

Supporting Information

Establishing Empirical Design Rules of Nucleic Acid Templates for Synthesis of Silver Nanoclusters with Tunable Photoluminescence and Functionalities Towards Targeted Bioimaging Applications

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Table S1. Single-stranded DNA nucleotide sequences used in the present study.

	Abbreviated Sequence	Full Sequence
Homo-oligonucleotides	dC ₂₀	5'-CCCCC CCCCC CCCCC CCCCC-3'
	dG ₂₀	5'-GGGGG GGGGG GGGGG GGGGG-3'
	dA ₂₀	5'-AAAAA AAAAA AAAAA AAAAA-3'
	dT ₂₀	5'-TTTTT TTTTT TTTTT TTTTT-3'
2-base sequences	dC ₁₅ G ₅	5'-CCCCC CCCCC CCCCC GGGGG-3'
	dC ₁₀ G ₁₀	5'-CCCCC CCCCC GGGGG GGGGG-3'
	dC ₅ G ₁₅	5'-CCCCCC GGGGG GGGGG GGGGG-3'
	dC ₁₅ A ₅	5'- CCCCC CCCCC CCCCC AAAAA-3'
	dC ₁₀ A ₁₀	5'-CCCCC CCCCC AAAAA AAAAA-3'
	dC ₅ A ₁₅	5'-CCCCC AAAAA AAAAA AAAAA-3'
	dC ₁₅ T ₅	5'- CCCCC CCCCC CCCCC TTTTT-3'
	dC ₁₀ T ₁₀	5'-CCCCC CCCCC TTTTT TTTTT-3'
	dC ₅ T ₁₅	5'- CCCCC TTTTT TTTTT TTTTT-3'
	dG ₁₅ A ₅	5'-GGGGG GGGGG GGGGG AAAAA-3'
	dG ₁₀ A ₁₀	5'-GGGGG GGGGG AAAAA AAAAA-3'
	dG ₅ A ₁₅	5'-GGGGG AAAAA AAAAA AAAAA-3'
	dG ₁₅ T ₅	5'-GGGGG GGGGG GGGGG TTTTT-3'
	dG ₁₀ T ₁₀	5'-GGGGG GGGGG TTTTT TTTTT-3'
	dG ₅ T ₁₅	5'-GGGGG TTTTT TTTTT TTTTT-3'
	dA ₁₅ T ₅	5'-AAAAA AAAAA AAAAA AAAAA-3'
	dA ₁₀ T ₁₀	5'-AAAAA AAAAA TTTTT TTTTT-3'
dA ₅ T ₁₅	5'-AAAAA TTTTT TTTTT TTTTT-3'	
Interdigitated sequences	d(CA) ₁₀	5'-CACAC ACACA CACAC ACACA-3'
	d(CT) ₁₀	5'-CTCTC TCTCT CTCTC TCTCT-3'
	d(GA) ₁₀	5'-GAGAG AGAGA GAGAG AGAGA-3'
	d(CG) ₁₀	5'-CGCGC GCGCG CGCGC GCGCG-3'

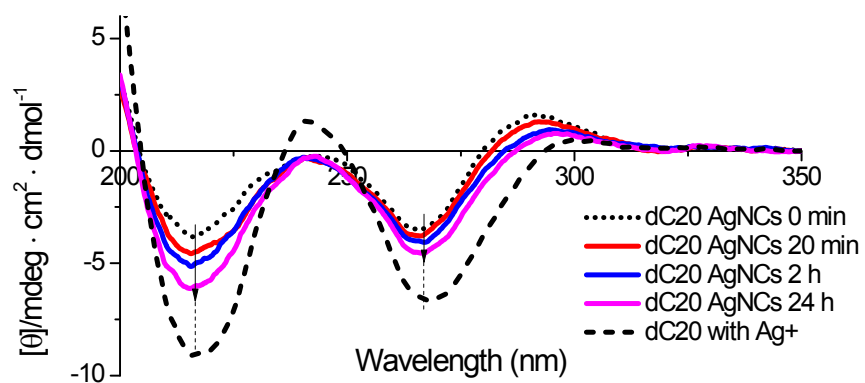


Fig. S1. Circular dichroism spectra showing the aging effects on the supramolecular structure of dC₂₀-templated AgNC at different time. CD spectra of DNA mixed with Ag⁺ (dashed line) and dC₂₀-AgNC immediately formed (ageing time = 0 min; dotted line) are included here for easier reference.

