Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material

Acid-base behaviour and binding to double stranded DNA/RNA of benzo[*g*]phthalazine-based ligands

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Supplementary Material include:

Figure S24. Fluorimetric titration of **1** at pH 6 with *duplex **TA***. Inset: fitting of fluorescence emission intensity.

Figure S25. Fluorimetric titration of **1** at pH 6 with *duplex **TC***. Inset: fitting of fluorescence emission intensity.

Figure S26. Fluorimetric titration of **1** at pH 6 with *duplex **TG***. Inset: fitting of fluorescence emission intensity.

Figure S27. Fluorimetric titration of **1** at pH 6 with *duplex **TT***. Inset: fitting of fluorescence emission intensity.

Figure S28. Fluorimetric titration of **2** at pH 6 with *duplex **TA***. Inset: fitting of fluorescence emission intensity.

Figure S29. Fluorimetric titration of **2** at pH 6 with *duplex **TC***. Inset: fitting of fluorescence emission intensity.

Figure S30. Fluorimetric titration of **2** at pH 6 with *duplex **TG***. Inset: fitting of fluorescence emission intensity.

Figure S31. Fluorimetric titration of **2** at pH 6 with *duplex **TT***. Inset: fitting of fluorescence emission intensity.

Figure S32. Minimum energy conformers calculated for the interaction of **2** (A) and **3** (B) with double stranded DNA.

Table S1.- Binding constants (K_a) and spectroscopic properties of complexes calculated from UV-Vis and fluorimetric titrations of compounds with mismatched and fully matched duplexes (sodium cacodylate 10 mM, NaCl 100 mM, pH 6.0).

	Oligonucleotide	log K_a (UV Vis)	log K_a (Fluorescence)	[a]I
1	duplex *TA*	5.5(2)	5.9(2)	0.39
	duplex *TC*	5.2(3)	5.7(1)	0.41
	duplex *TG*	5.0(1)	5.9(1)	0.52
	duplex *TT*	5.2(1)	5.7(1)	0.41
2	duplex *TA*	4.9(3)	6.1(1)	0.37
	duplex *TC*	5.4(1)	5.5(2)	0.48
	duplex *TG*	5.0(2)	5.7(3)	0.36
	duplex *TT*	5.1(1)	6.2(2)	0.39

[a]Emission change; I = I(complex)/I(ligand).

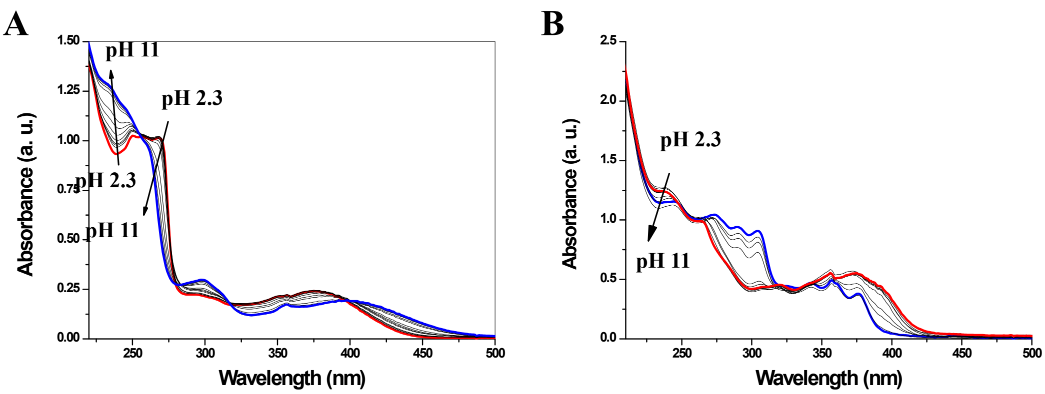

Figure S1.- UV-Vis spectra changes with the pH of compound **1** (A) and **2** (B). Blue line is the most basic UV-Vis spectra (pH ~ 11) and red line is the most acidic UV-Vis one (pH ~ 2)

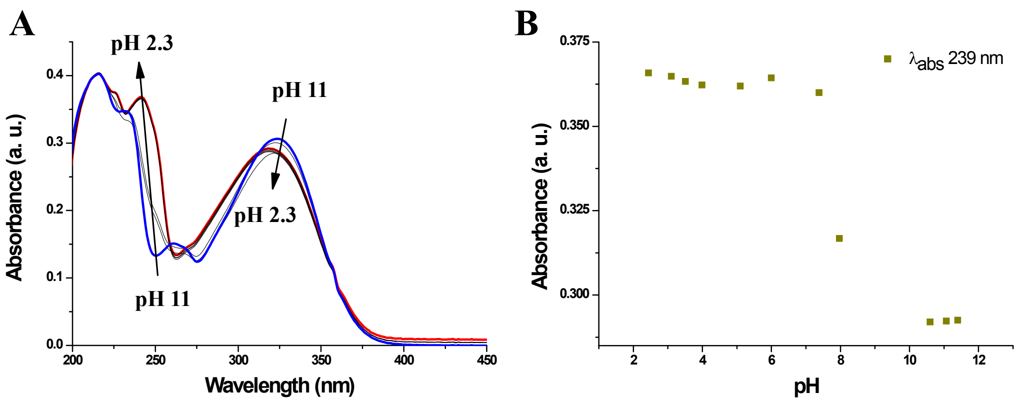

Figure S2.- UV-Vis spectra changes with the pH of phthalazine **3** (A) and absorption maxima at 239 nm with the pH (B). Blue line is the most basic UV-Vis spectra (pH ~ 11) and red line is the most acidic UV-Vis one (pH ~ 2)

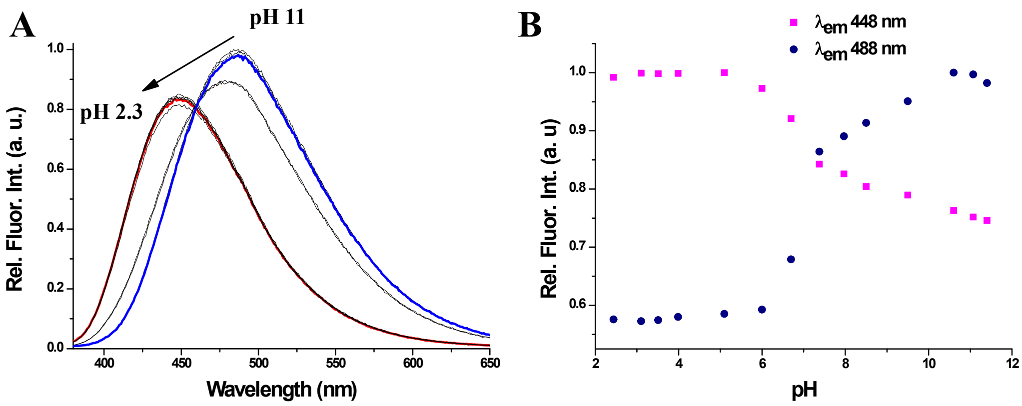

Figure S3.- Emission fluorescence spectra changes with the pH of phthalazine **3** (A) and emission maxima at 448 and 488 nm respectively with the pH (B). Blue line is the most basic UV-Vis spectra (pH ~ 11) and red line is the most acidic UV-Vis one (pH ~ 2)

