Supporting Information for:

METAL ION CHELATES AS SURROGATES OF NUCLEOBASES FOR THE RECOGNITION OF NUCLEIC ACID SEQUENCES: THE Pd^{2+} COMPLEX OF 2,6-BIS(3,5-DIMETHYLPYRAZOL-1-YL)PURINE RIBOSIDE

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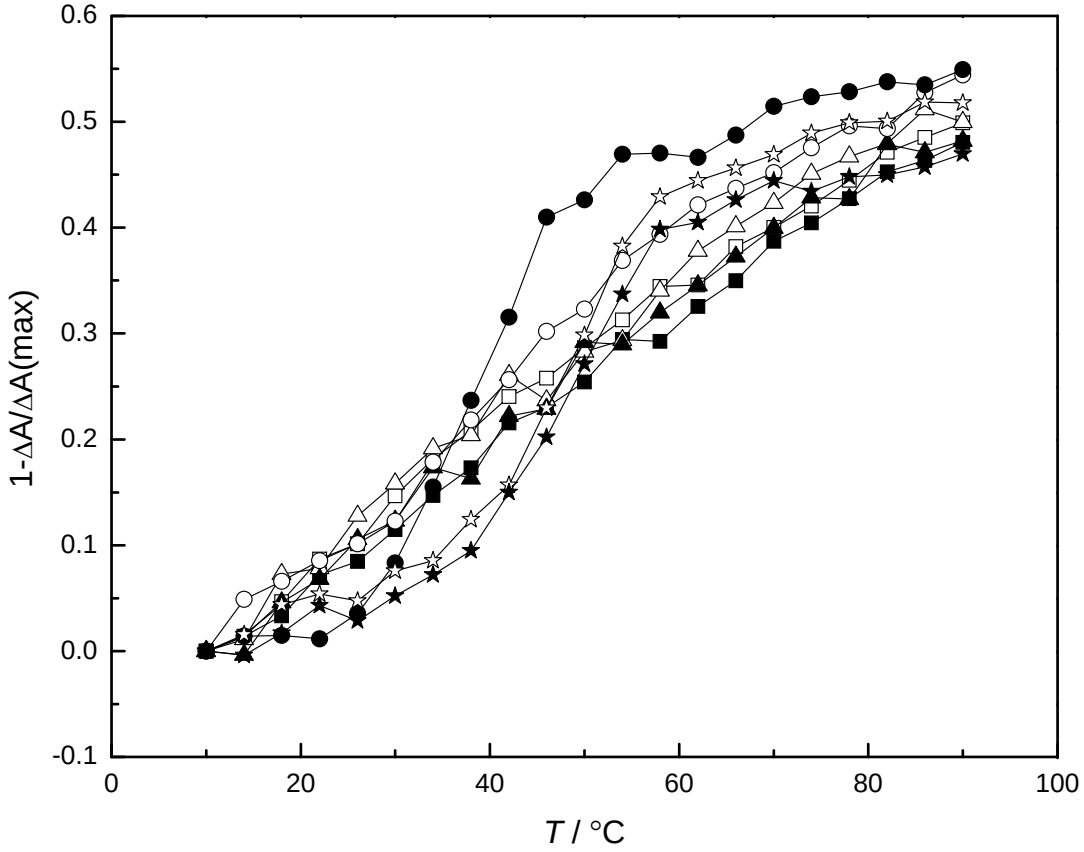

Figure S1. Temperature vs. 1- ΔA/ΔA(max) profiles of the heteroduplexes formed between **7A** and DNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; $I(NaClO_4)$ = 0.1 M; pH = 7.4. (□) **7A**:**10C**, (■) **7A**:**10C** + Pd^{2+}, (○) **7A**:**10G**, (●) **7A**:**10G** + Pd^{2+}, (☆) **7A**:**10T**, (★) **7A**:**10T** + Pd^{2+}, (△) **7A**:**10A**, (▲) **7A**:**10A** + Pd^{2+}.

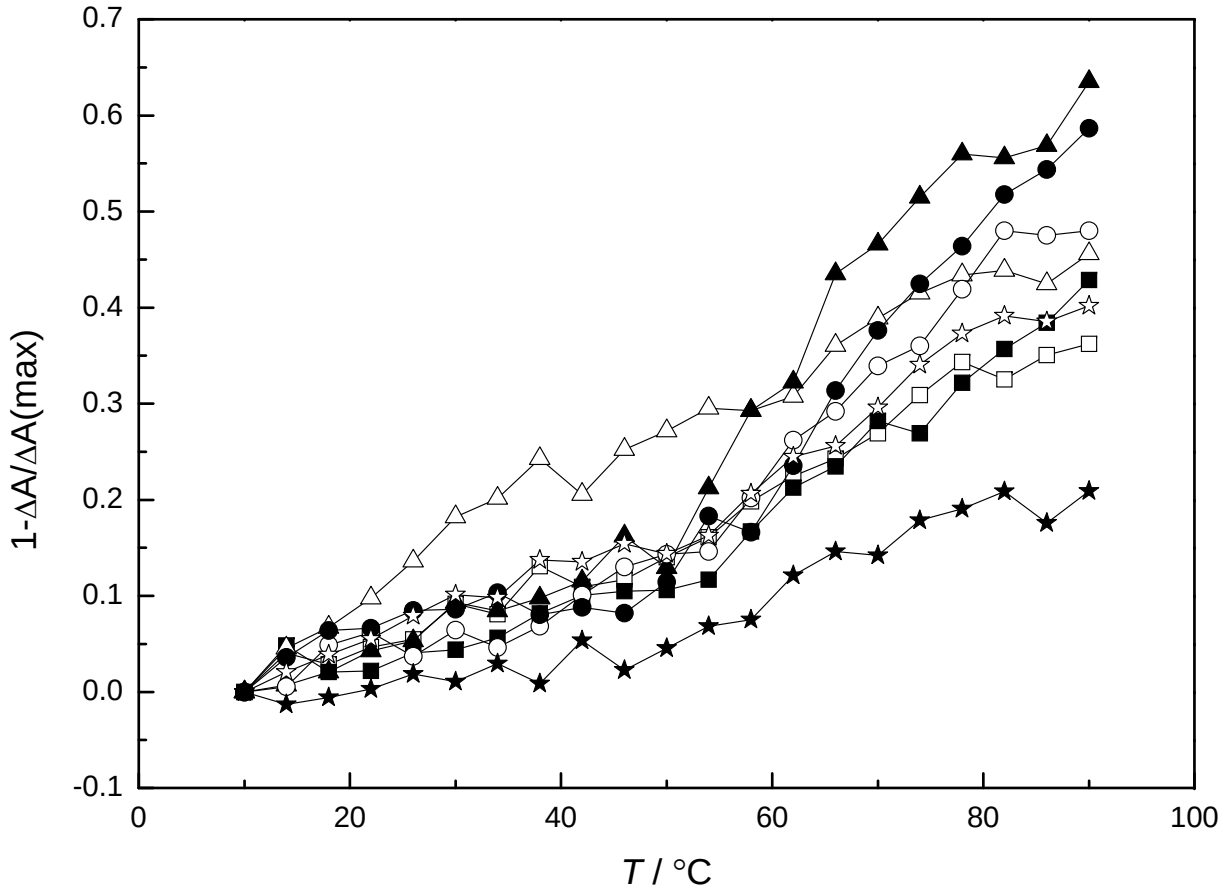

Figure S2. Temperature vs. 1- ΔA/ΔA(max) profiles of the heteroduplexes formed between **7X** and DNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; $I(NaClO_4)$ = 0.1 M; pH = 7.4. (□) **7X**:**10C**, (■) **7X**:**10C** + Pd^{2+}, (○) **7X**:**10G**, (●) **7X**:**10G** + Pd^{2+}, (☆) **7X**:**10T**, (★) **7X**:**10T** + Pd^{2+}, (△) **7X**:**10A**, (▲) **7X**:**10A** + Pd^{2+}.

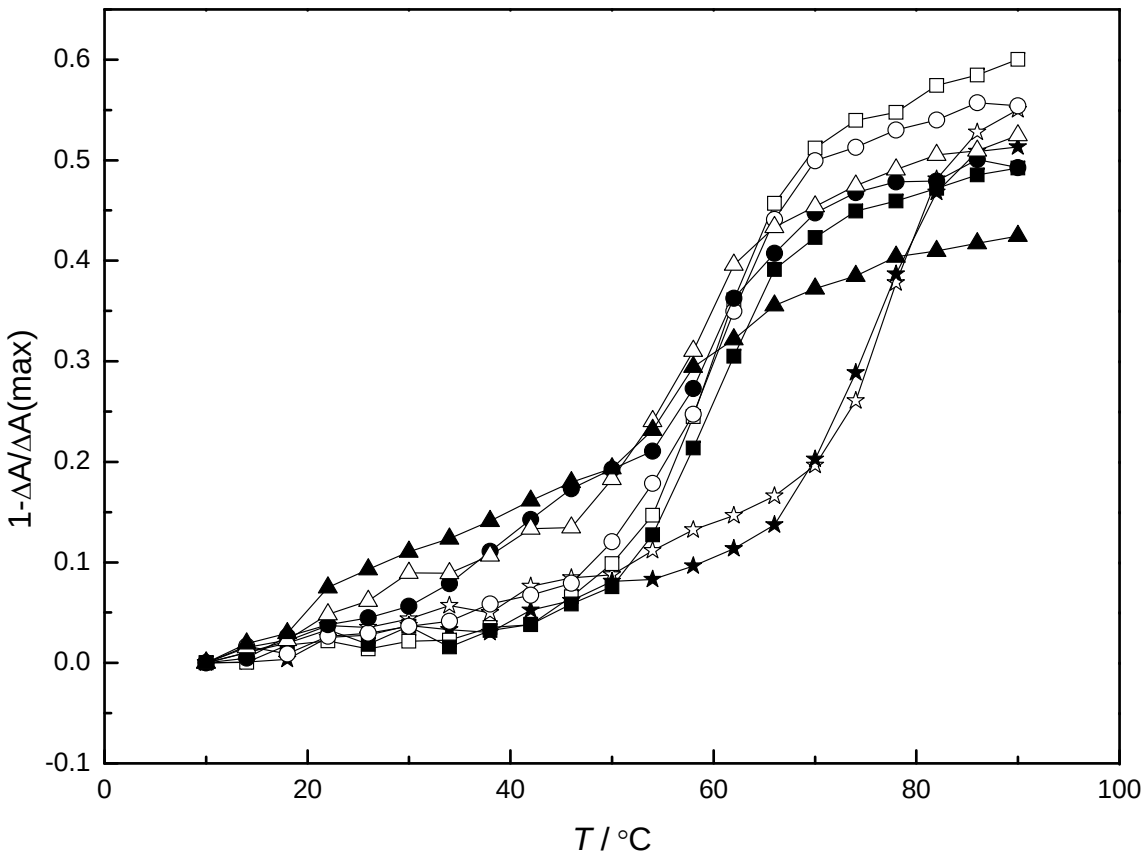

Figure S3. Temperature vs. 1- ΔA/ΔA(max) profiles of the homoduplexes formed between **7A** and 2′-*O*-methyl-RNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; *I*($NaClO_4$) = 0.1 M; pH = 7.4. (□) **7A**:**8C**, (■) **7A**:**8C** + Pd^{2+}, (○) **7A**:**8G**, (●) **7A**:**8G** + Pd^{2+}, (☆) **7A**:**8U**, (★) **7A**:**8U** + Pd^{2+}, (△) **7A**:**8A**, (▲) **7A**:**8A** + Pd^{2+}.