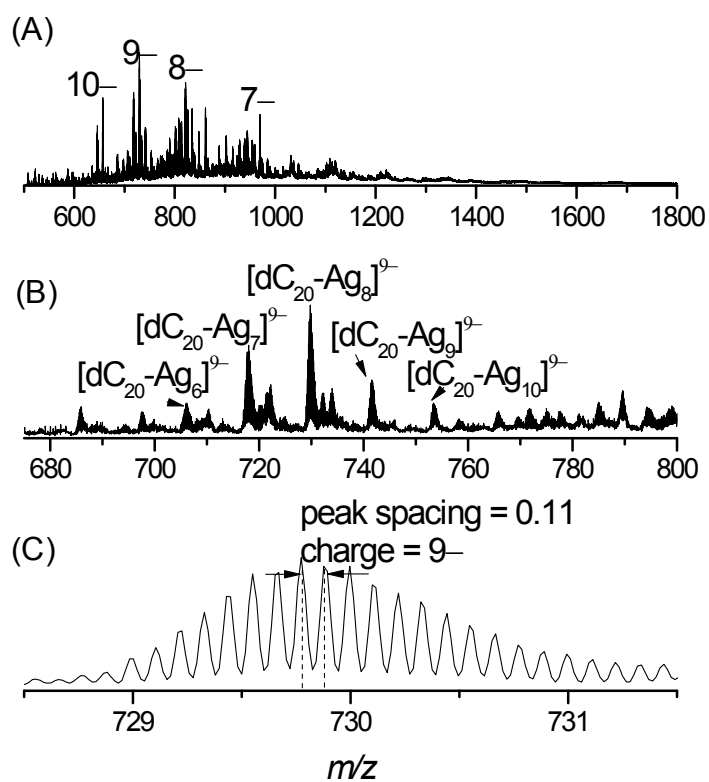


Fig. S2. (A) Wide range ESI mass spectrum of dC₂₀-AgNCs (the number represents the charge of ionized species) and (B) zoomed-in mass spectrum of the 9⁻ peak in (A) showing AgNCs with 6–10 Ag atoms; (C) isotope pattern of the [dC₂₀-Ag₈]⁹⁻ peak in (B).

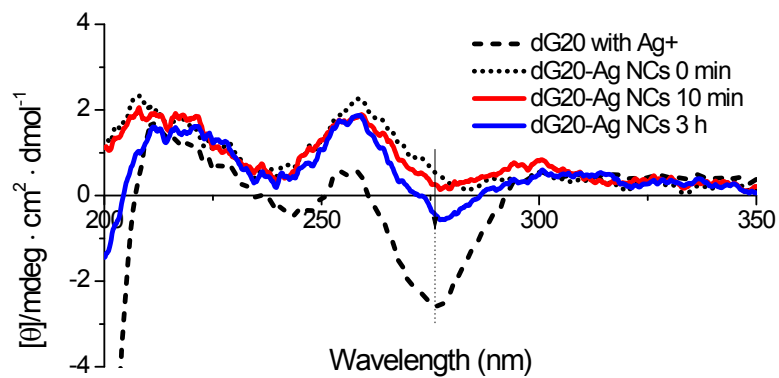


Fig. S3. Circular dichroism spectra showing the aging effects on the supramolecular structure of dG₂₀-templated AgNC at different time. The CD spectra of DNA mixed with Ag⁺ (dashed line) and dG₂₀-AgNC immediately formed (ageing time = 0 min; dotted line) are included here for easier reference.