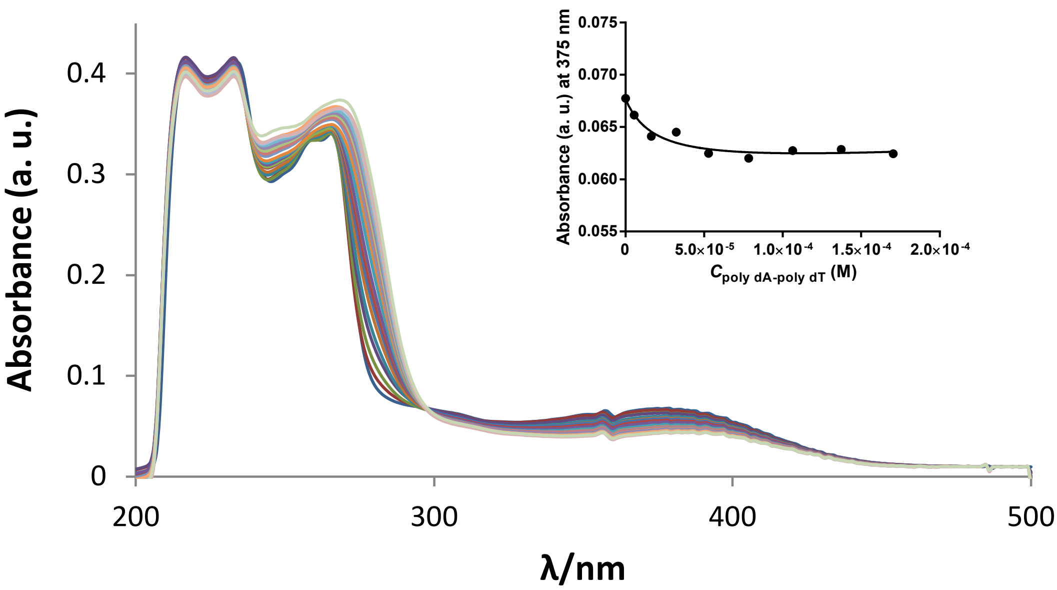

Figure S4. UV-Vis titration of **1** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly dA-poly dT. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

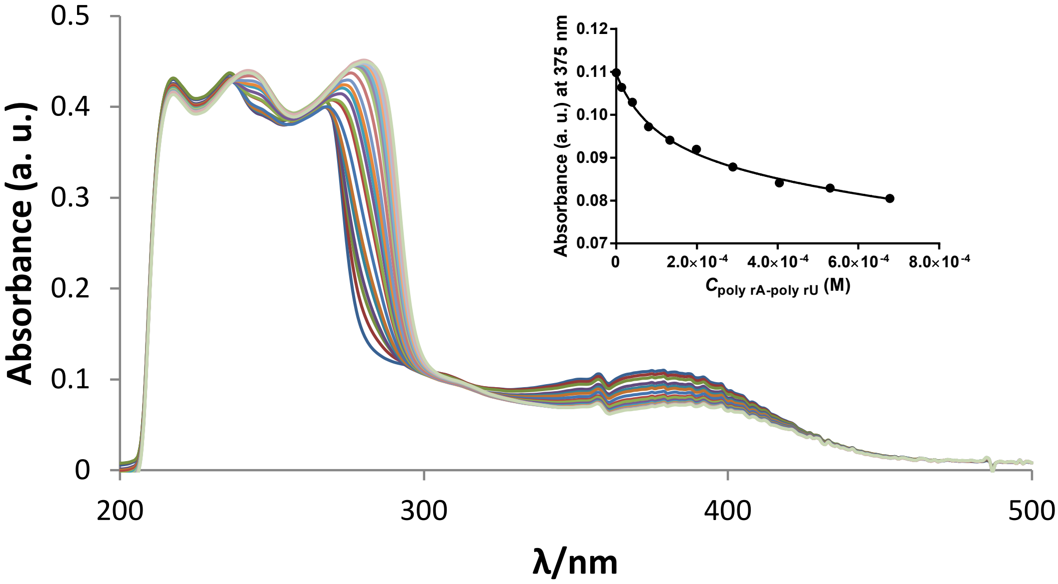

Figure S5. UV-Vis titration of **1** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly rA-poly rU. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

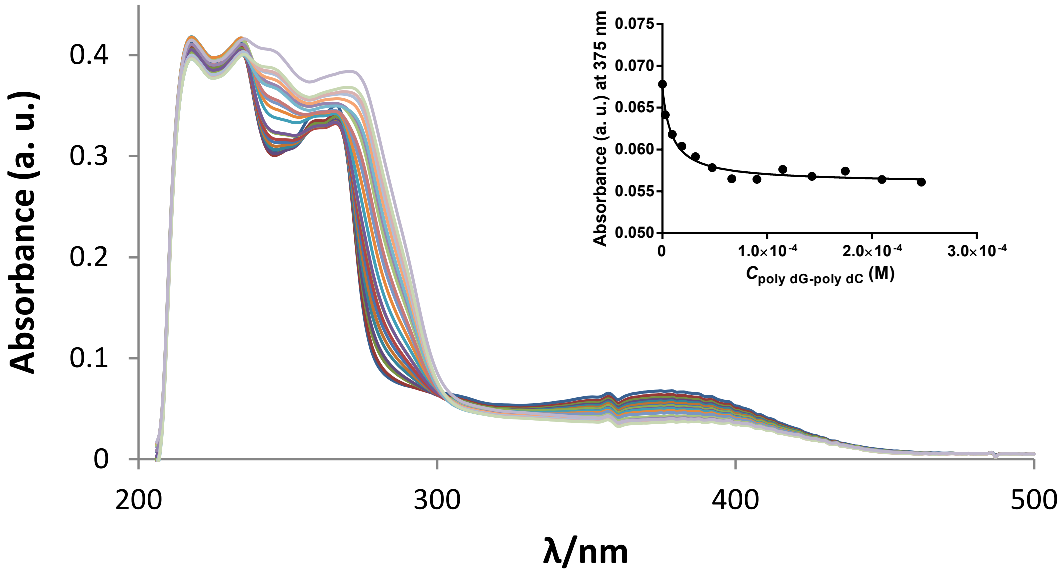

Figure S6. UV-Vis titration of **1** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly dG-poly dC. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

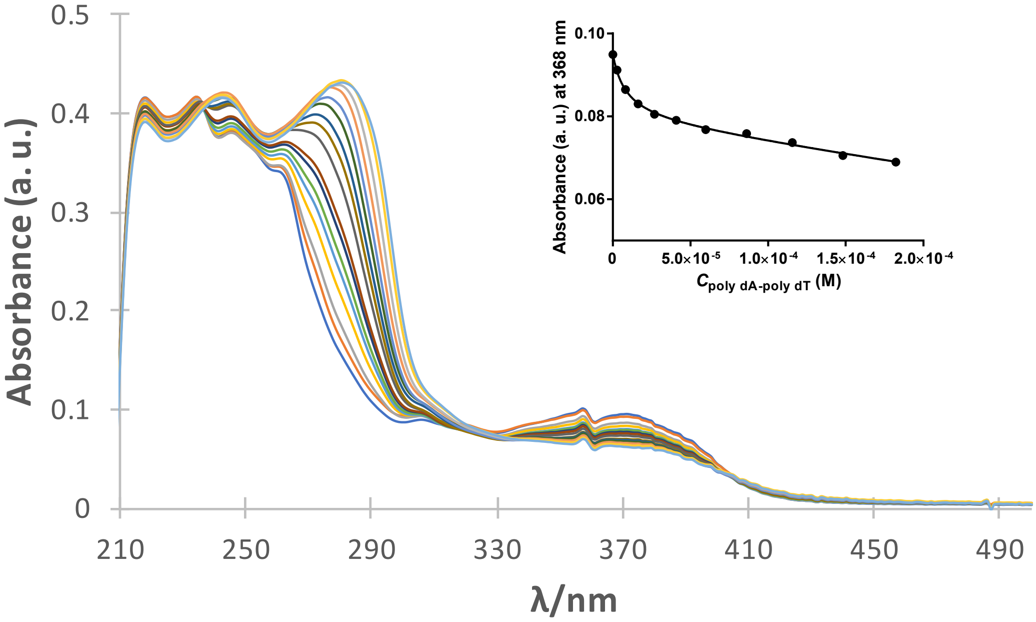

Figure S7. UV-Vis titration of **2** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly dA-poly dT. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