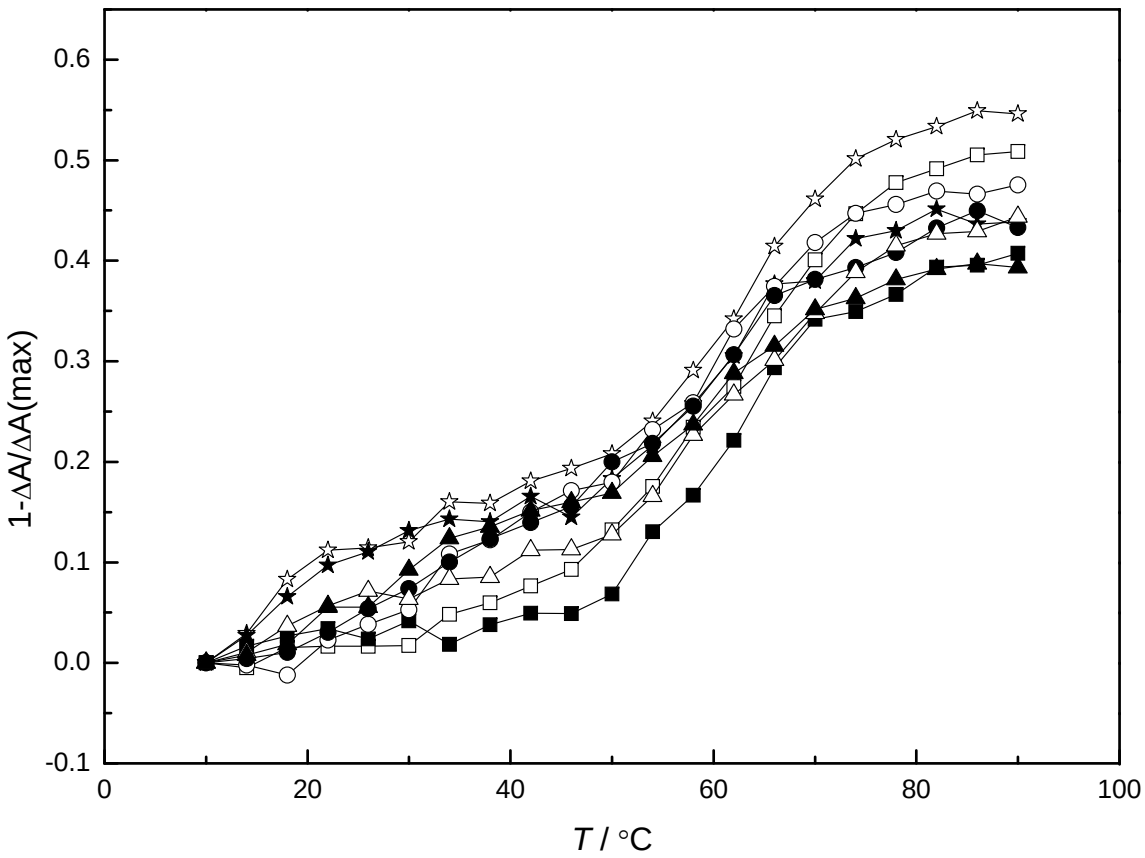

Figure S4. Temperature vs. 1- ΔA/ΔA(max) profiles of the homoduplexes formed between **7A** and 2′-*O*-methyl-RNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; *I*($NaClO_4$) = 0.1 M; pH = 7.4. (□) **7A**:**8C**, (■) **7A**:**8C** + Pd^{2+}, (○) **7A**:**8G**, (●) **7A**:**8G** + Pd^{2+}, (☆) **7A**:**8U**, (★) **7A**:**8U** + Pd^{2+}, (△) **7A**:**8A**, (▲) **7A**:**8A** + Pd^{2+}.

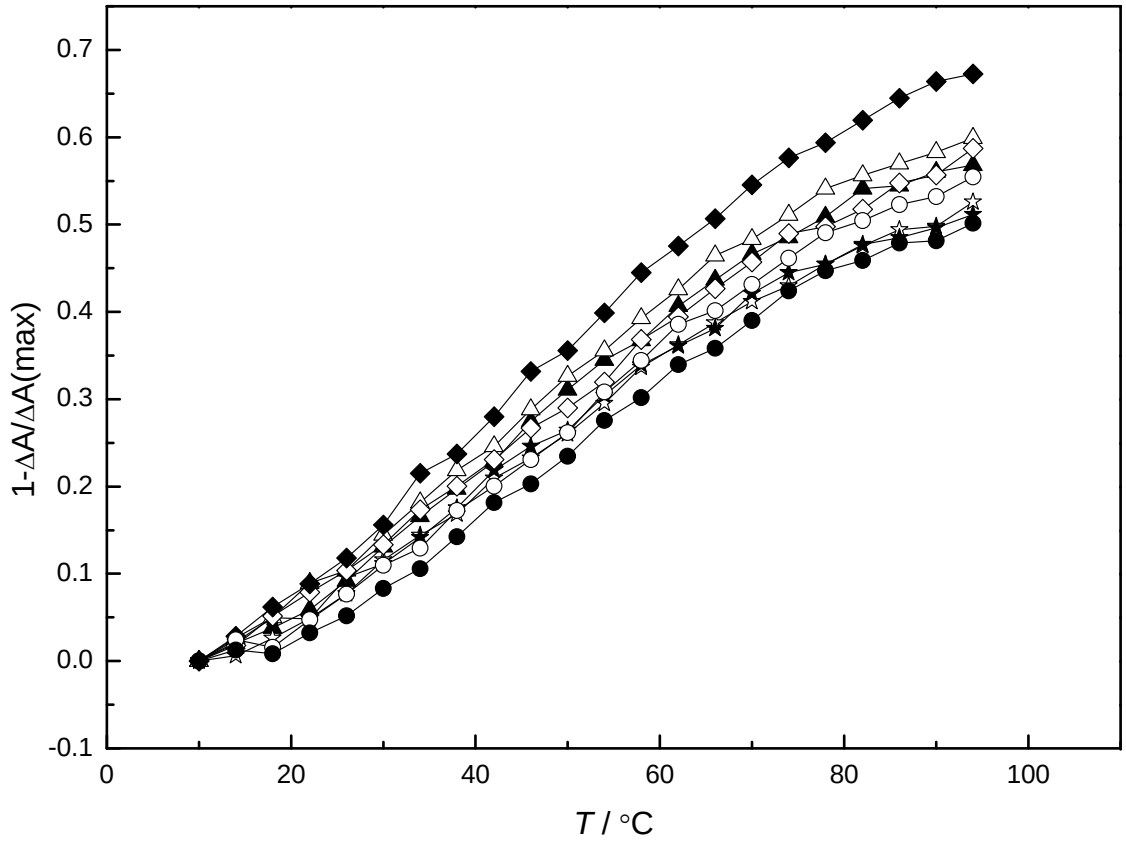

Figure S5. Temperature vs. 1- ΔA/ΔA(max) profiles of the mismatched homoduplexes formed between **7A** and 2′-*O*-methyl-RNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; *I*($NaClO_4$) = 0.1 M; pH = 7.4. (◇) **7A**:**9C**, (◆) **7A**:**9C** + Pd^{2+}, (△) **7A**:**9A**, (▲)**7A**:**9A** + Pd^{2+}, (○) **7A**:**9G**, (●) **7A**:**9G** + Pd^{2+}, (☆) **7A**:**9U**, (★) **7A**:**9U** + Pd^{2+}.

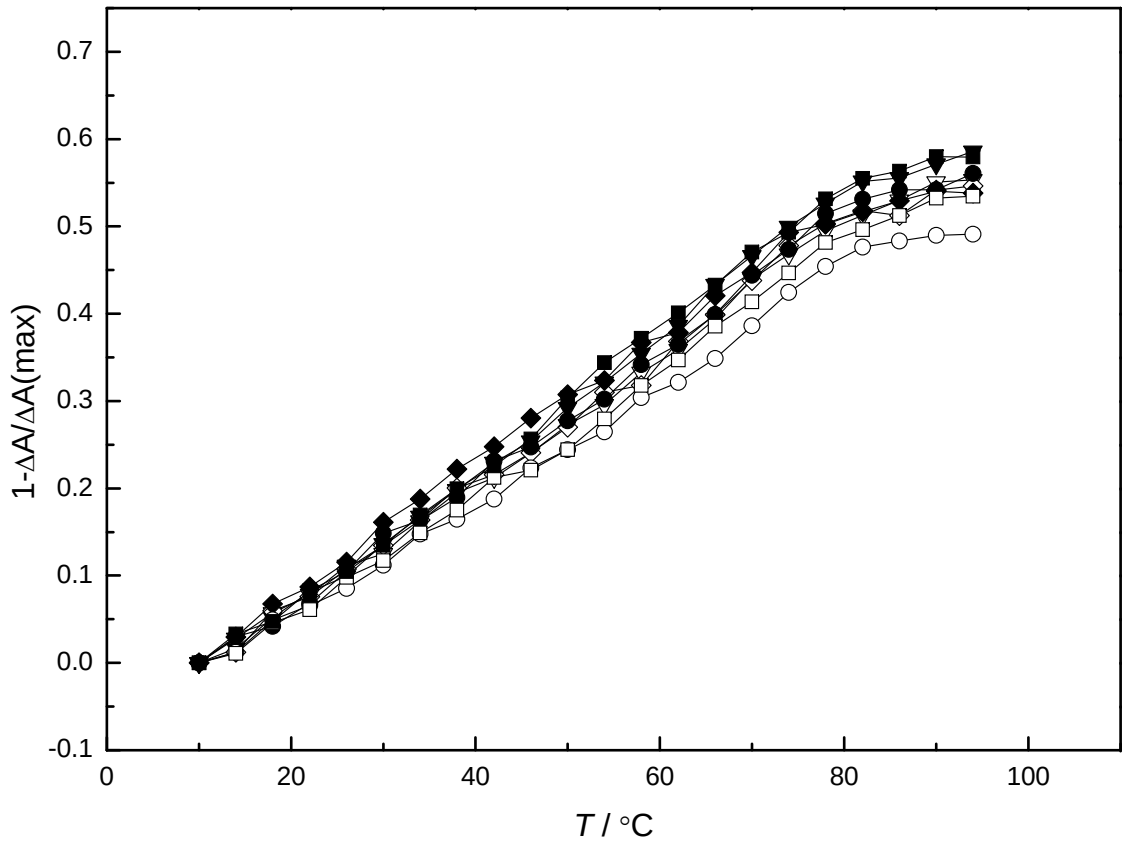

Figure S6. Temperature vs. 1- ΔA/ΔA(max) profiles of the mismatched homoduplexes formed between **7A** and 2′-*O*-methyl-RNA oligonucleotides in the presence and absence of Pd^{2+}; scan range 220 – 320 nm; $I(NaClO_4)$ = 0.1 M; pH = 7.4. (□) **7X**:**9C**, (■) **7X**:**9C** + Pd^{2+}, (▽) **7X**:**9A**, (▼) **7X**:**9A** + Pd^{2+}, (○) **7X**:**9G**, (●) **7X**:**9G** + Pd^{2+}, (◇) **7X**:**9U**, (◆) **7X**:**9U** + Pd^{2+}.