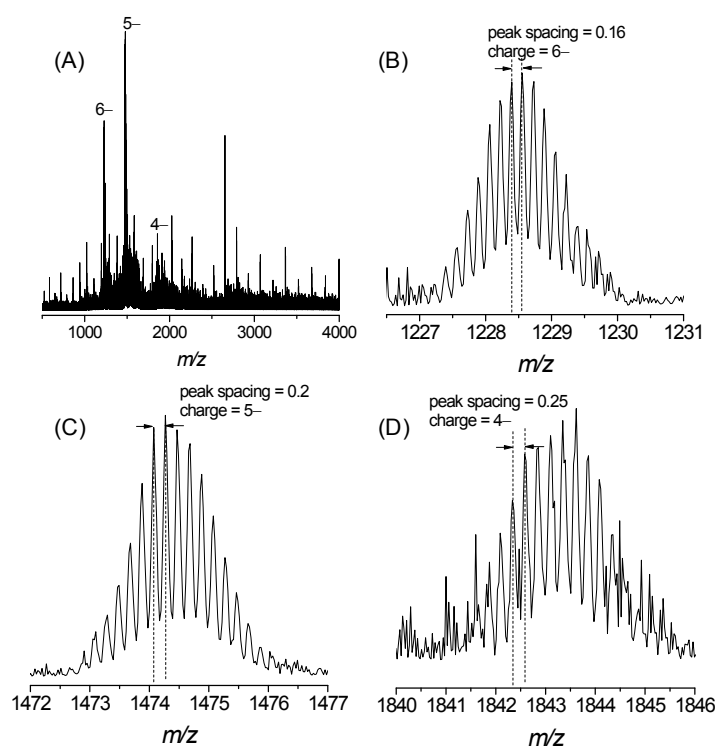


Fig. S4. (A) Wide range ESI mass spectrum of dG₂₀-Ag₈NCs and (B-D) isotope patterns determining the charges of major peaks observed in (A).

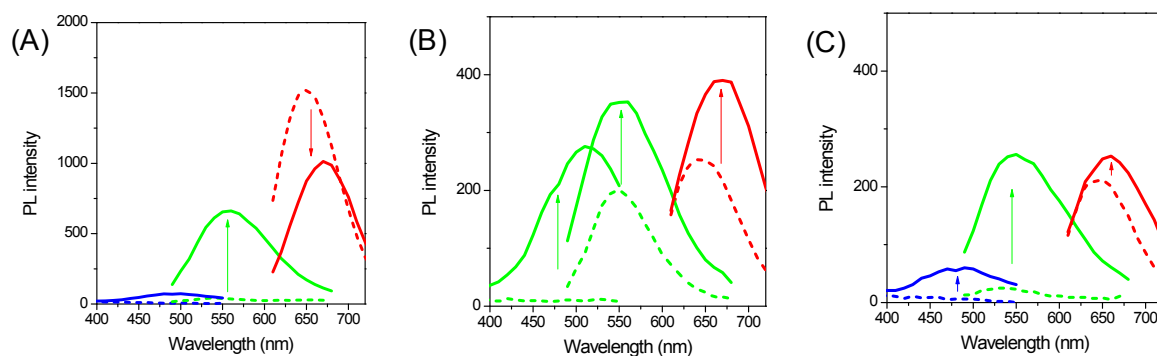


Fig. S5. Photoluminescence spectra of freshly prepared ($t = 0.3$ h, dash lines) and aged ($t = 24$ h, solid lines) AgNCs templated by (A) $dC_{15}A_5$, (B) $dC_{10}A_{10}$, (C) dC_5A_{15} DNA sequences. The blue, green and red emission spectra were obtained at the excitation wavelength (λ_{ex}) of 340, 450 and 570 nm respectively.