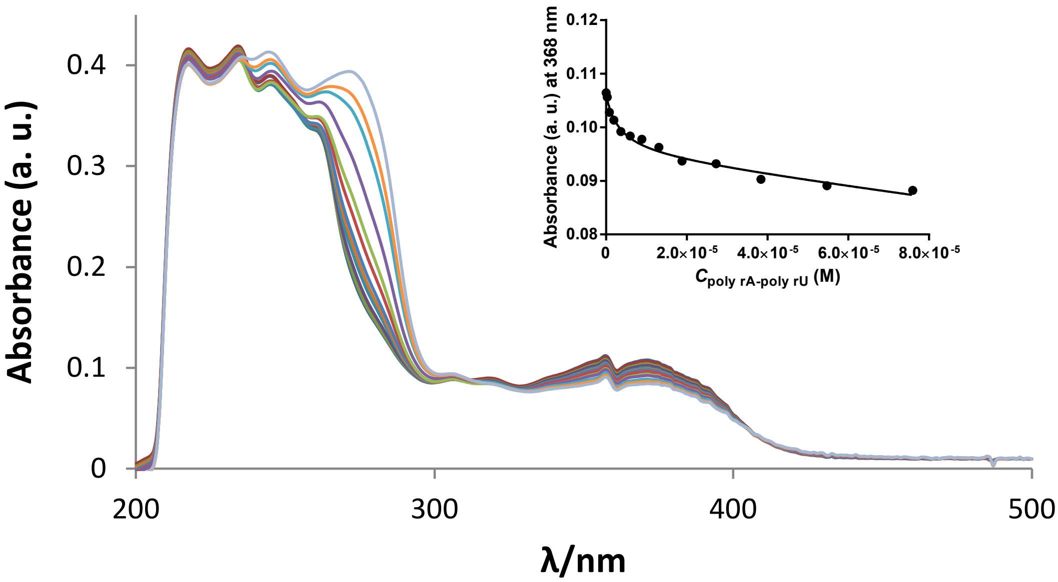

Figure S8. UV-Vis titration of **2** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly rA-poly rU. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

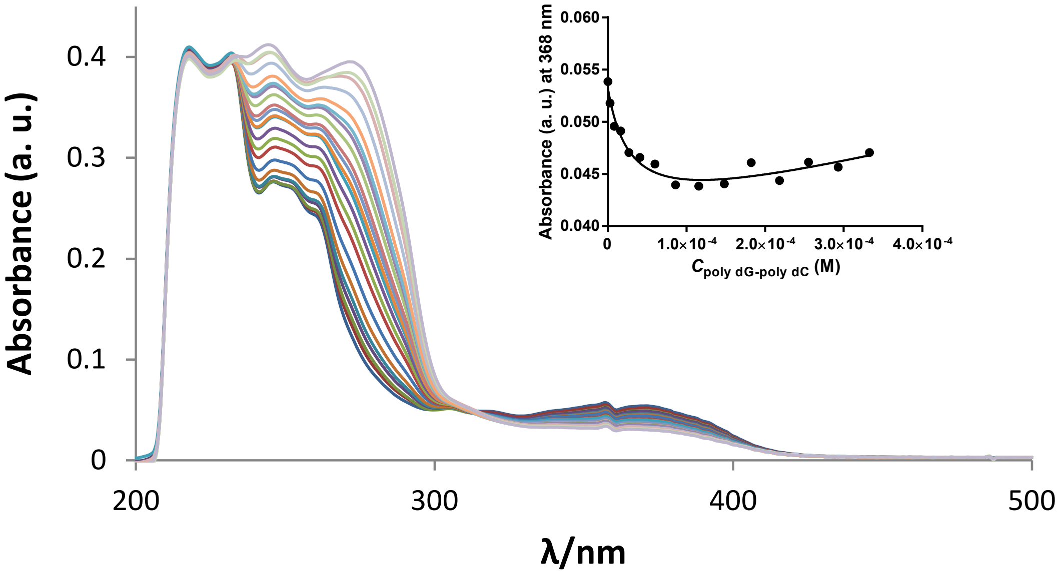

Figure S9. UV-Vis titration of **2** ($c = 5 \times 10^{-6}$ M) at pH 7 with poly dG-poly dC. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

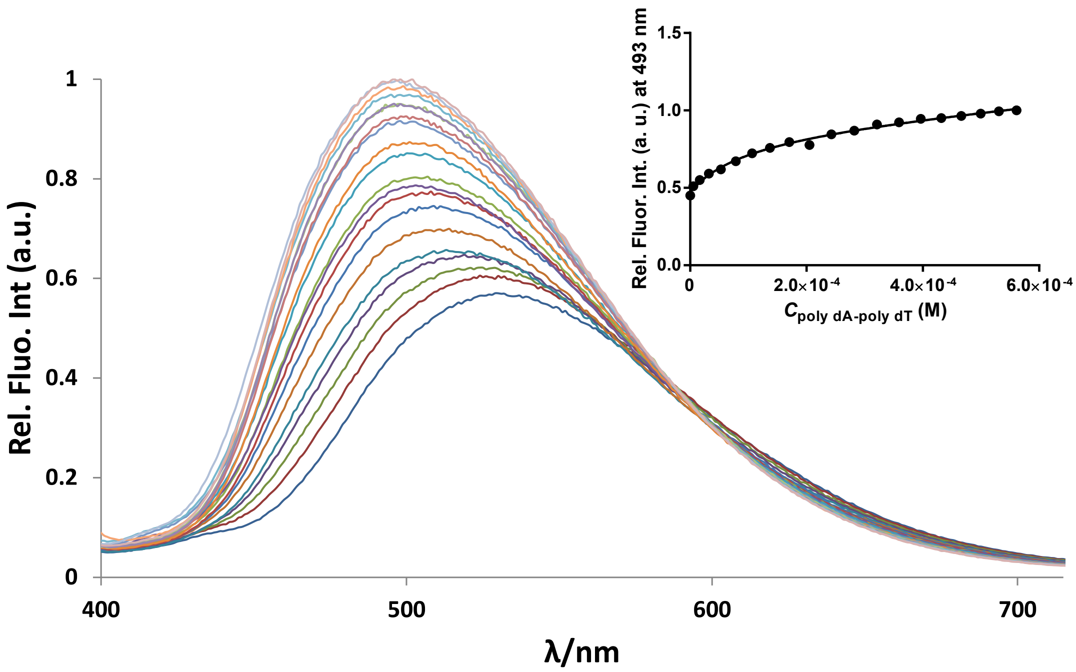

Figure S10. Fluorimetric titration of **1** ($c = 5 \times 10^{-6}$ M, λ_{exc}=380 nm) at pH 7 with poly dA-poly dT. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, I = 0.05 M.

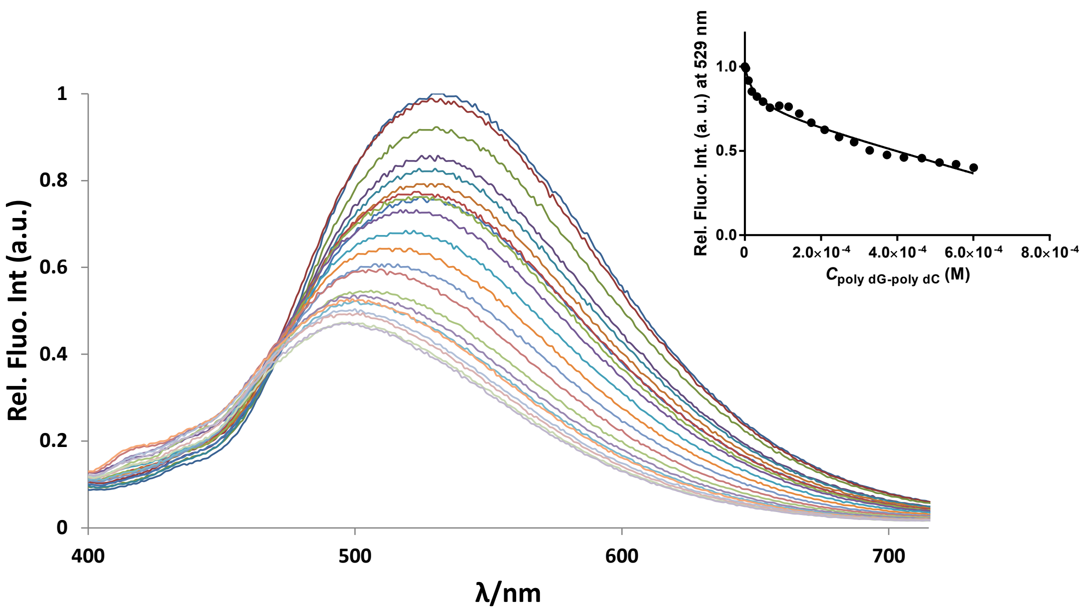

Figure S11. Fluorimetric titration of **1** ($c = 5 \times 10^{-6}$ M, λ_{exc}=380 nm) at pH 7 with poly dG-poly dC. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, I = 0.05 M.

