Supplementary Information

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Abstract: Using UV-vis absorption and circular dichroism (CD) spectroscopies, we explored the binding interactions of 3,3′-diethylthiatricarbocyanine iodide (**Cy7**) with polynucleotides of different sequences and helicity. CD showed to be a very diagnostic tool giving different spectroscopic chiroptical signatures for all explored DNA sequences upon **Cy7** binding. **Cy7** was able to spectroscopically discriminate between the right handed B-DNA of poly(dG-dC)$_2$ and its left handed Z-DNA counterpart induced by spermine or Co(III)hexamine via nearly opposite induced circular dichroic signal.

Keywords: Cy7 cyanine dye; left-handed Z-DNA; circular dichroism; DNA recognition; sensing

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Figure S1. Intensity change of the CD signals at 622 nm, 770 nm, and 800 nm as a function of the **Cy7** concentration when titrated with poly(dA-dT)$_2$ (red curve with triangles), poly(dG-dC)$_2$ (blue curve with squares), poly(dG).poly(dC) (green curve with spheres). Titration step: [Cy7] = 2.0 μM. Conditions: [DNA] = 50 μM, 10 mM NaCl, 5% MeOH + Na-cacodylate buffer (1mM, pH = 7.0).

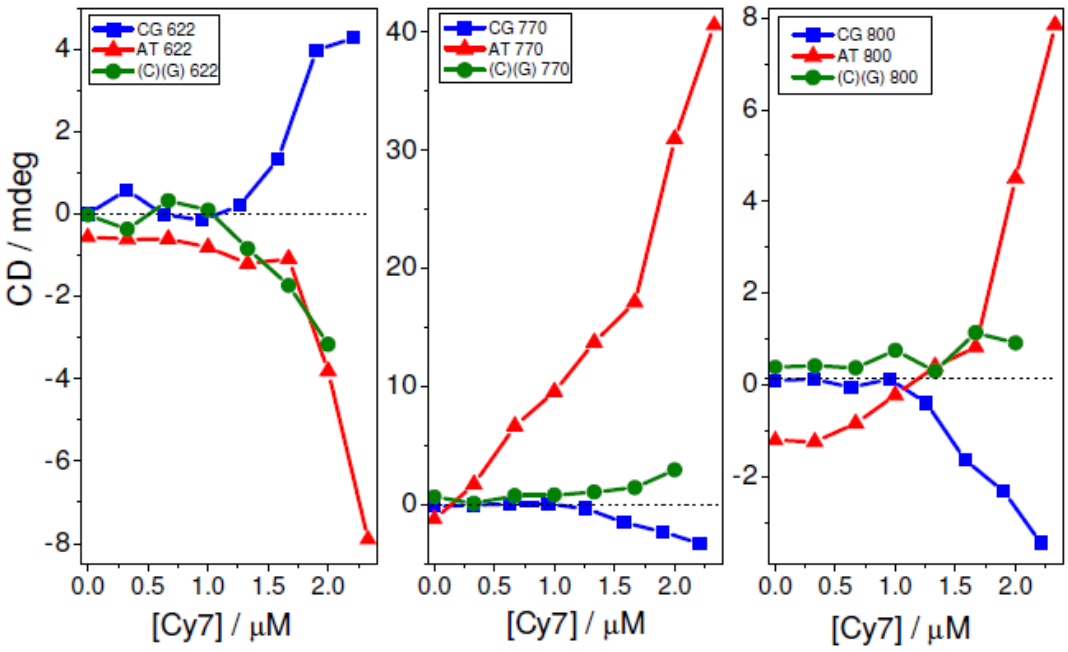

Figure S2. CD spectra of **Cy7** titrated to Co(III) induced Z-poly(dG-dC)$_2$. Titration step: [Cy7] = 2.0 μM. Conditions: [Z-poly(dG-dC)2] = 50 μM, [Co(III)] = 12 μM, [NaCl] = 10 mM, 5% MeOH + Na-cacodylate buffer (1mM, pH = 7.0).

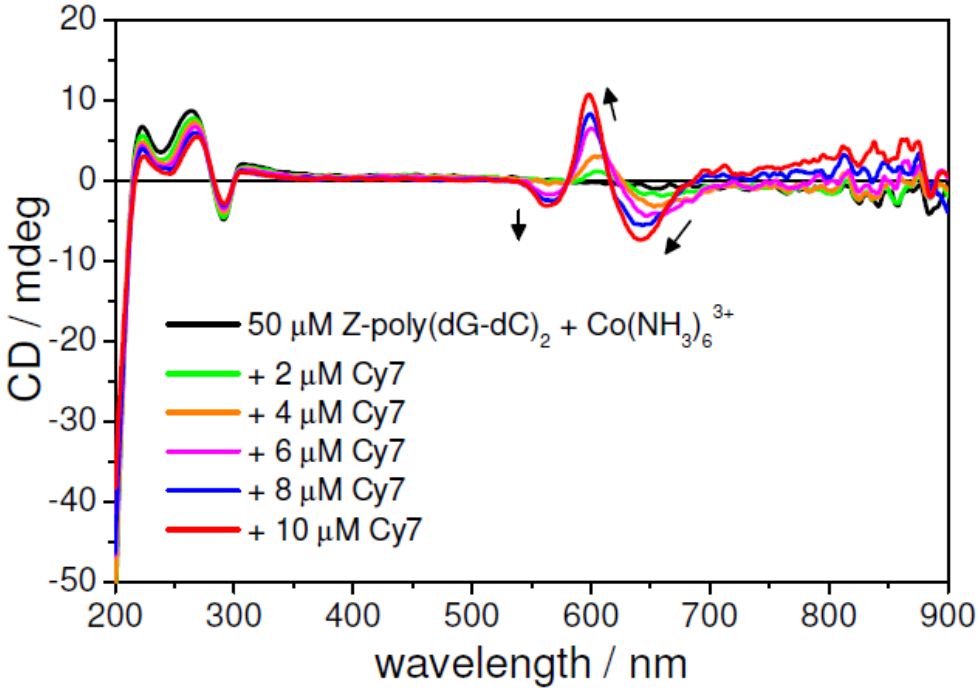

Figure S3. CD spectra comparison of **Cy7** bound to poly(dG-dC)$_2$ (blue) and Co(III) induced Z-poly(dGdC)$_2$ (red). Inset: intensity change of the CD signal at 645 nm as a function of the **Cy7** concentration. Conditions: [DNA] = 50 μM, [Co(III)] = 12 μM, [NaCl] = 10 mM, 5% MeOH + Na-cacodylate buffer (1mM, pH = 7.0). Titration step: [Cy7] = 2.0 μM.