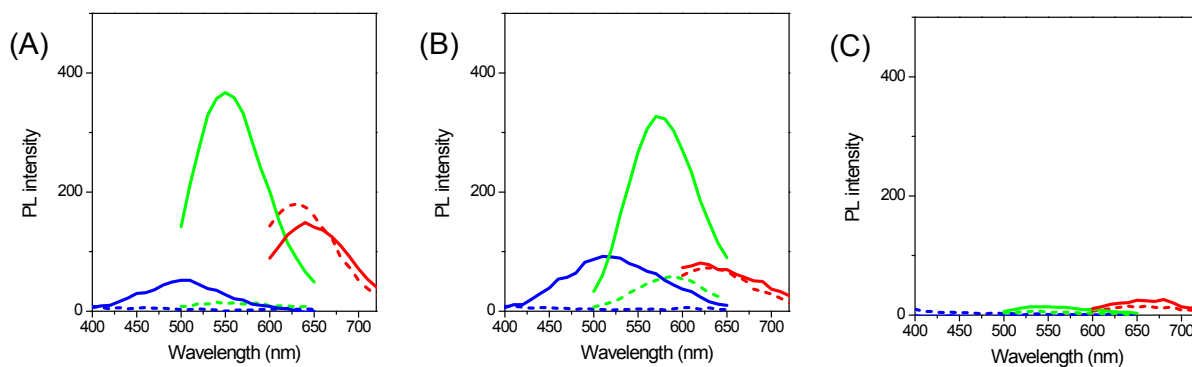


Fig. S6. Photoluminescence spectra of freshly prepared ($t = 0.3$ h, dash lines) and aged ($t = 24$ h, solid lines) AgNCs templated by (A) dC₁₅T₅, (B) dC₁₀T₁₀, (C) dC₅T₁₅ DNA sequences. The blue, green and red emission spectra were obtained at $\lambda_{\text{ex}} = 340, 450$ and 540 nm respectively.

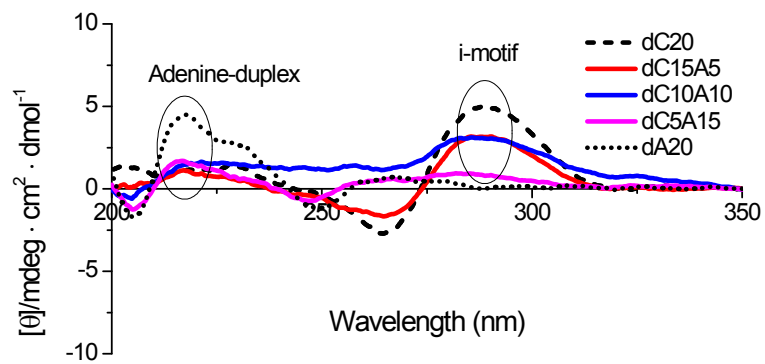


Fig. S7. Circular dichroism spectra of the 5'-d[C_{5n}A_(20-5n)]-3' DNA sequences (n is an integer from 0 to 4).

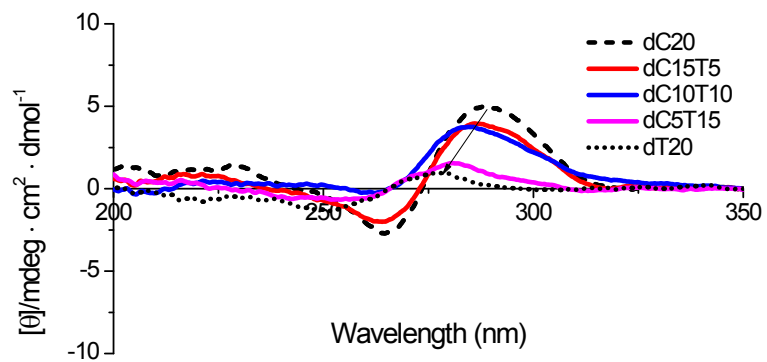


Fig. S8. Circular dichroism spectra of the 5'-d[C_{5n}T_(20-5n)]-3' DNA sequences (n is an integer from 0 to 4).