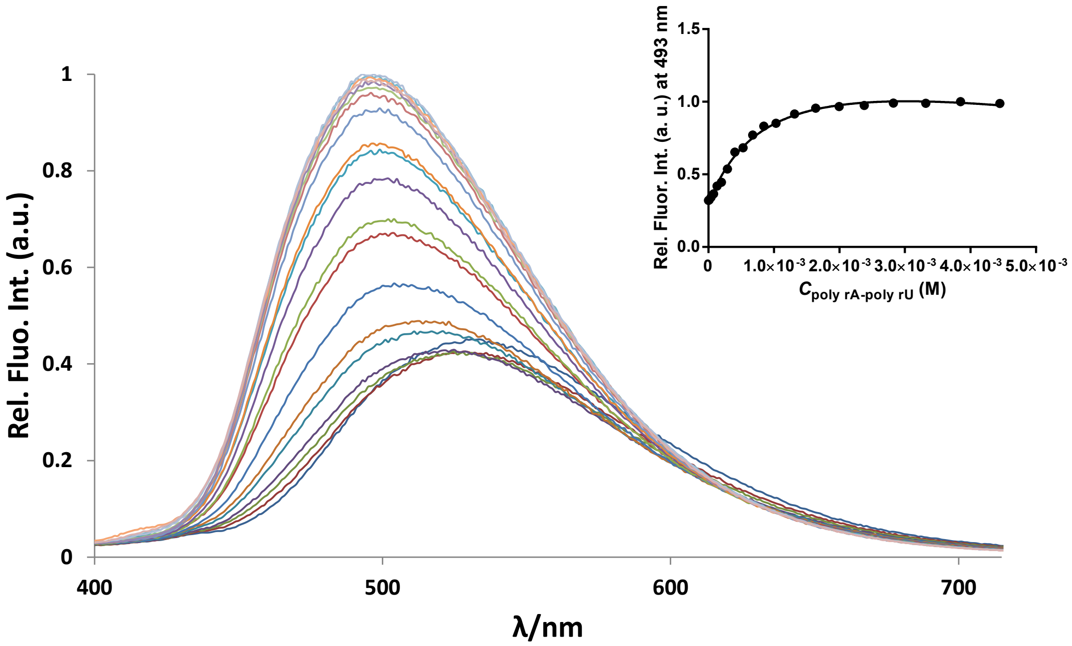

Figure S12. Fluorimetric titration of **1** ($c = 5 \times 10^{-6}$ M, λ_{exc}=380 nm) at pH 7 with poly rA-poly rU. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, I = 0.05 M.

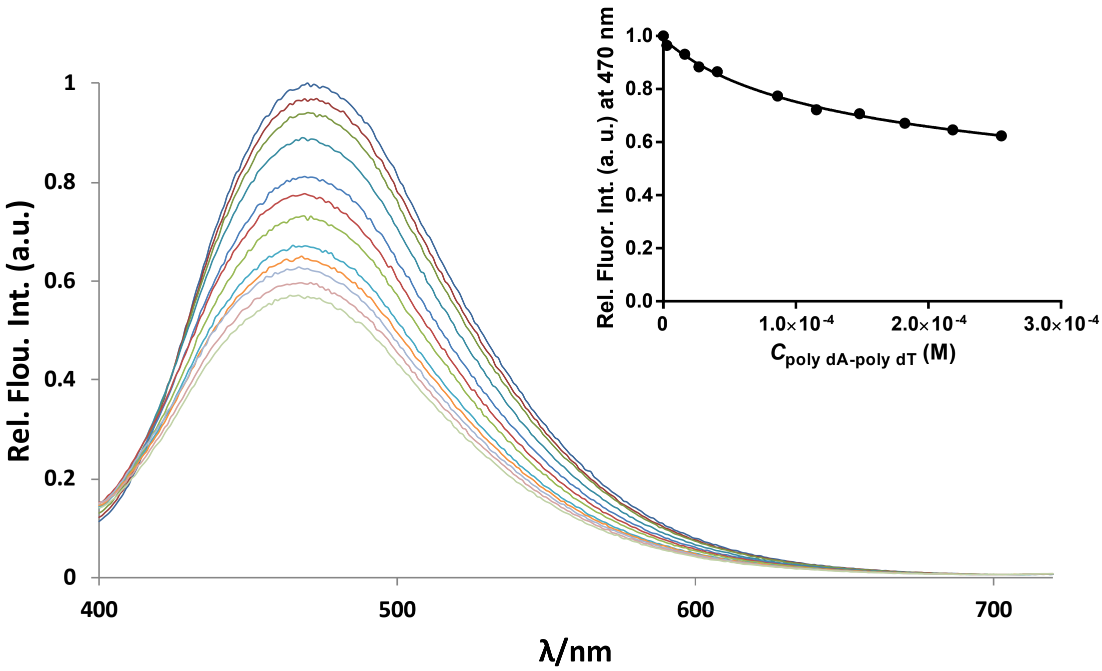

Figure S13. Fluorimetric titration of **2** ($c = 5 \times 10^{-6}$ M, λ_{exc}=380 nm) at pH 7 with poly dA-poly dT. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

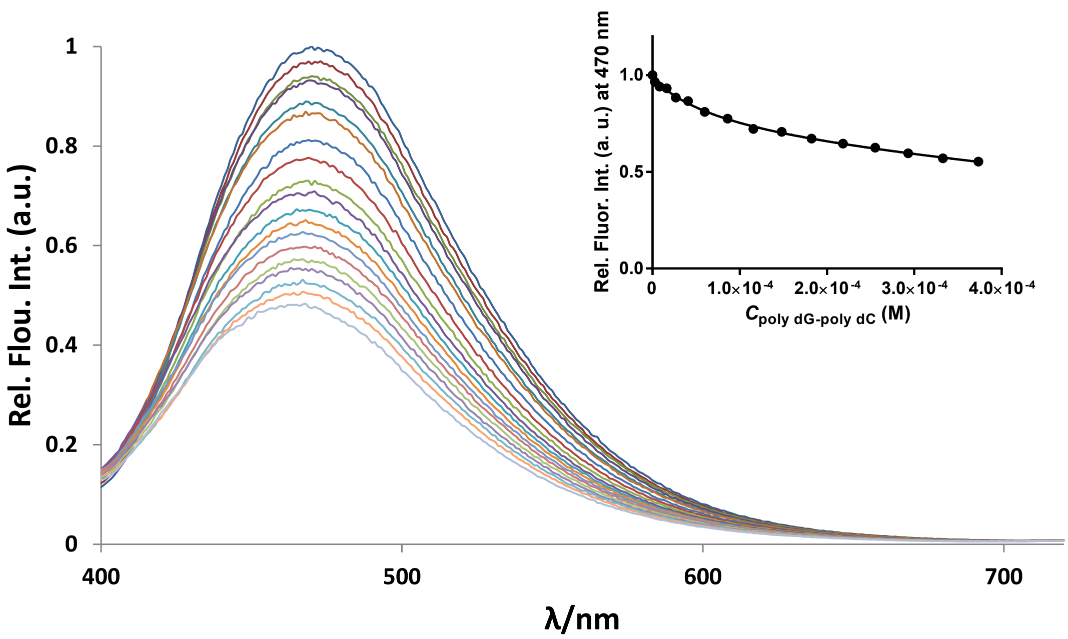

Figure S14. Fluorimetric titration of **2** ($c = 5 \times 10^{-6}$ M, λ_{exc}=380 nm) at pH 7 with poly dG-poly dC. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, $I = 0.05$ M.