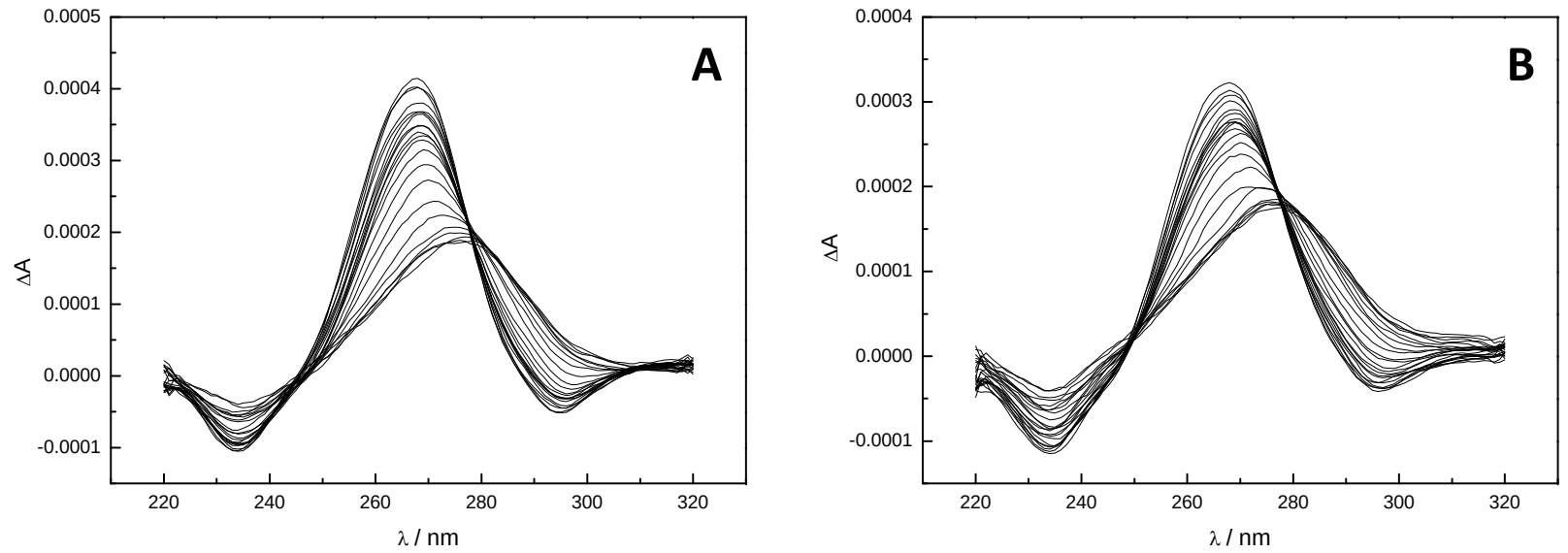

Figure S7. CD spectra of the homoduplex **7X**:**8U** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

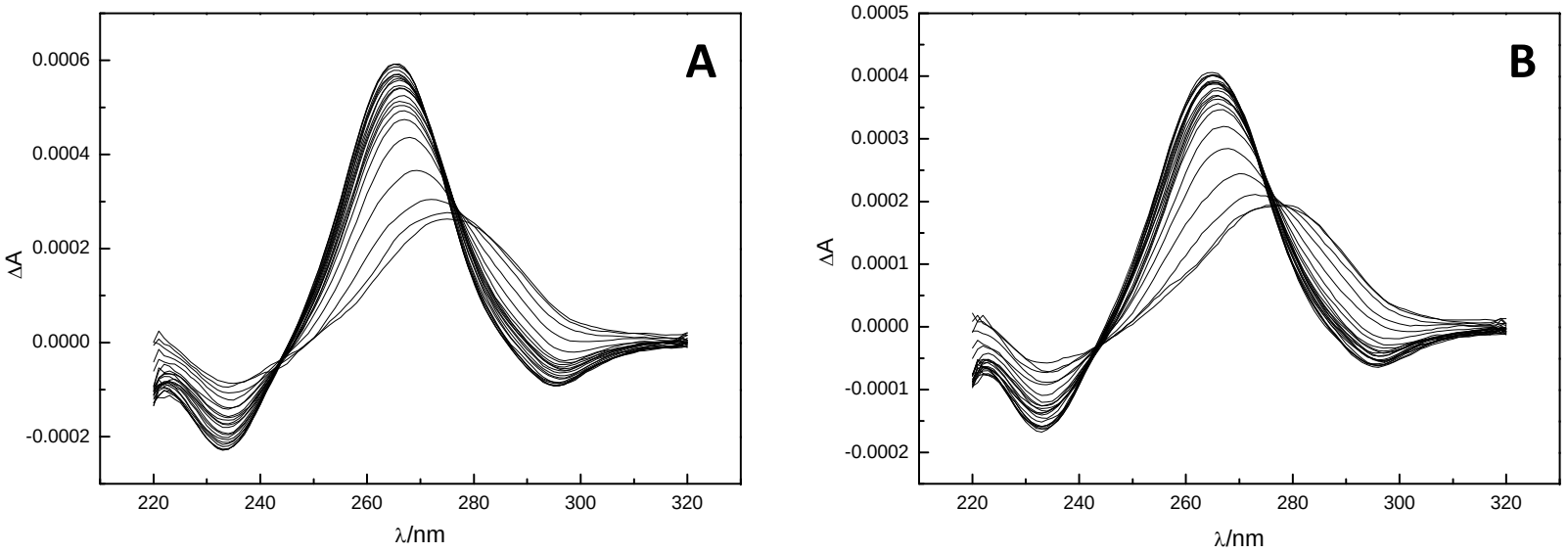

Figure S8. CD spectra of the homoduplex **7A**:**8U** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

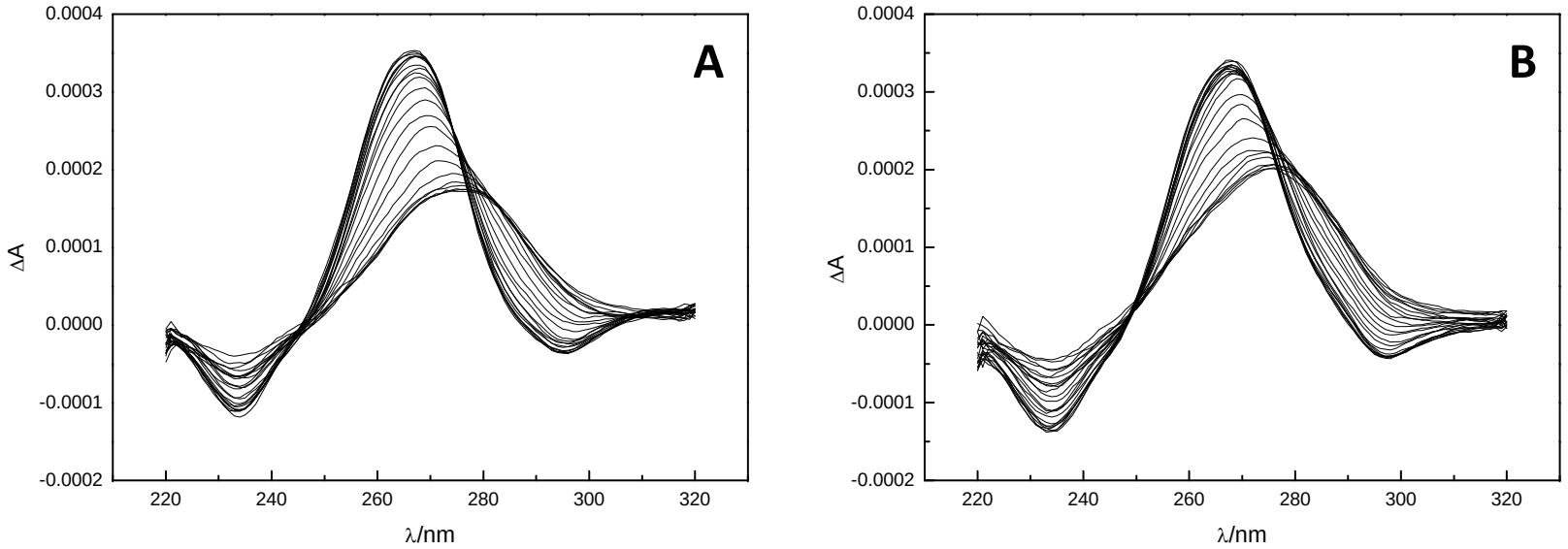

Figure S9. CD spectra of the homoduplex **7X**:**8C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

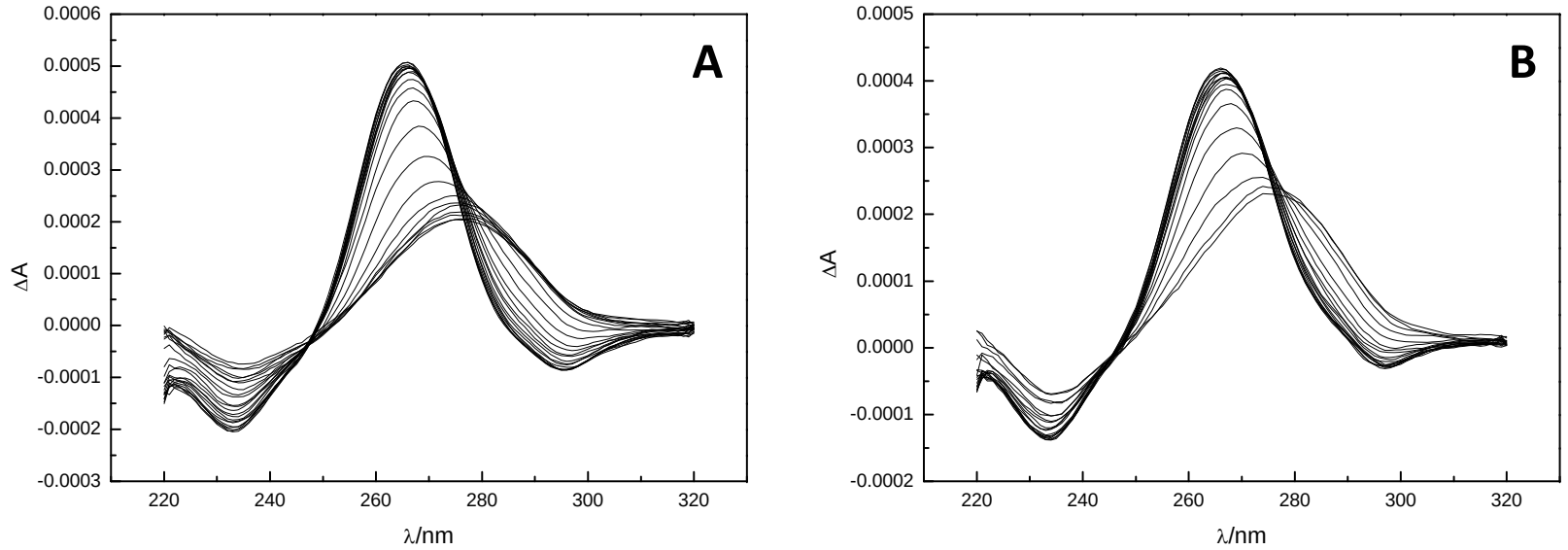

Figure S10. CD spectra of the homoduplex **7A**:**8C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