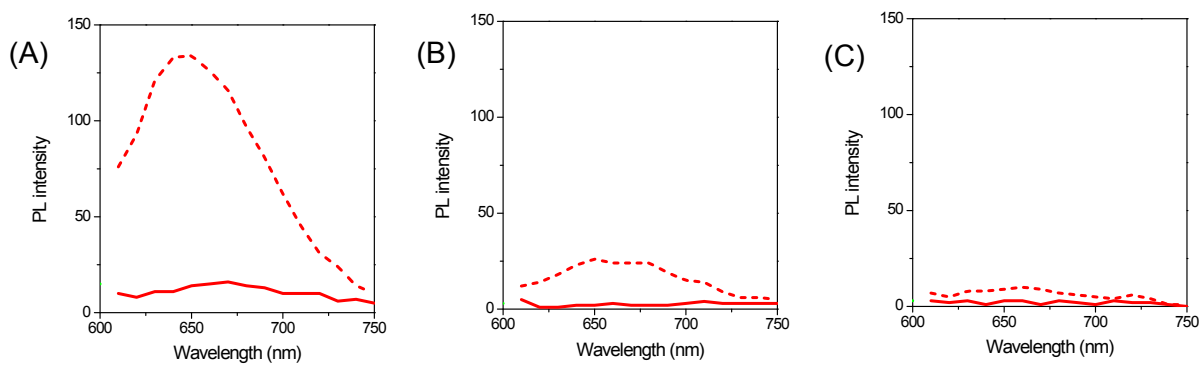


Fig. S9. Photoluminescence spectra of freshly prepared ($t = 0.3$ h, dash lines) and aged ($t = 24$ h, solid lines) AgNCs templated by (A) dG₁₅T₅, (B) dG₁₀T₁₀, (C) dG₅T₁₅ DNA sequences ($\lambda_{\text{ex}} = 580$ nm).

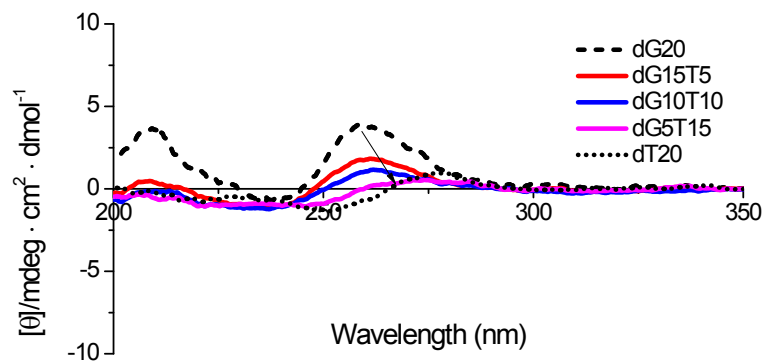


Fig. S10. Circular dichroism spectra of the 5'-d[G_{5n}T_(20-5n)]-3' DNA sequences (n is an integer from 0 to 4).

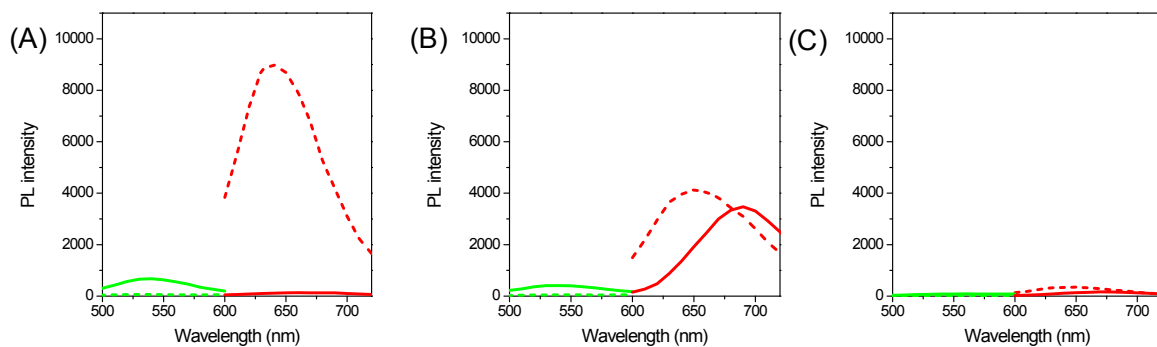


Fig. S11. Photoluminescence spectra of freshly prepared ($t = 0.3$ h, dash lines) and aged ($t = 24$ h, solid lines) AgNCs templated by (A) dC₁₅G₅, (B) dC₁₀G₁₀, (C) dC₅G₁₅ DNA sequences. The green and red emission spectra were obtained at $\lambda_{\text{ex}} = 440$ and 570 nm respectively.