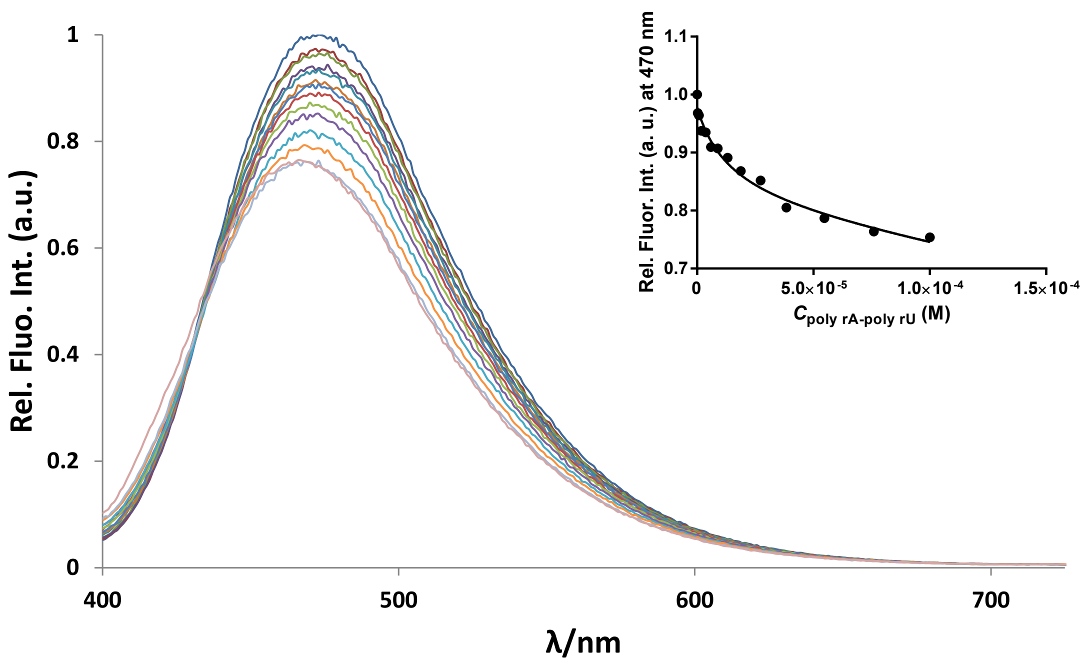

Figure S15. Fluorimetric titration of **2** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 7 with poly rA-poly rU. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer, I = 0.05 M.

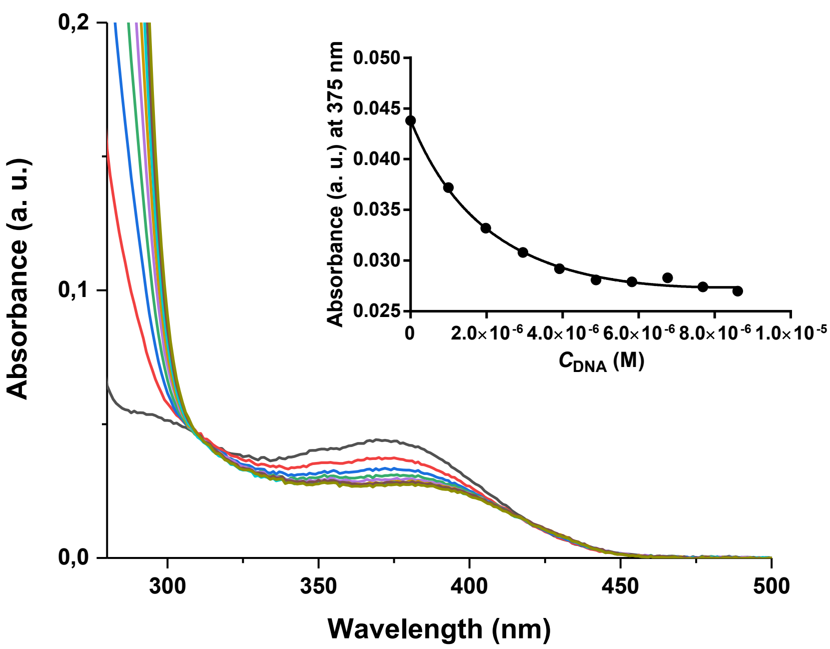

Figure S16. UV-Vis titration of **1** (c = 5 × 10^{-6} M) at pH 6 with *duplex **TA***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

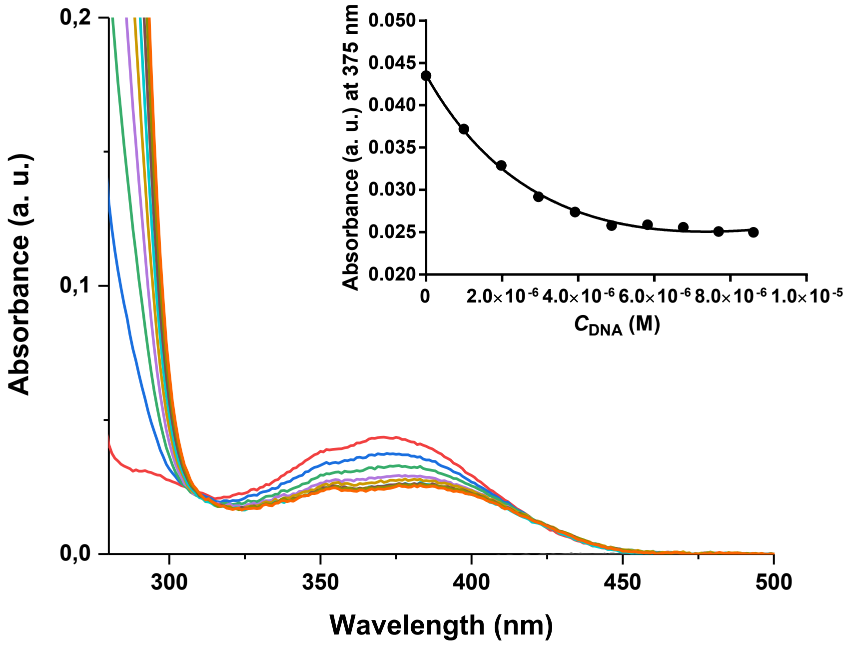

Figure S17. UV-Vis titration of **1** ($c = 5 \times 10^{-6}$ M) at pH 6 with *duplex* ***TC***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

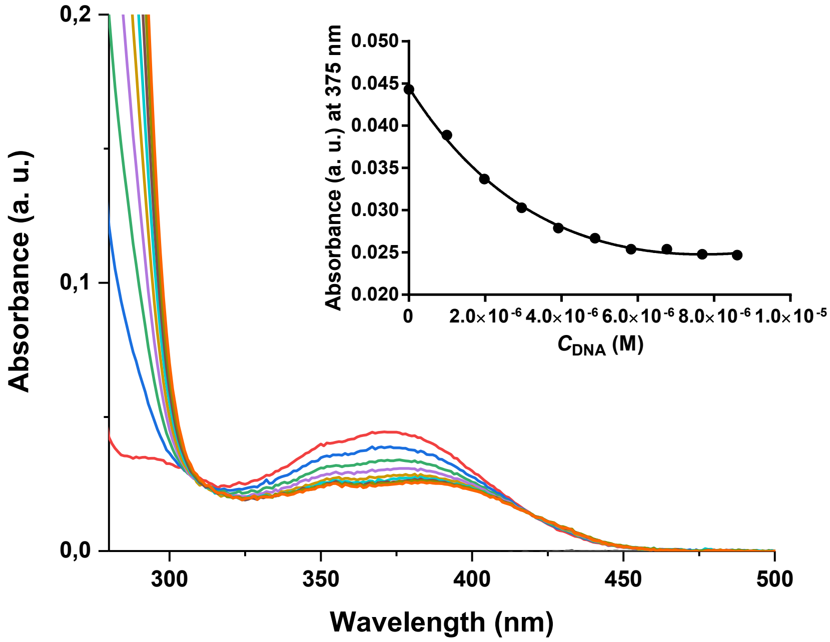

Figure S18. UV-Vis titration of **1** ($c = 5 \times 10^{-6}$ M) at pH 6 with *duplex* ***TG***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