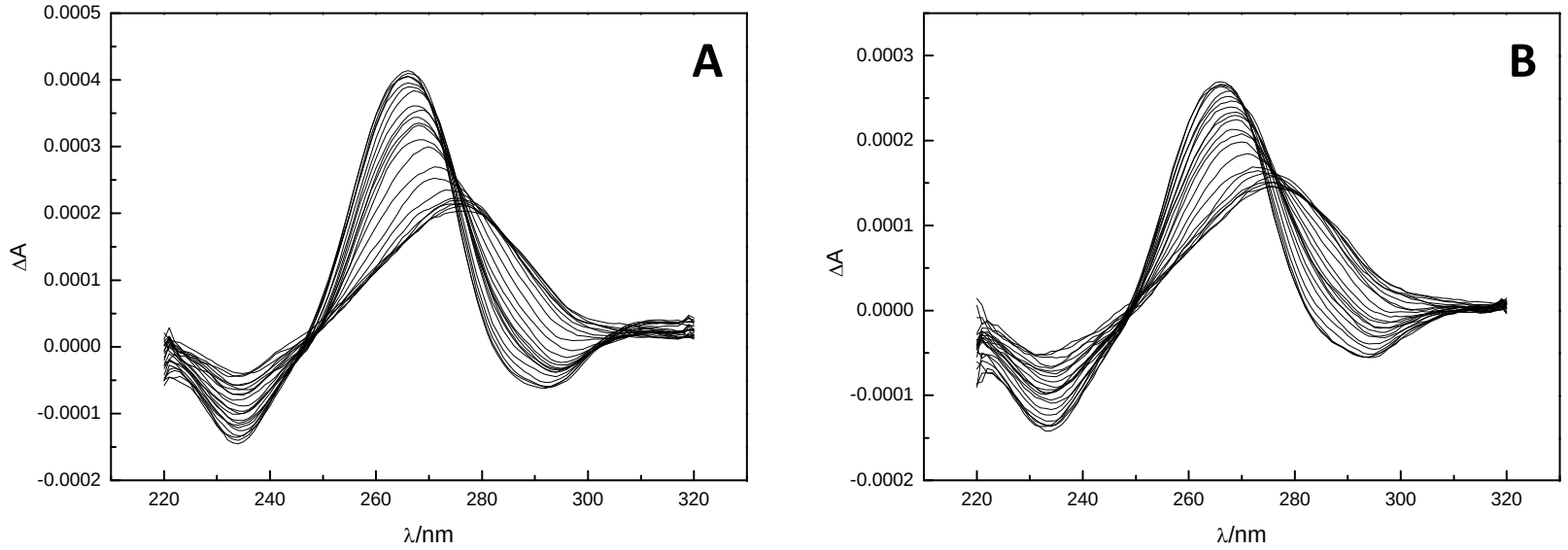

Figure S11. CD spectra of the homoduplex **7X**:**8G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

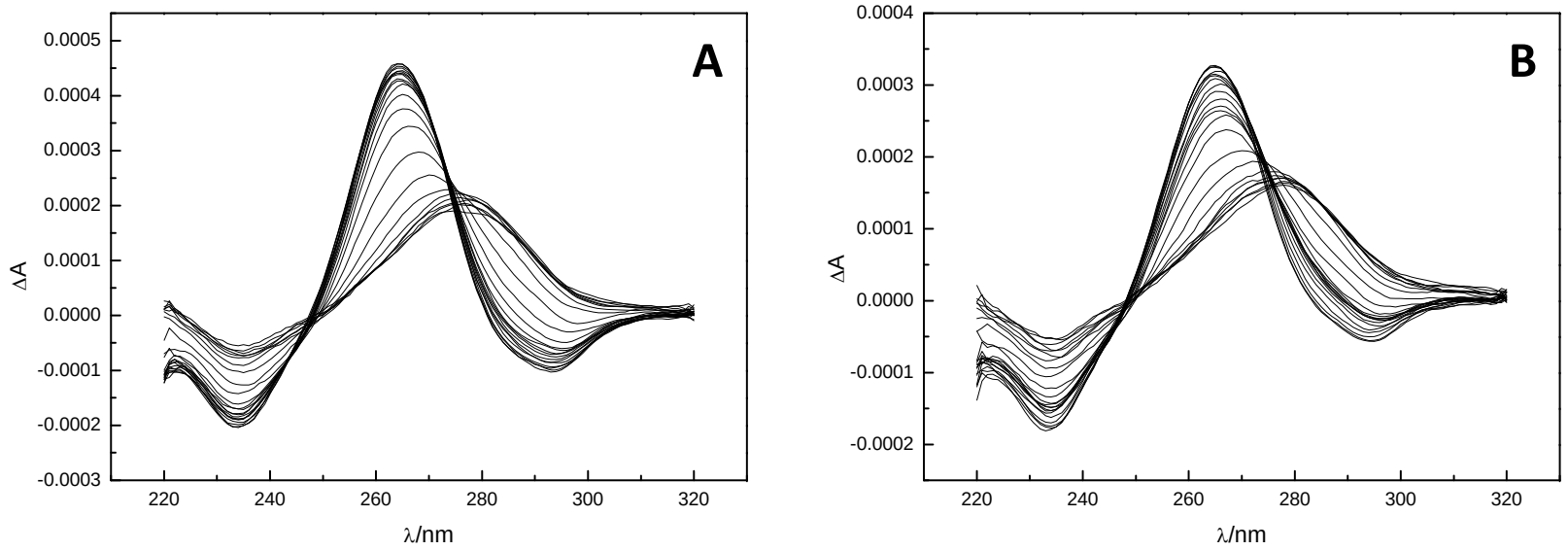

Figure S12. CD spectra of the homoduplex **7A**:**8G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

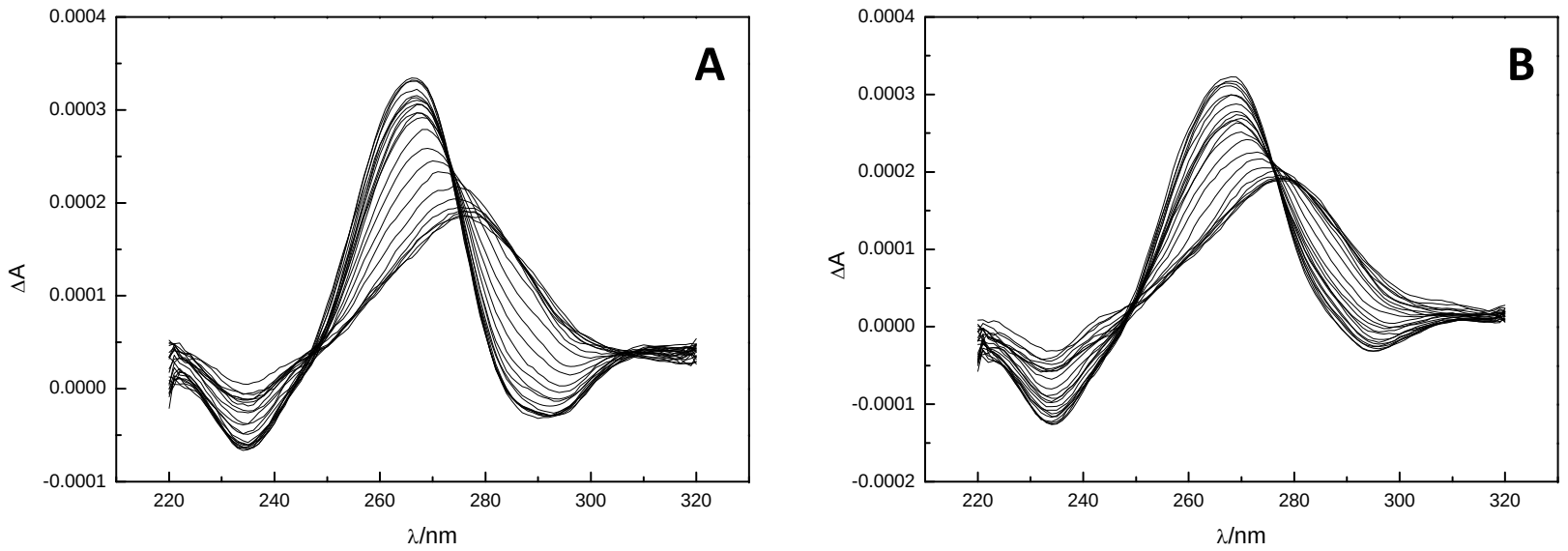

Figure S13. CD spectra of the homoduplex **7X**:**8A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

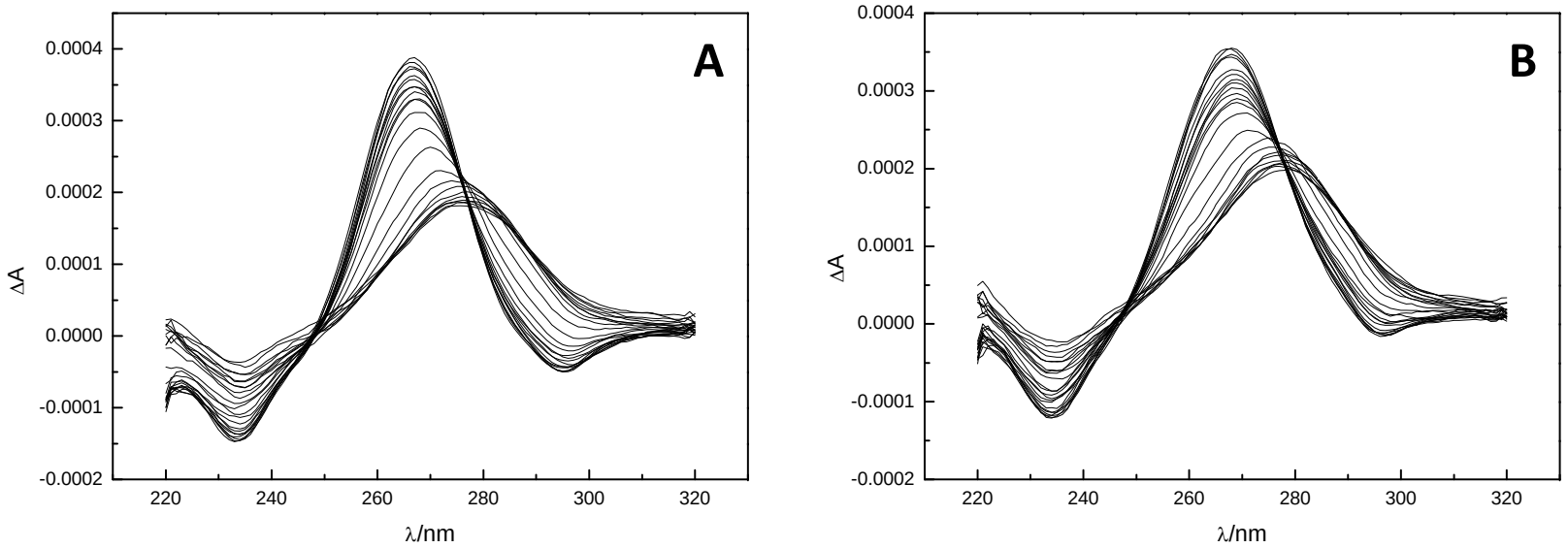

Figure S14. CD spectra of the homoduplex **7A**:**8A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