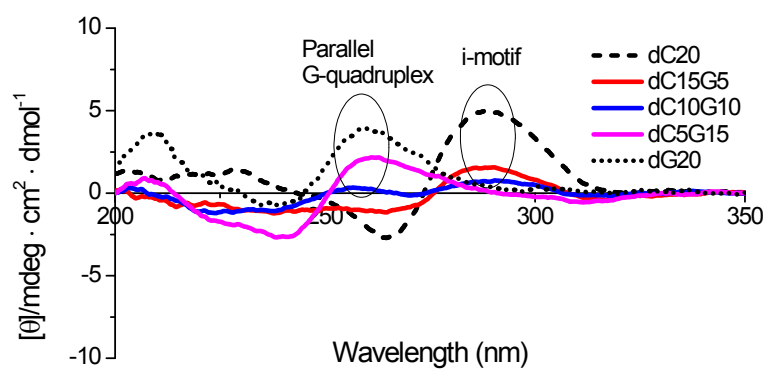


Fig. S12. Circular dichroism spectra of the 5'-d[C_{5n} G_(20-5n)]-3' DNA sequences (n is an integer from 0 to 4).

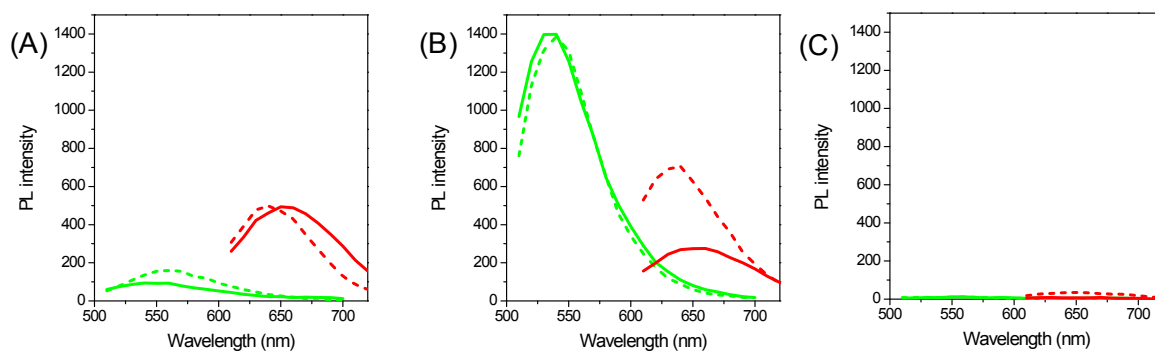


Fig. S13. Photoluminescence spectra of freshly prepared ($t = 0.3$ h, dash lines) and aged ($t = 24$ h, solid lines) AgNCs templated by (A) dG₁₅A₅, (B) dG₁₀A₁₀, (C) dG₅A₁₅ DNA sequences. The green and red emission spectra were obtained at $\lambda_{\text{ex}} = 470$ and 570 nm respectively.

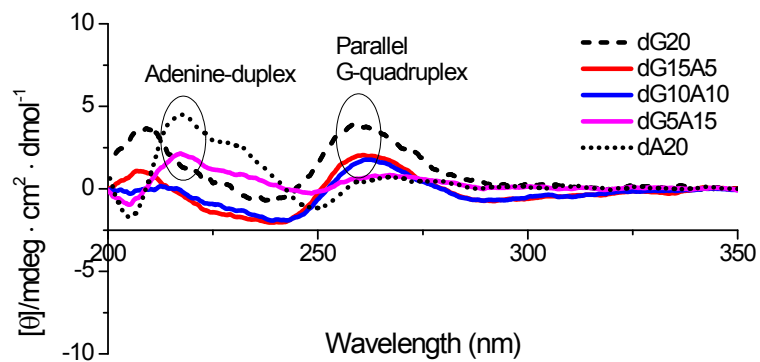


Fig. S14. Circular dichroism spectra of the 5'-d[G_{5n} A_(20-5n)]-3' DNA sequences (n is an integer from 0 to 4).