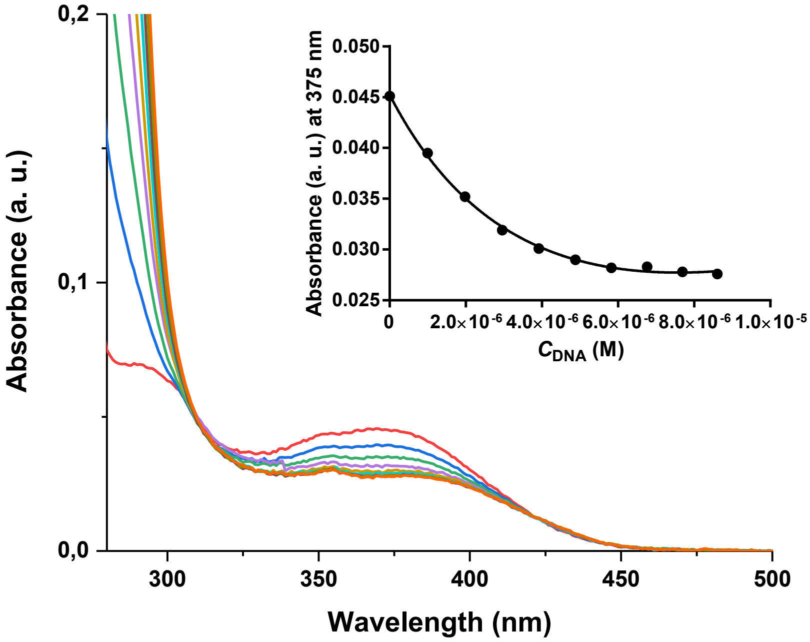

Figure S19. UV-Vis titration of **1** (c = 5 × 10^{-6} M) at pH 6 with *duplex* ***TT***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

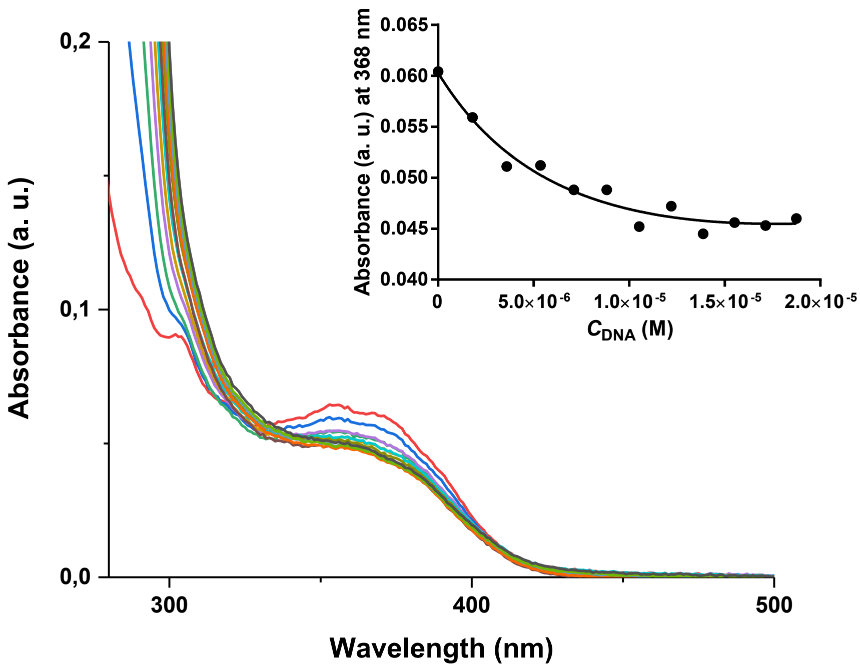

Figure S20. UV-Vis titration of **2** (c = 5 × 10^{-6} M) at pH 6 with *duplex* ***TA***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

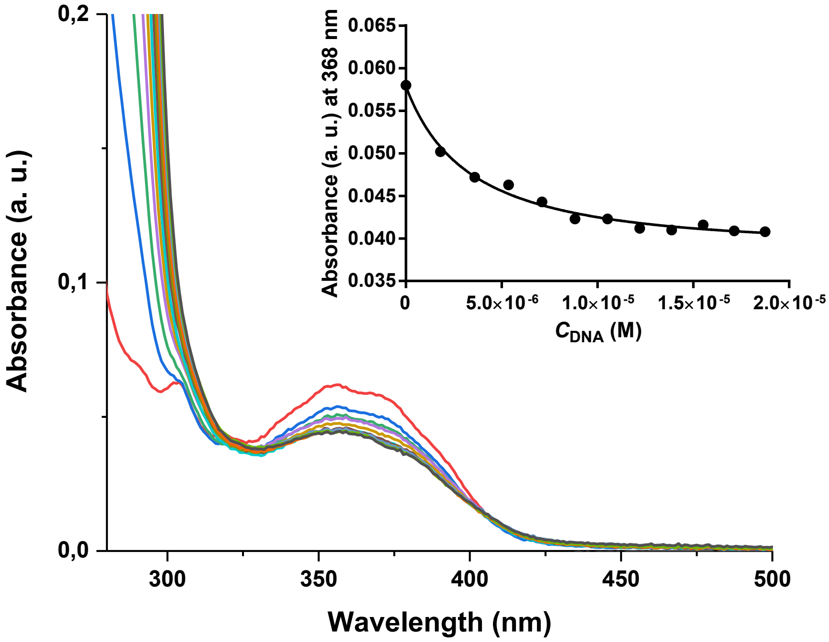

Figure S21. UV-Vis titration of **2** ($c = 5 \times 10^{-6}$ M) at pH 6 with *duplex* ***TC***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

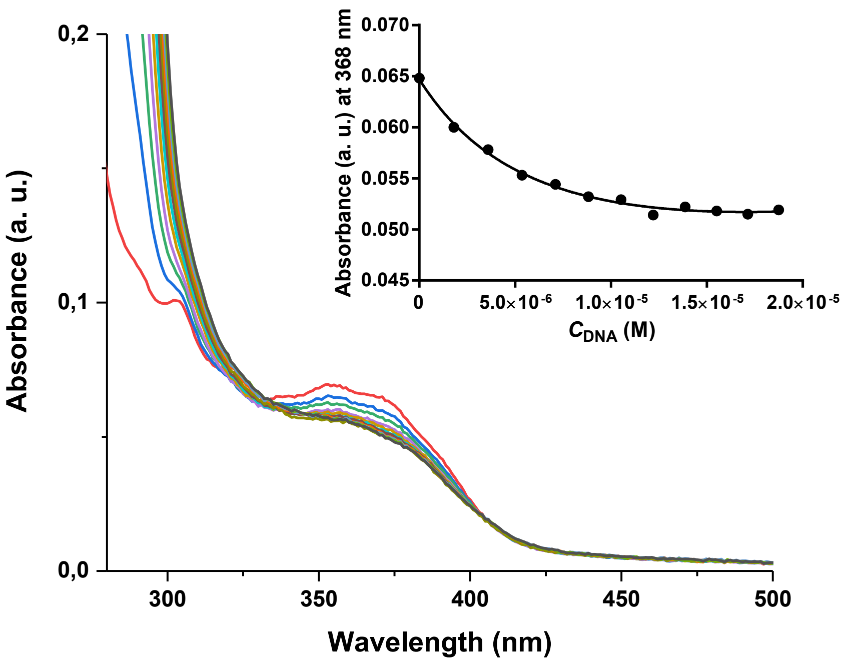

Figure S22. UV-Vis titration of **2** ($c = 5 \times 10^{-6}$ M) at pH 6 with *duplex* ***TG***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