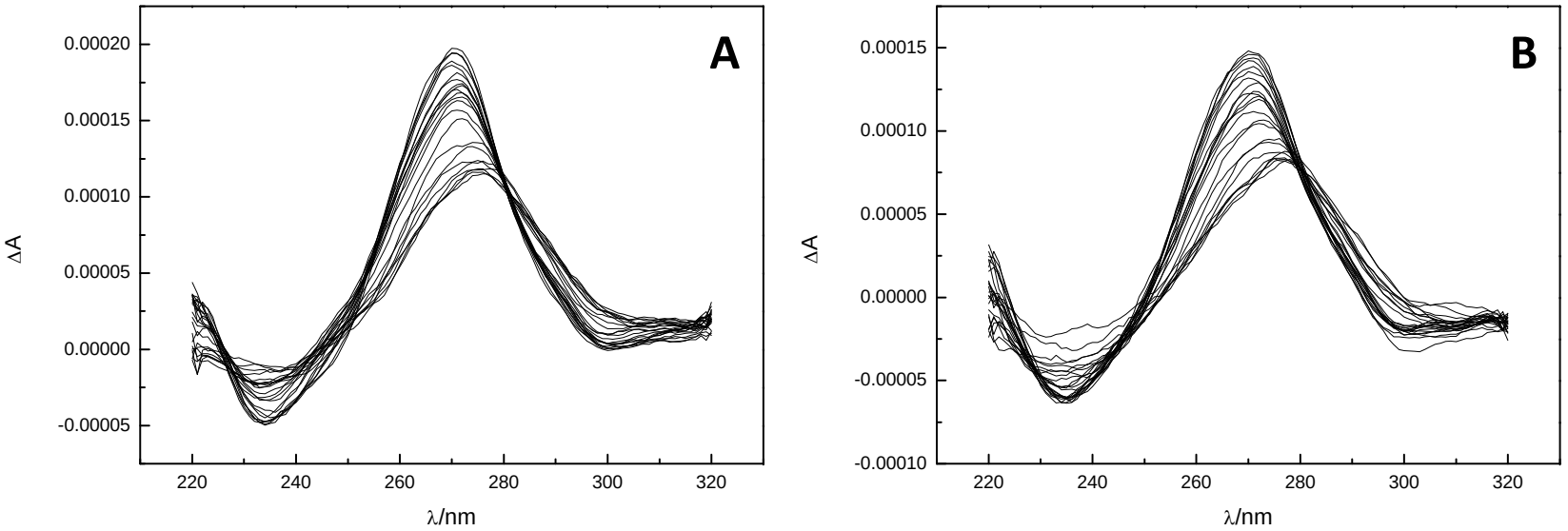

Figure S15. CD spectra of the heteroduplex **7X**:**10A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

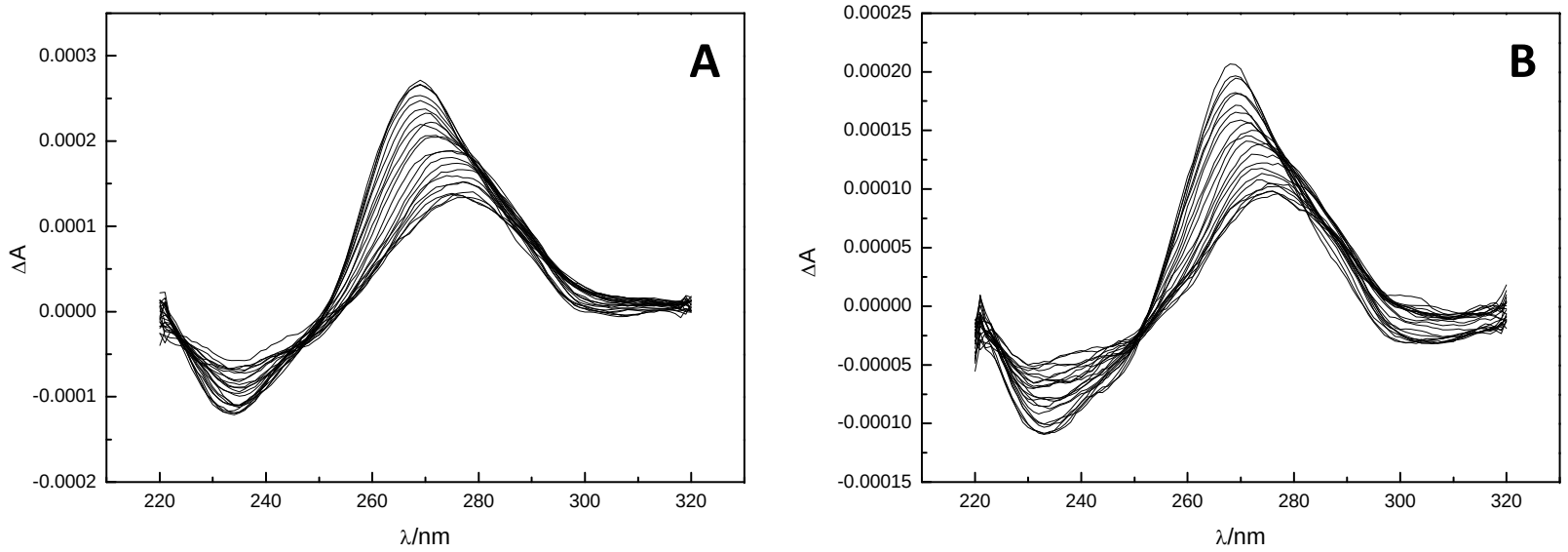

Figure S16. CD spectra of the heteroduplex **7A**:**10A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

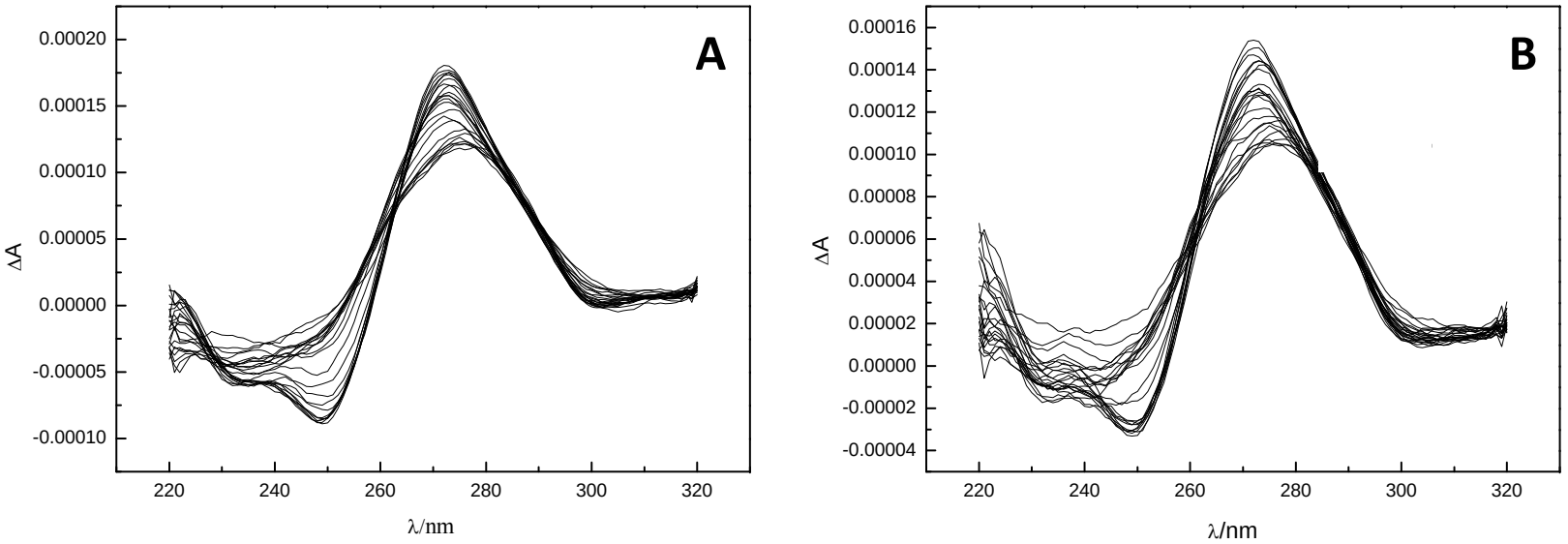

Figure S17. CD spectra of the heteroduplex **7X**:**10C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

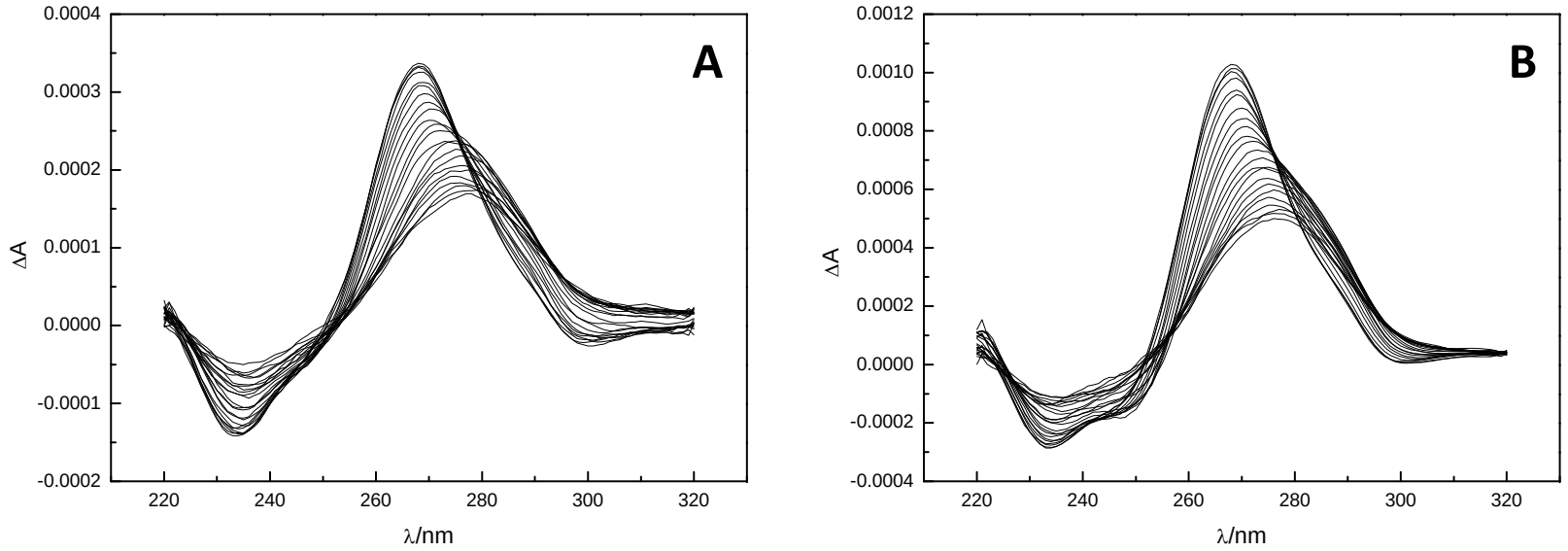

Figure S18. CD spectra of the heteroduplex **7A**:**10C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

