Supporting Information for

The Dynamics and Efficiency of Hole Transport in LNA:DNA Hybrid Diblock Oligomers

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Materials and Methods

Materials. **Sa** and **Sd** were prepared, purified, and characterized as previously described.[1, 2] Oligonucleotide syntheses was carried out using phosphoramidite chemistry on a Expedite synthesizer. For LNA monomers the coupling time and oxidation time were modified as per manufacture protocol. The oligonucleotides were deprotected using 30% ammonium hydroxide at room temperature for 24 h, purified by HPLC and characterized by MALDI-TOF spectroscopy (Table S1). Emission spectra were recorded on SPEX Fluoromax fluorimeter for the $\mathbf{A_6}$ and $^{\mathbf{L}}\mathbf{A_6}$ conjugates and is shown in Figure S1.Thermal dissociation profiles were recorded on a Perkin Elmer Lambda 2 UV/VIS spectrometer with a Peltier Temperature Programmer and are shown in Figure S2. Incomplete melting and broad transitions are observed in all cases. Circular dichroism (CD) spectra were recorded on a Jasco-J-815 CD spectrometer and are shown in Figure S2.

Methods. Transient Absorption Spectra. Femtosecond (fs) time resolved transient absorption spectra of solutions containing ca. 50 μM hairpin in 10 mM phosphate buffer (pH 7.2) containing 0.1 M NaCl were obtained as previously described[3,4] using 350 nm excitation (which provides selective excitation of **Sa**) from a Ti-sapphire-based system having a time resolution of ca. 180 fs, a spectral range of 425-800 nm, and a time window of 0-6 ns.

Table S1. m/z values for oligomer sequences determined by MALDI-TOF mass spectrometry.

Sequences	Calculated	Found
$^{L}A_6$	4617.08	4615.10
$^{L}A_2G_4$	4509.00	4511.04
$^{L}A_3G_3$	4536.02	4537.02
$^{L}A_4G_2$	4563.04	4562.88
$A_2{}^{L}G_4$	4565.02	4566.11
$A_3{}^{L}G_3$	4536.02	4534.98
$A_2{}^{L}G_6$	5857.78	5860.11
$A_2{}^{L}G_8$	7150.54	7154.22
$^{L}A_2{}^{L}G_4$	4641.04	4640.56
$^{L}A_3{}^{L}G_3$	4635.05	4635.10
$T_2{}^{L}C_4$	4621.14	4620.19
$^{L}T_2{}^{L}C_4$	4677.16	4678.98
$^{L}(A_2G_4)$	4845.22	4845.99

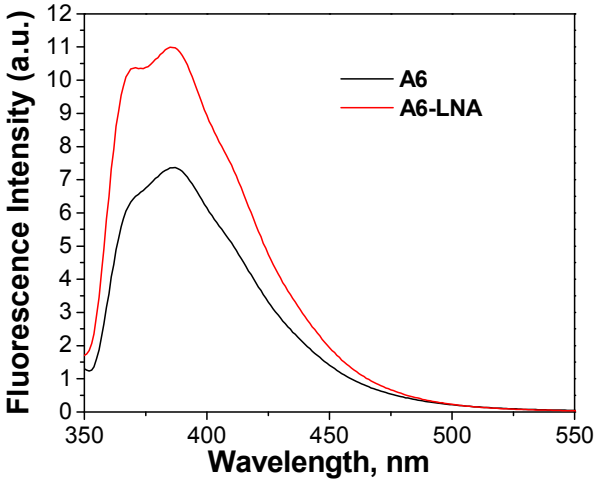

Figure S1. Emission spectra of A_6 (black) and $^{L}A_6$ (red) in phosphate buffer (10 mM phosphate, 0.1 M NaCl, pH 7.2). Excitation wavelength 340 nm.