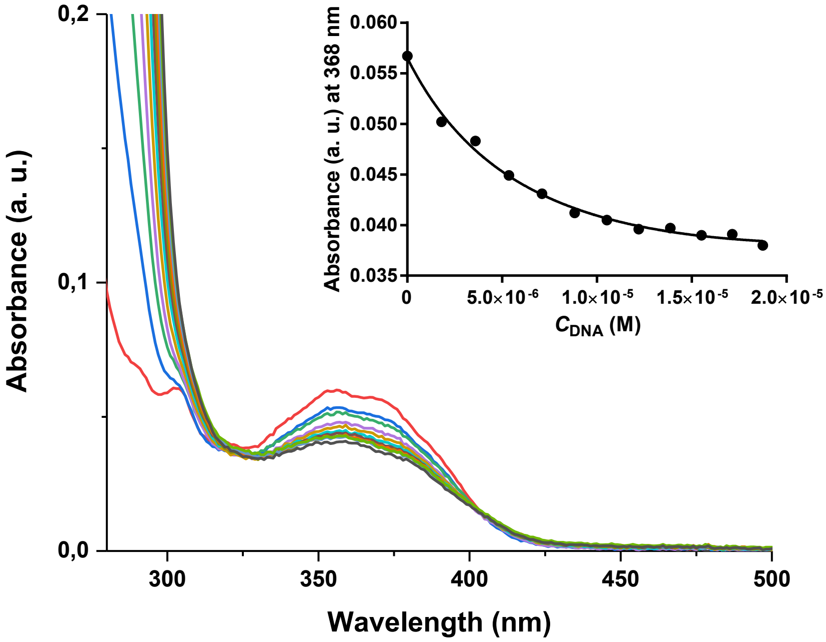

Figure S23. UV-Vis titration of **2** (c = 5 × 10^{-6} M) at pH 6 with *duplex* ***TT***. Inset: fitting of absorbance intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

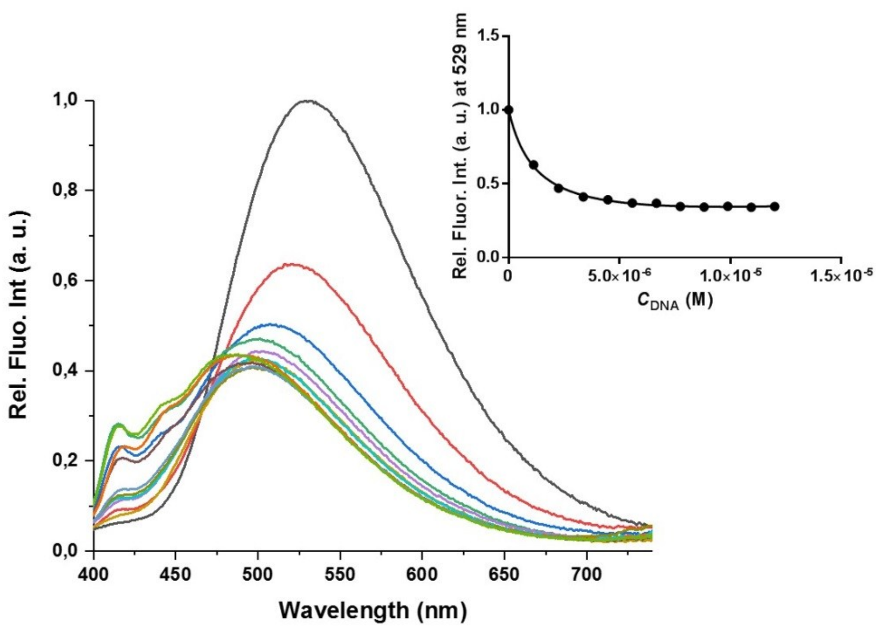

Figure S24. Fluorimetric titration of **1** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TA***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

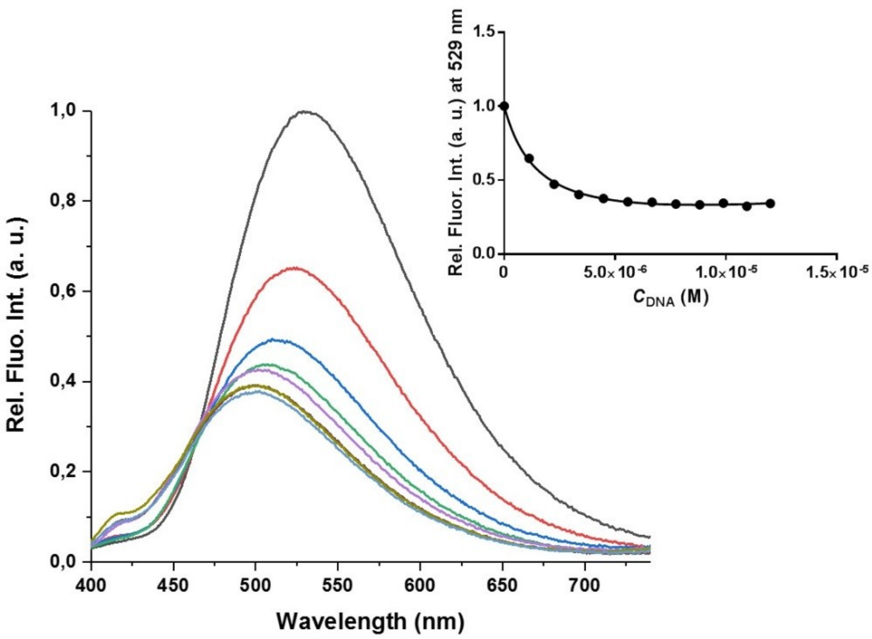

Figure S25. Fluorimetric titration of **1** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TC***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

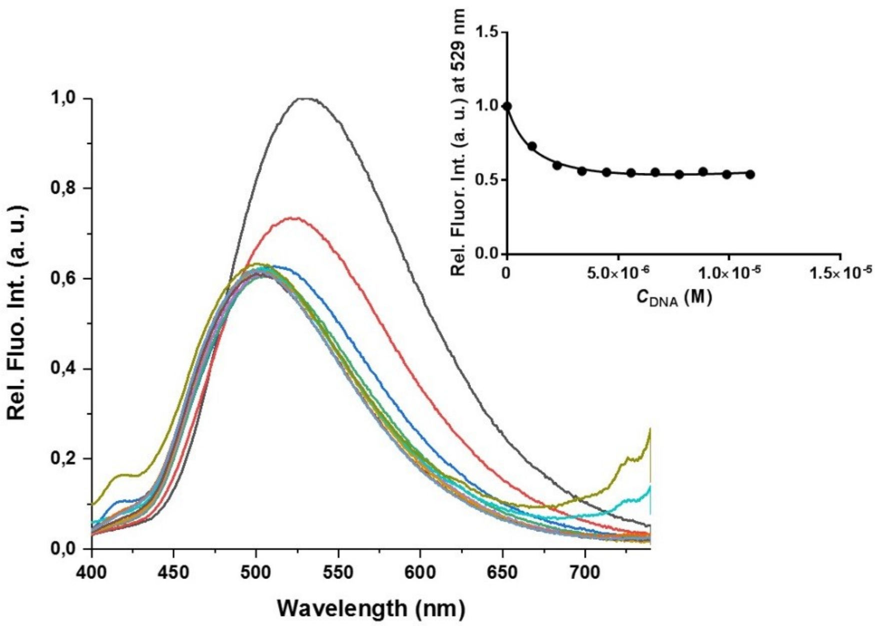

Figure S26. Fluorimetric titration of **1** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TG***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

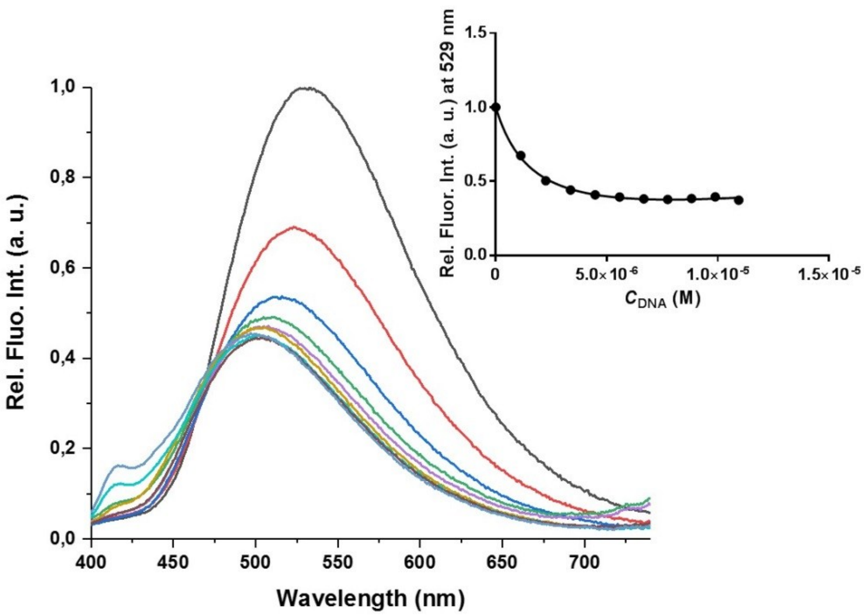

Figure S27. Fluorimetric titration of **1** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TT***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