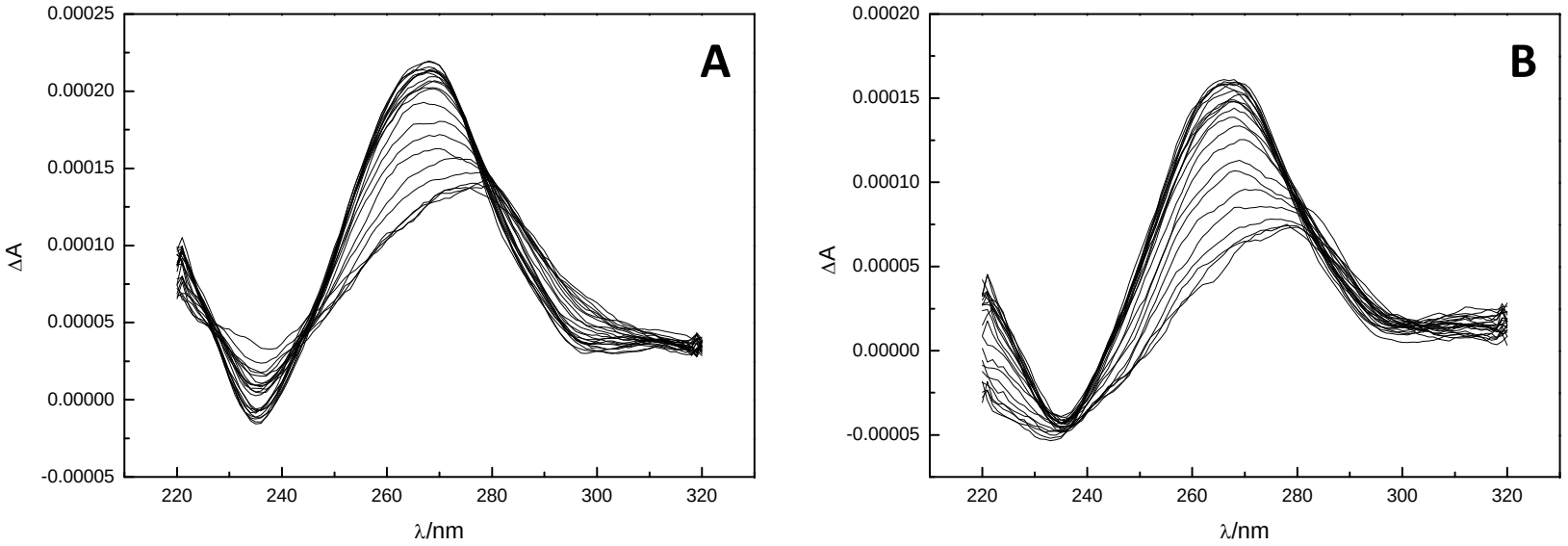

Figure S19. CD spectra of the heteroduplex **7X**:**10G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

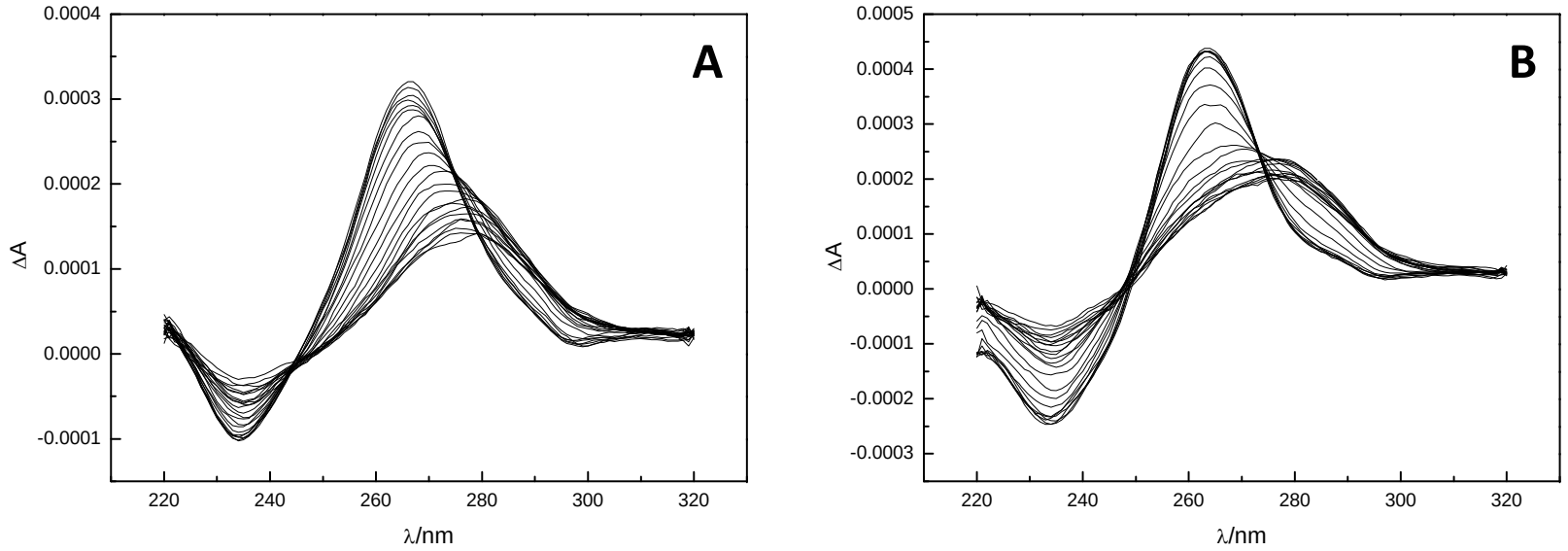

Figure S20. CD spectra of the heteroduplex **7A**:**10G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

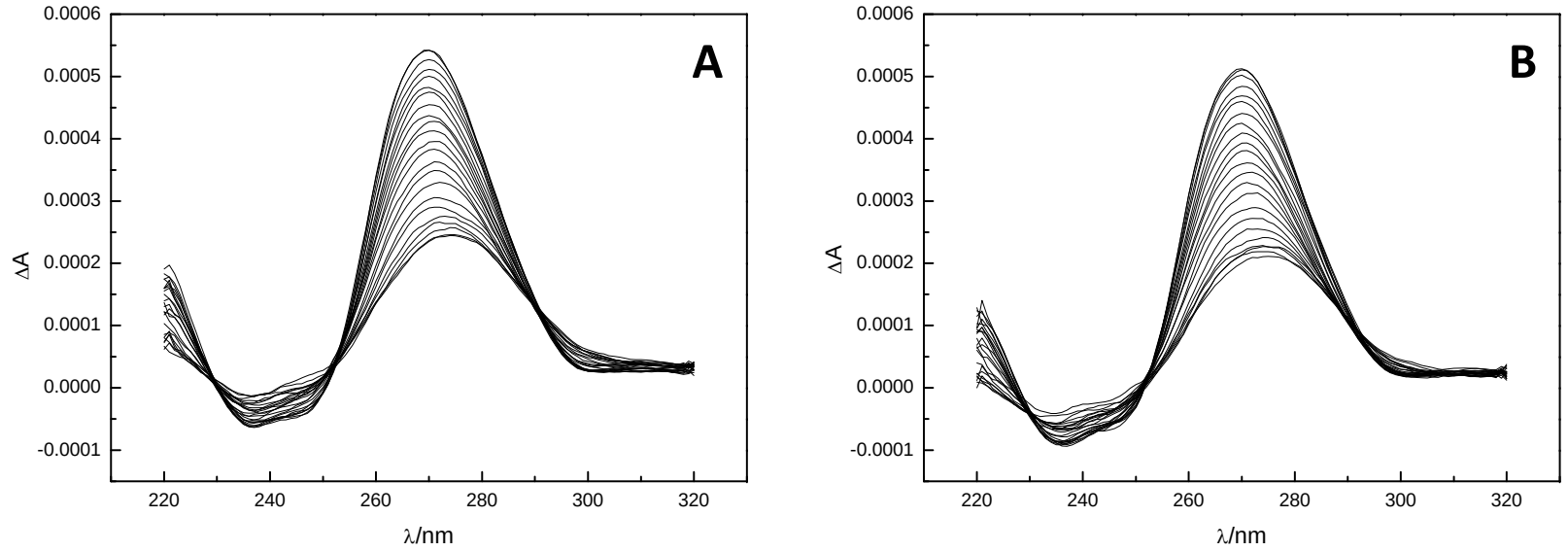

Figure S21. CD spectra of the mismatched homoduplex **7X**:**9A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

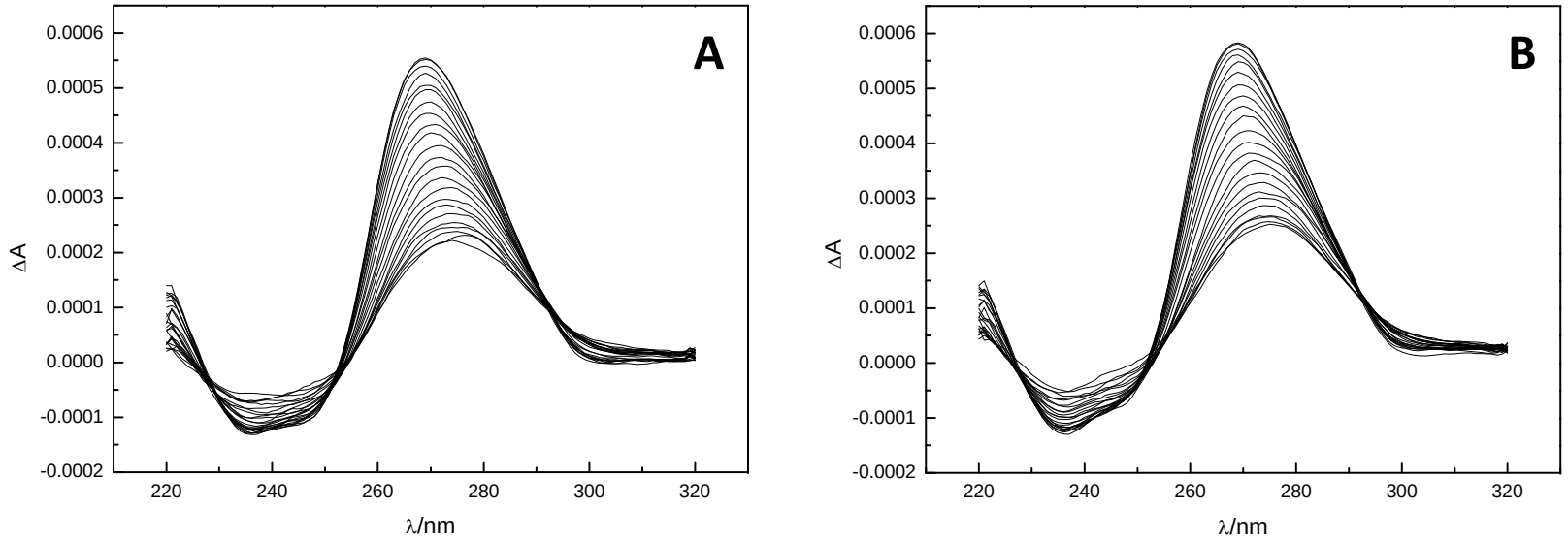

Figure S22. CD spectra of the mismatched homoduplex **7A**:**9A** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