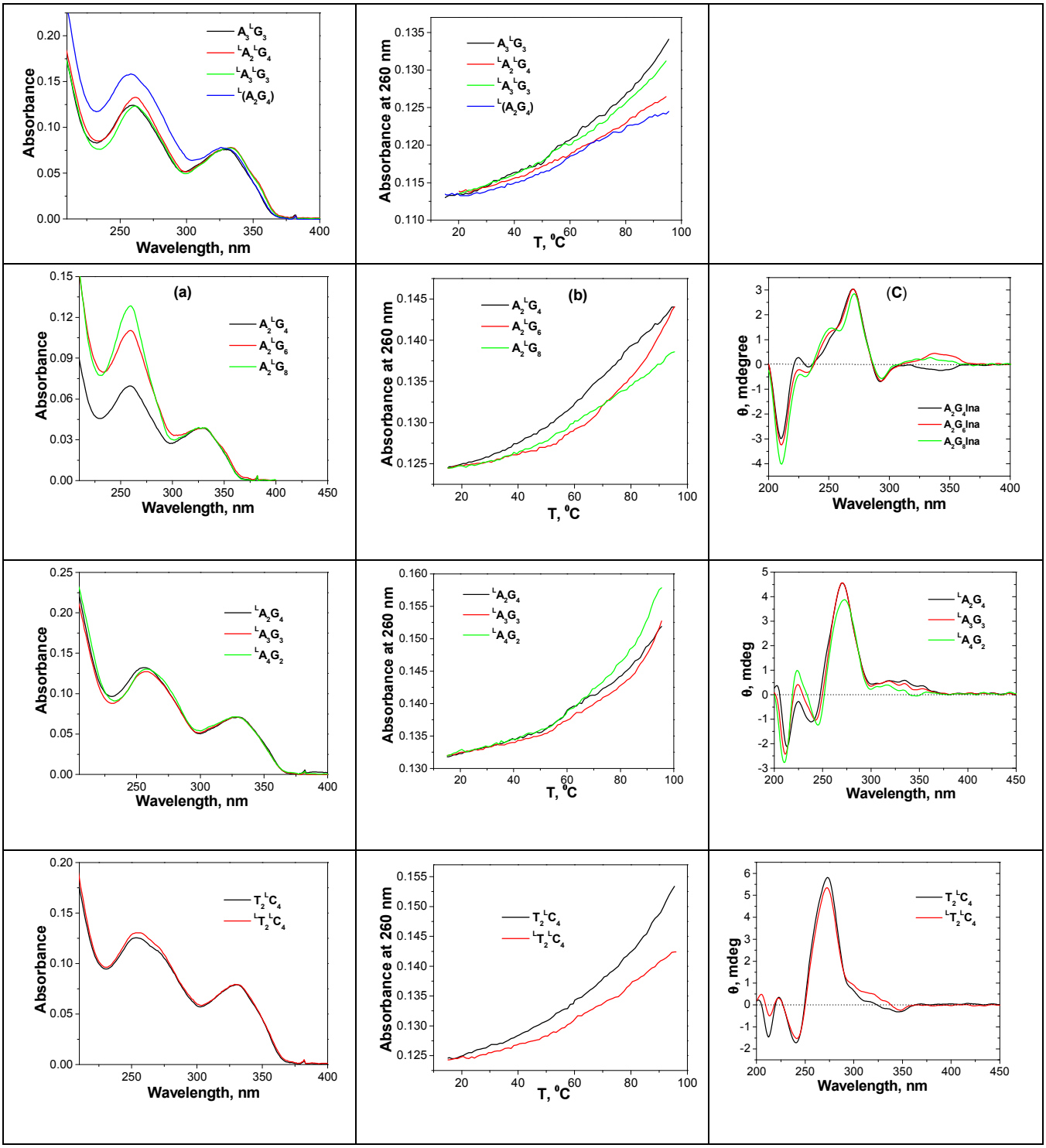

Figure S2. Absorption spectra (normalized at 330 nm) (a), thermal dissociation profile (b) and circular dichroism spectra (c) for the conjugates in 10 mM phosphate buffer, pH~ 7.2 (100 mM NaCl). See Chart 1 for structures.

References

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(3) Lewis, F. D.; Zhu, H.; Daublain, P.; Fiebig, T.; Raytchev, M.; Wang, Q.; Shafirovich, V. *J. Am. Chem. Soc.* **2006**, *128*, 791-800.

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