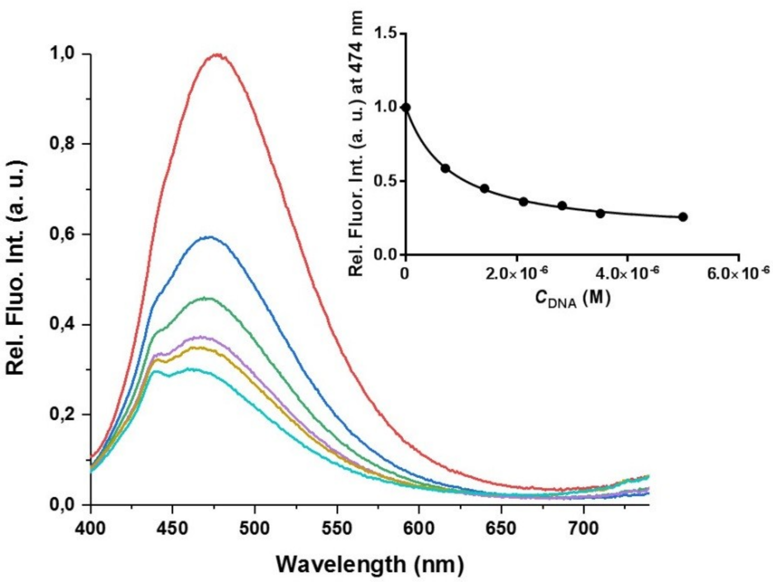

Figure S28. Fluorimetric titration of **2** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TA***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

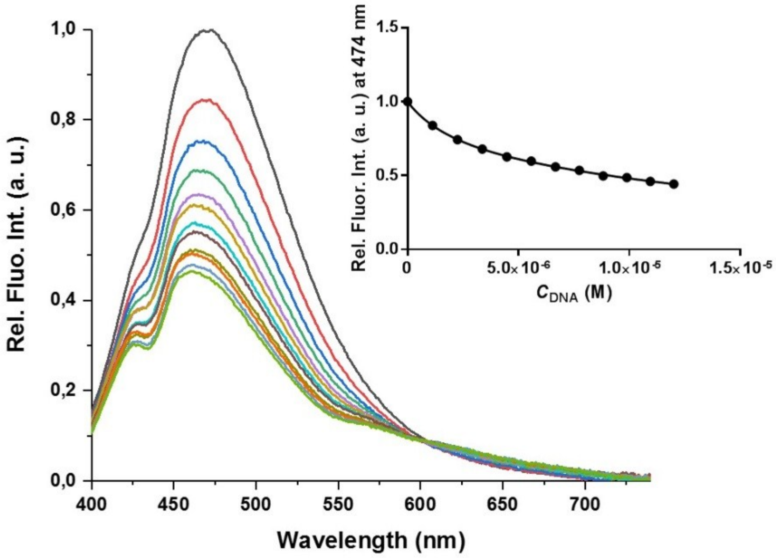

Figure S29. Fluorimetric titration of **2** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TC***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

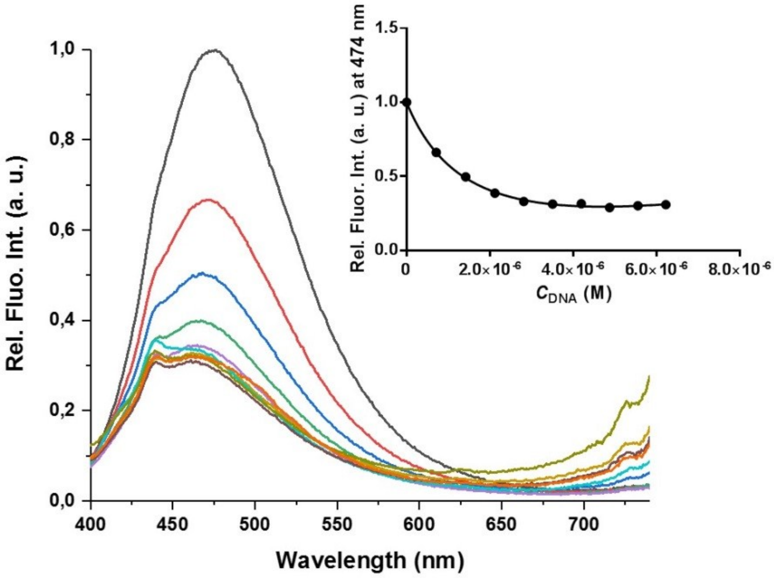

Figure S30. Fluorimetric titration of **2** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex* ***TG***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

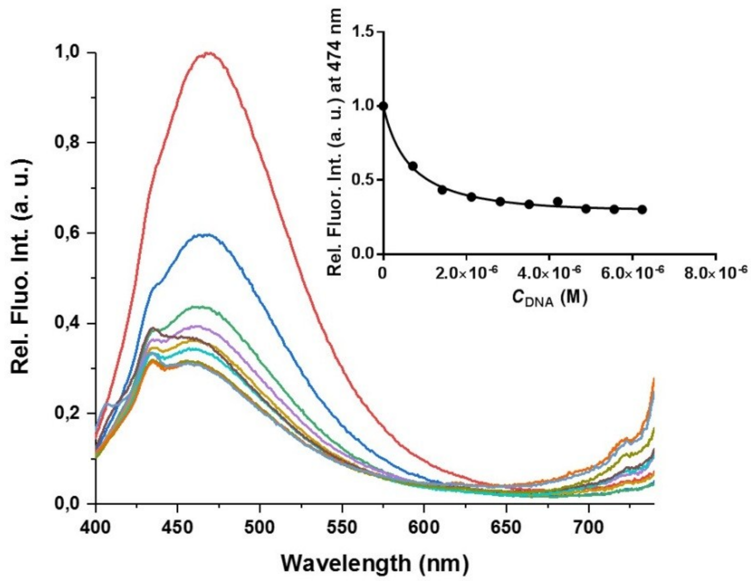

Figure S31. Fluorimetric titration of **2** (c = 5 × 10^{-6} M, λ_{exc}=380 nm) at pH 6 with *duplex **TT***. Inset: fitting of fluorescence emission intensity. Performed in sodium cacodylate buffer (NaCacodylate 10 mM, NaCl 100 mM).

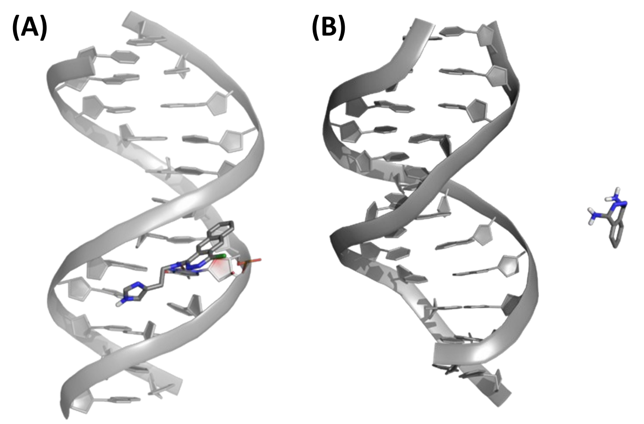

Figure S32. Minimum energy conformers calculated for the interaction of **2** (A) and **3** (B) with double stranded DNA.