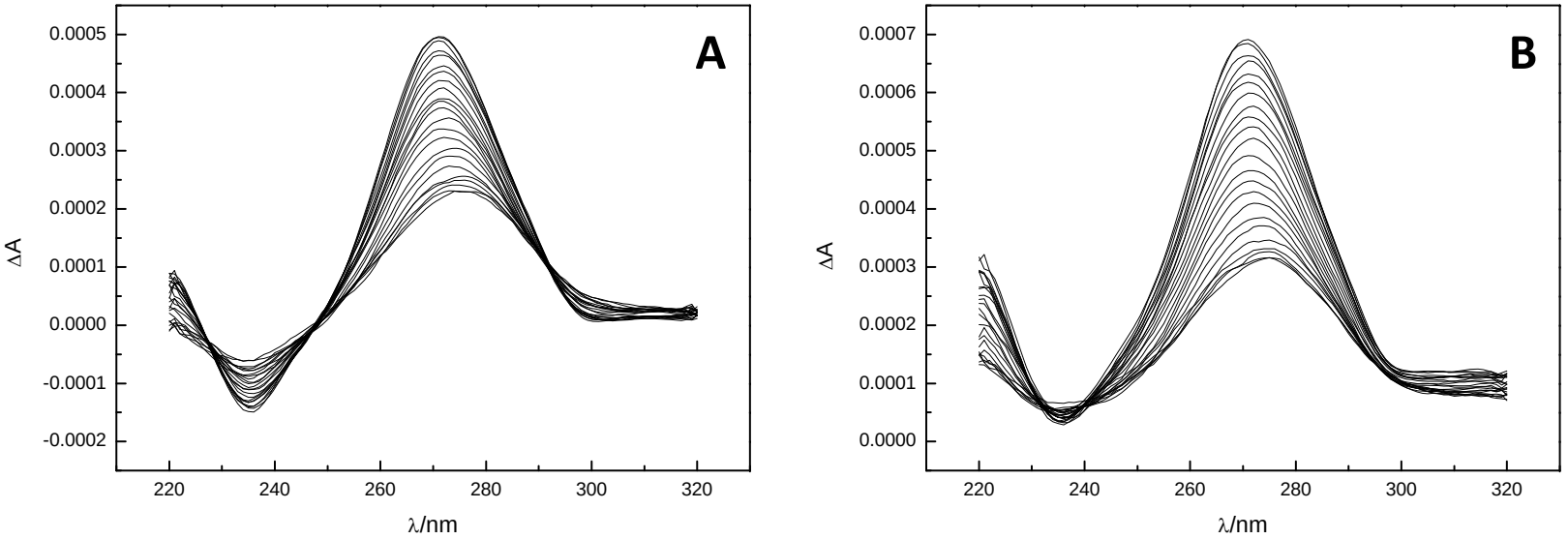

Figure S23. CD spectra of the mismatched homoduplex **7X**:**9C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

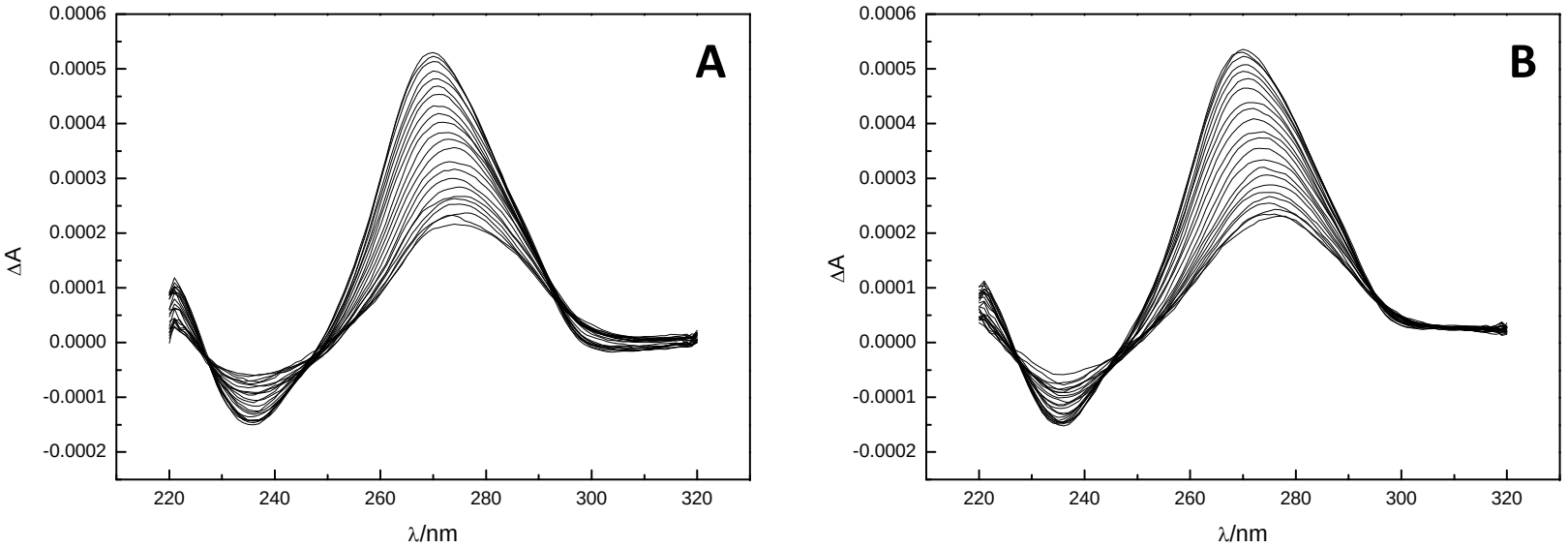

Figure S24. CD spectra of the mismatched homoduplex **7A**:**9C** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

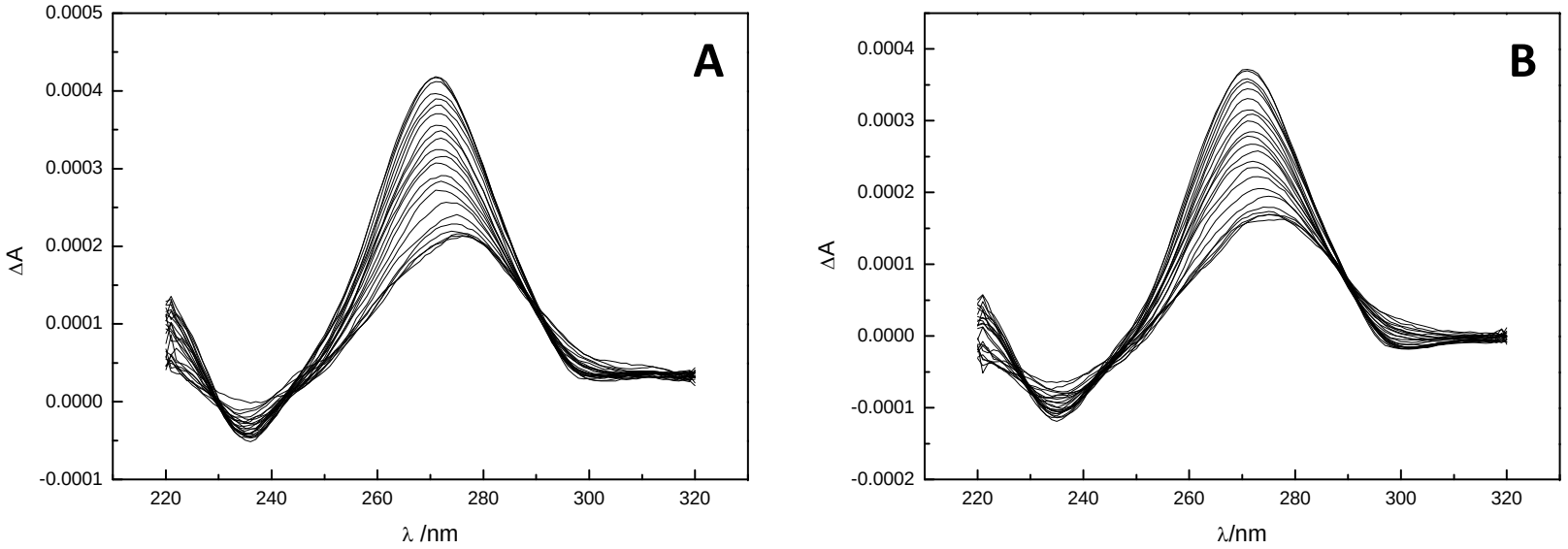

Figure S25. CD spectra of the mismatched homoduplex **7X**:**9G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