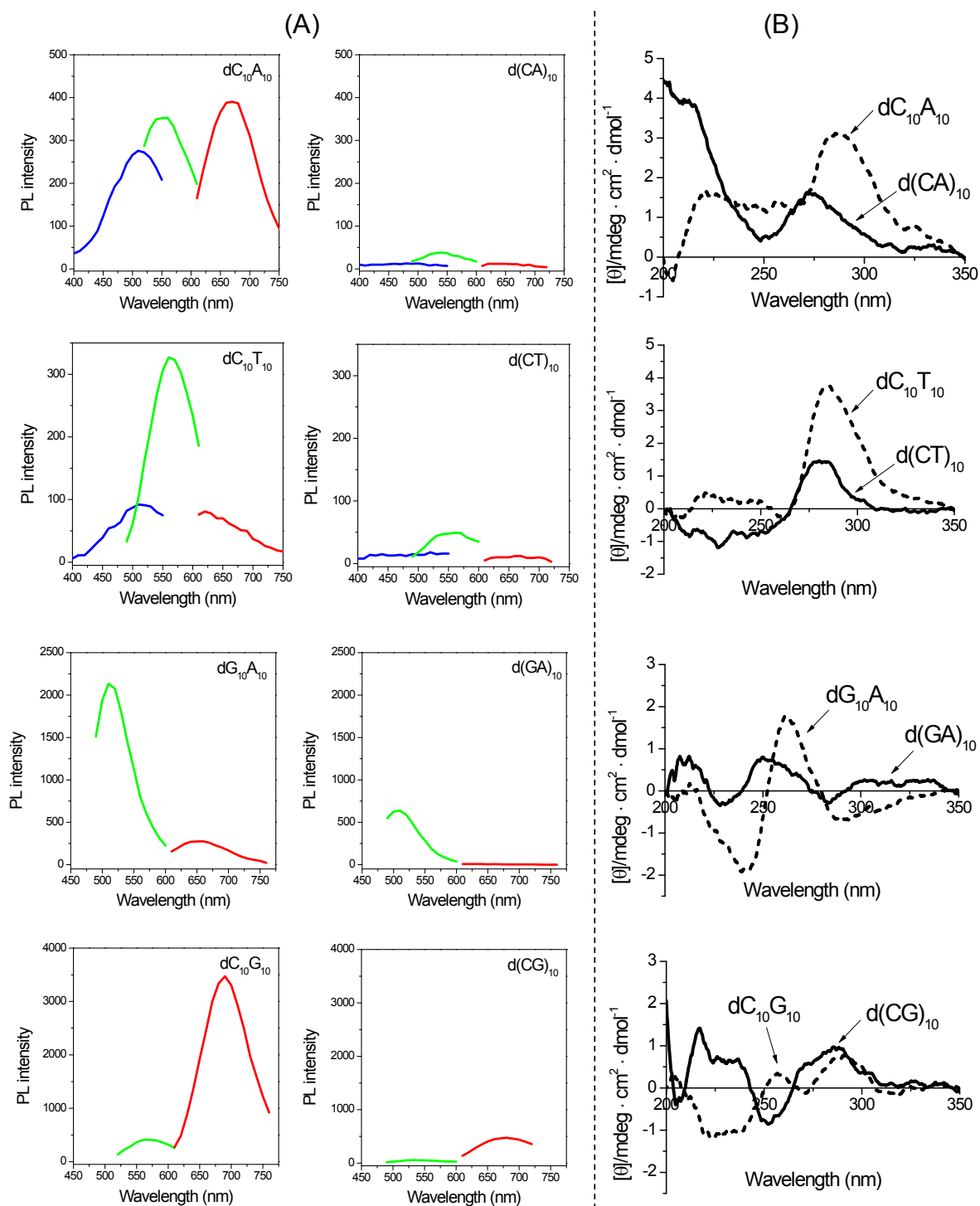


Fig. S15. (A) Fluorescence spectra of AgNCs templated by dC₁₀A₁₀, dC₁₀T₁₀, dG₁₀A₁₀, dC₁₀G₁₀ and their interdigitated counterparts (middle panel) bearing the general formula of d(XY)₁₀. All fluorescence spectra were taken at 24 hours after the AgNCs were synthesised. For cytosine-containing sequences, λ_{ex} for blue, green and red emissions are 340, 450 and 570 nm respectively, whilst for guanine-containing sequences, λ_{ex} for green and red emissions are 470 and 570 nm respectively (B) CD spectra of the dX₁₀Y₁₀ (dashed lines) and d(XY)₁₀ DNA sequences (solid lines) in aqueous solution.