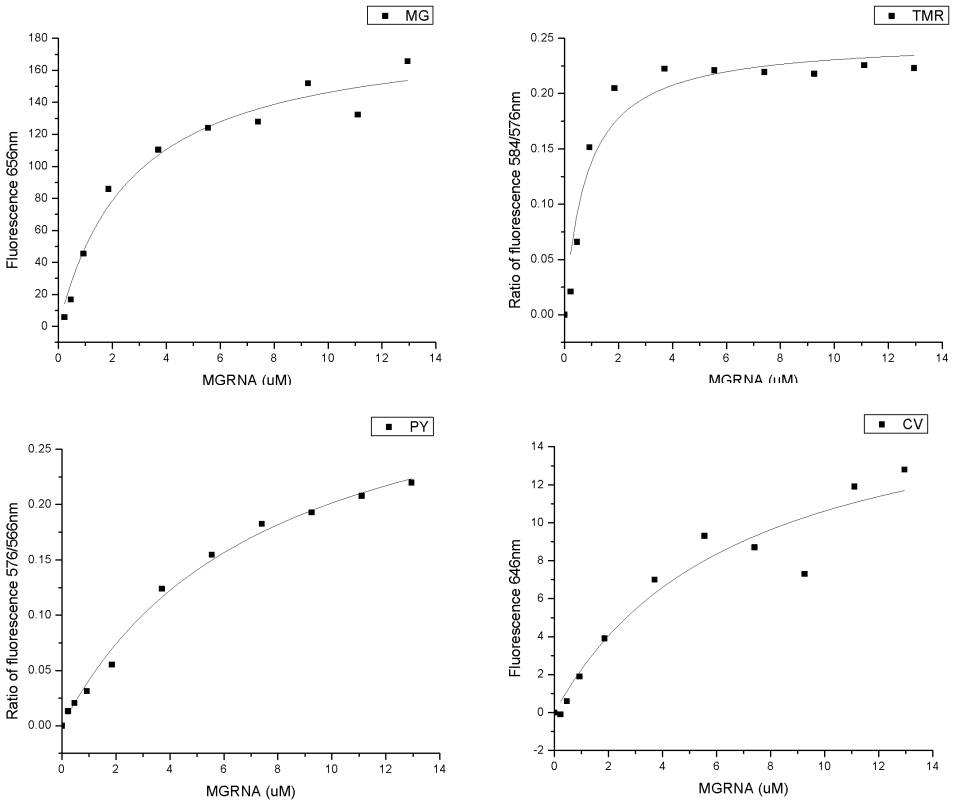
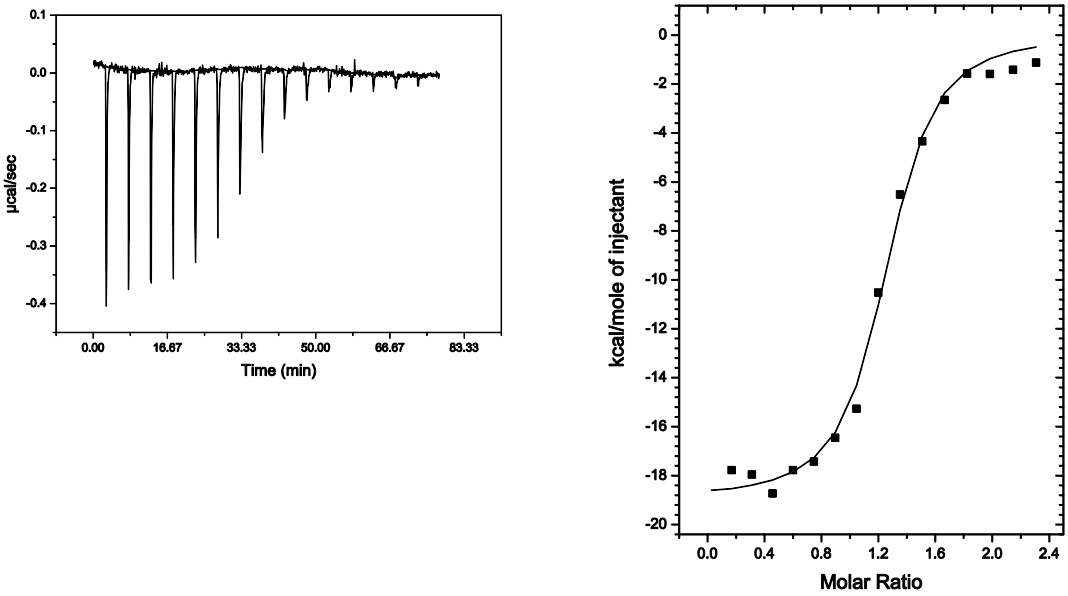


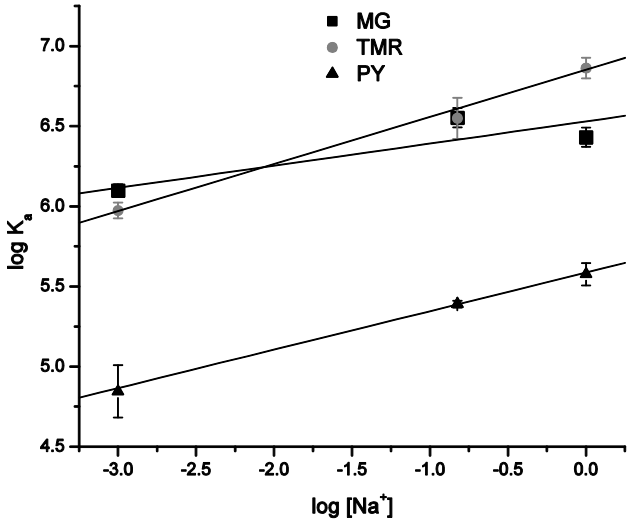
S1: Binding curves from equilibrium dialysis experiments preformed at 100mM phosphate buffer, 50mM NaCl, pH6.0. The binding curves were fit using Origin using the equation $y = (B_{max} * x) / (K_d + x)$.



S2: Binding curves from Nanodrop fluorescence experiments preformed at 50mM phosphate buffer, 150mM NaCl, pH6.7. The binding curves were fit using Origin using the equation $y = (B_{max} * x) / (K_d + x)$..



S3: Right: Typical ITC raw data showing heat generated over time as dye is injected into cell containing MGA RNA. Left: Integrated data fitted using Origin to a single binding site model which provides K_d, ΔH, ΔS values. Experiments were preformed at 10mM phosphate buffer with varying salt concentrations (1mM, 150mM, 1M) , pH 6.7.



S4: Plot of log K_a versus log [Na^+] for MG, TMR and PY binding to MGA. Data points were fit using linear regression (Excel) to generate lines and equations. Linear regression fits of shown as solid lines (——) MG data ($y = 0.1306x + 6.5273$, $R^2 = 0.7426$), TMR data ($y = 0.29x + 6.8315$, $R^2 = 0.9925$), and PY data ($y = 0.245x + 5.5827$, $R^2 = 0.9996$).