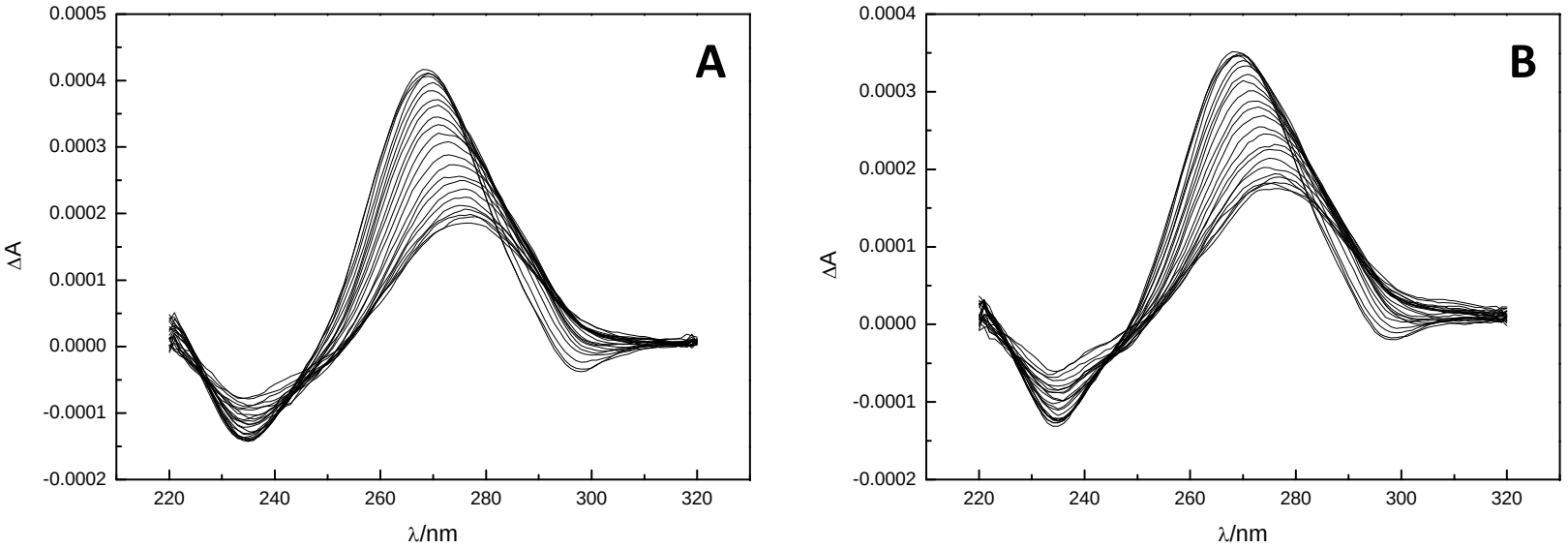

Figure S26. CD spectra of the mismatched homoduplex **7A**:**9G** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

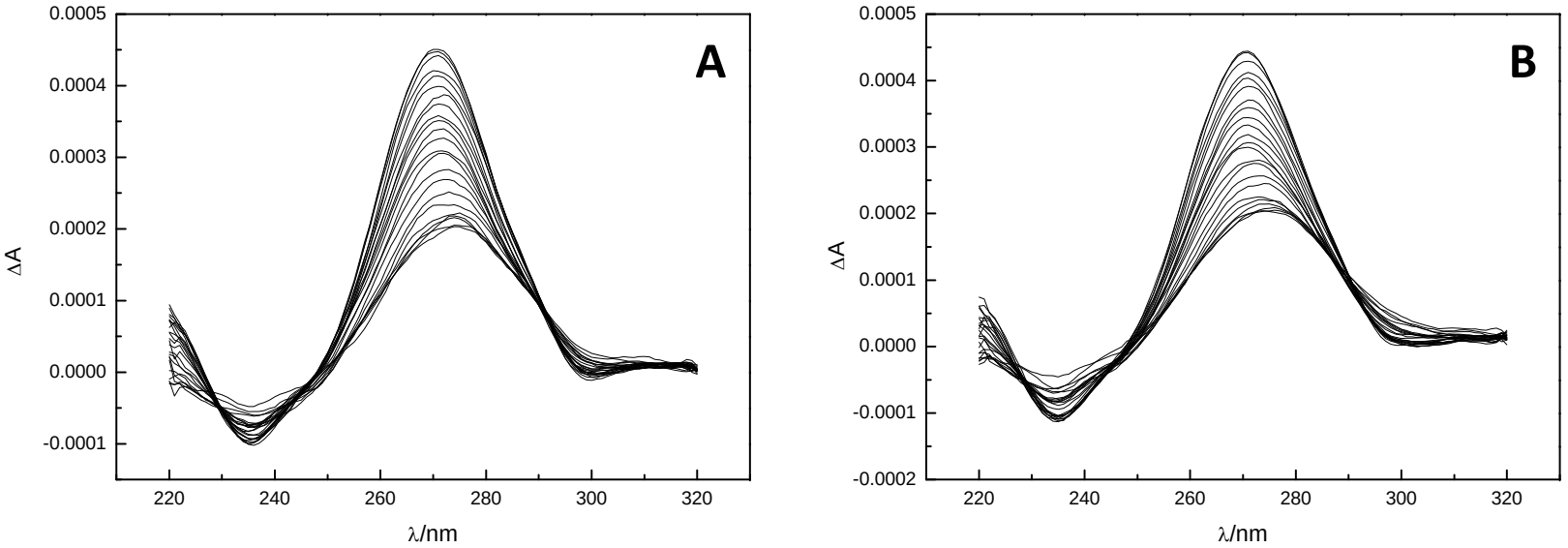

Figure S27. CD spectra of the mismatched homoduplex **7X**:**9U** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

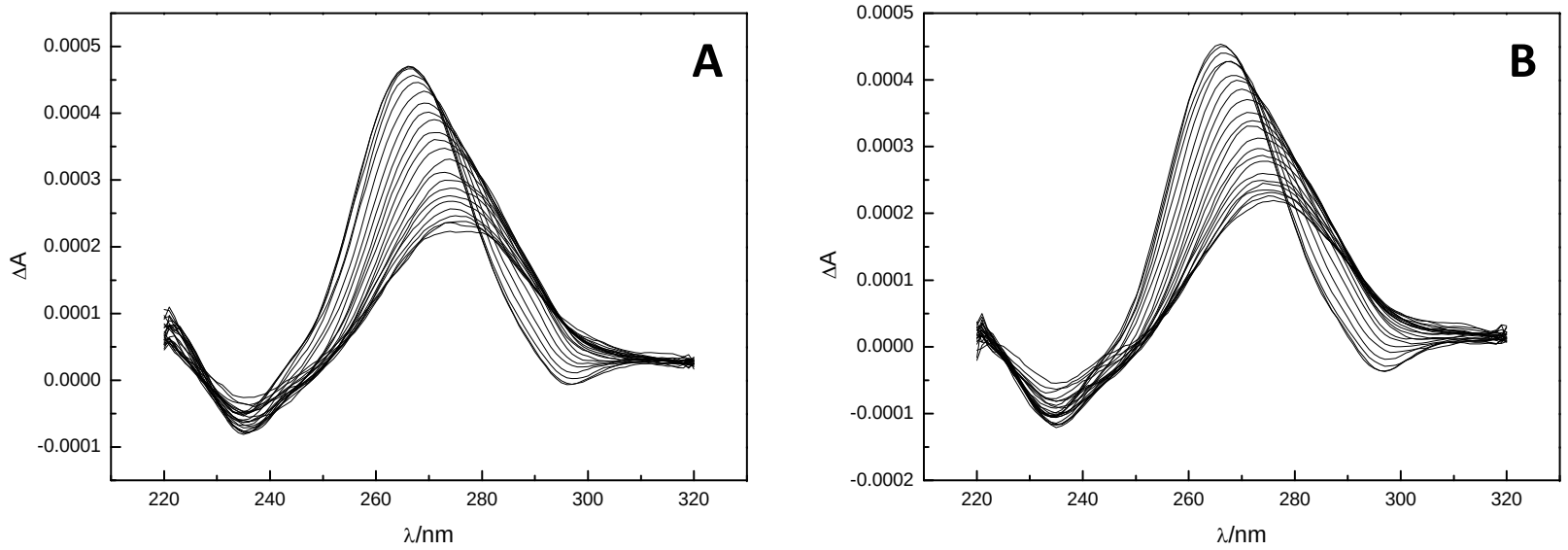

Figure S28. CD spectra of the mismatched homoduplex **7A**:**9U** in the absence (A) and presence (B) of Pd^{2+}; $I(NaClO_4)$ = 0.1 mol L^{-1}, pH = 7.4.

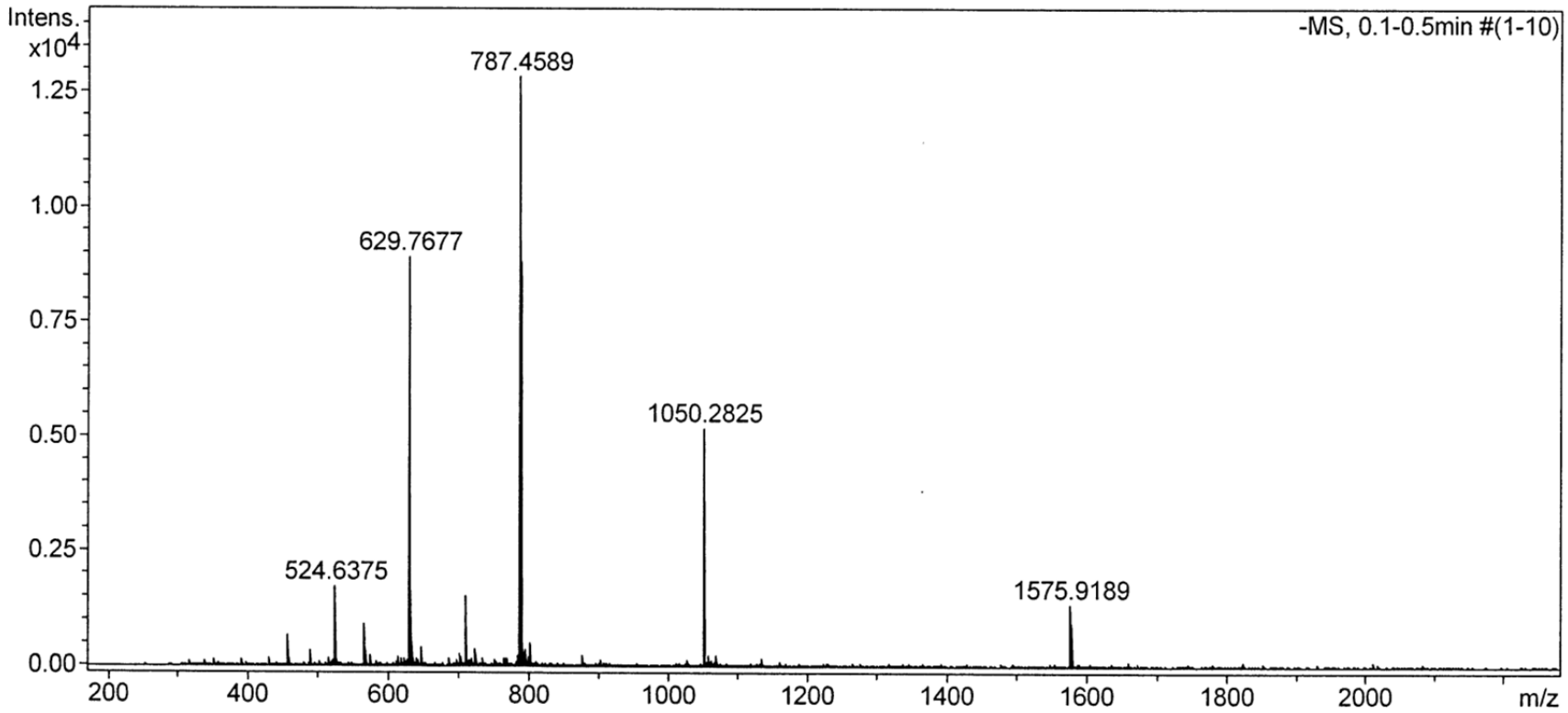

Figure S29. ESI⁻ mass spectrum of the modified oligonucleotide **7X**.