Supplementary Information

Jung Kyu Choi 1, Alessandro D’Urso 1,2, Mitch Trauernicht 2, Murtaza Shabbir-Hussain 1, Andrea E. Holmes 2 and Milan Balaz 1,*

1 Department of Chemistry, University of Wyoming, Laramie, WY 82071, USA; E-Mails: jchoi4@uwyo.edu (J.K.C.); adurso@unict.it (A.D.); mshabbir@uwyo.edu (M.S.-H.)
2 Doane College, 1014 Boswell, Crete, NE 68333, USA; E-Mails: mitchell.trauernicht@doane.edu (M.T.); andrea.holmes@doane.edu (A.E.H.)

* Author to whom correspondence should be addressed; E-Mail: mbalaz@uwyo.edu; Tel.: +1-307-766-4330; Fax: +1-307-766-2807.

Received: 21 October 2011; in revised form: 2 November 2011 / Accepted: 7 November 2011 / Published: 16 November 2011

Abstract: Using UV-vis absorption and circular dichroism (CD) spectrosopies, 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
**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 (1 mM, pH = 7.0). Titration step: [Cy7] = 2.0 µM.

© 2011 by the authors; licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (http://creativecommons.org/licenses/by/3.0/).