

Electronic supplementary information

Photoreversible DNA end capping for the formation of hairpin structures

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Scheme S1. Photochemical 5'-end capping of ODNs with ^{CNV}K.

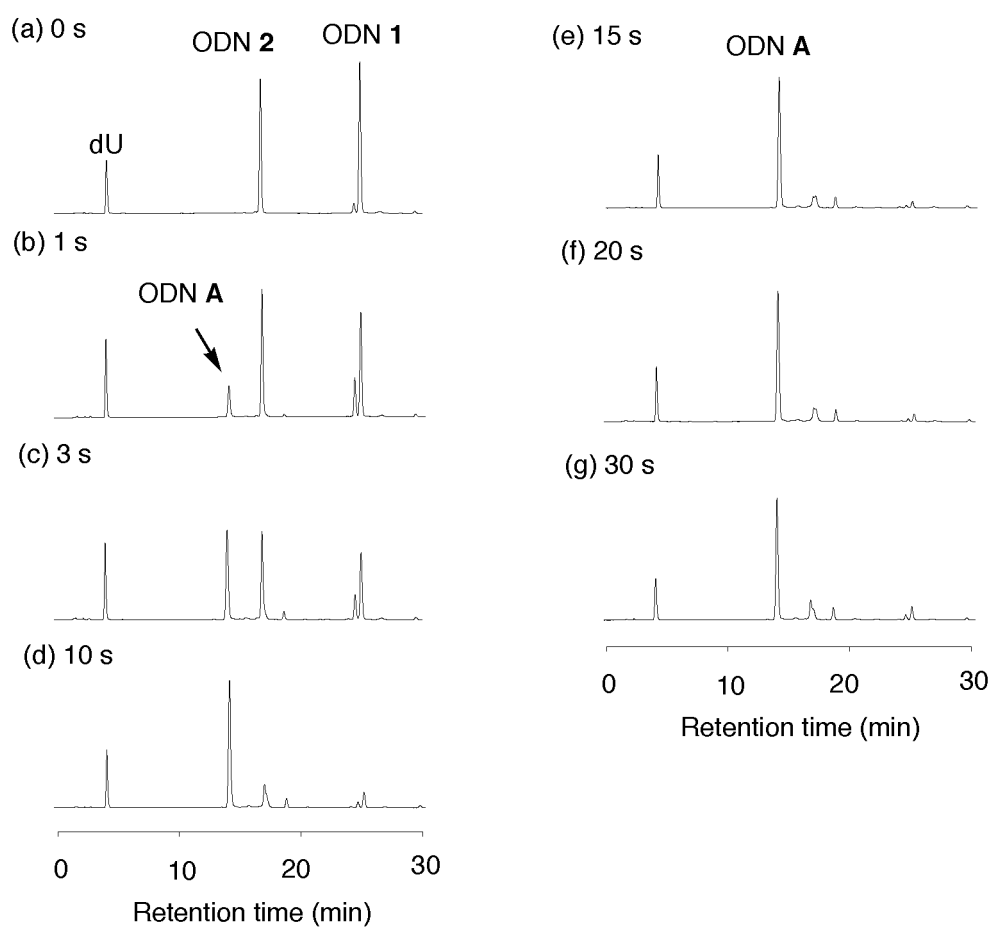
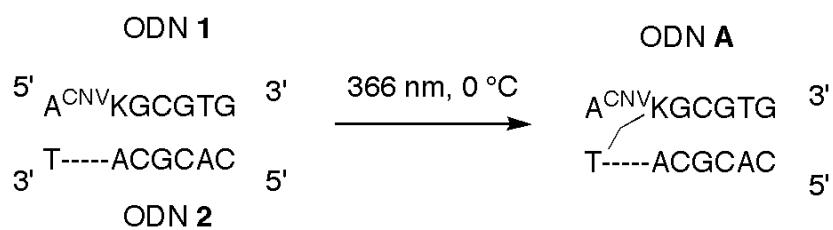


Figure S1. HPLC analysis of the irradiated ODN 1 in the presence of ODN 2. 2'-Deoxyuridine (dU) was used as an internal standard.

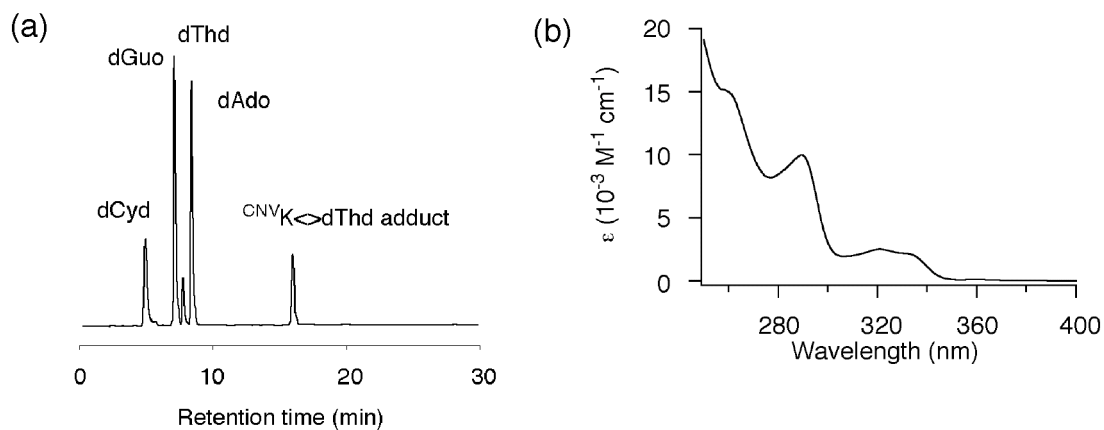


Figure S3. (a) HPLC analysis of products during enzymatic digestion process of ODN A, (b) UV spectrum of $\text{CNV K} \leftrightarrow \text{T}$ photoadduct.

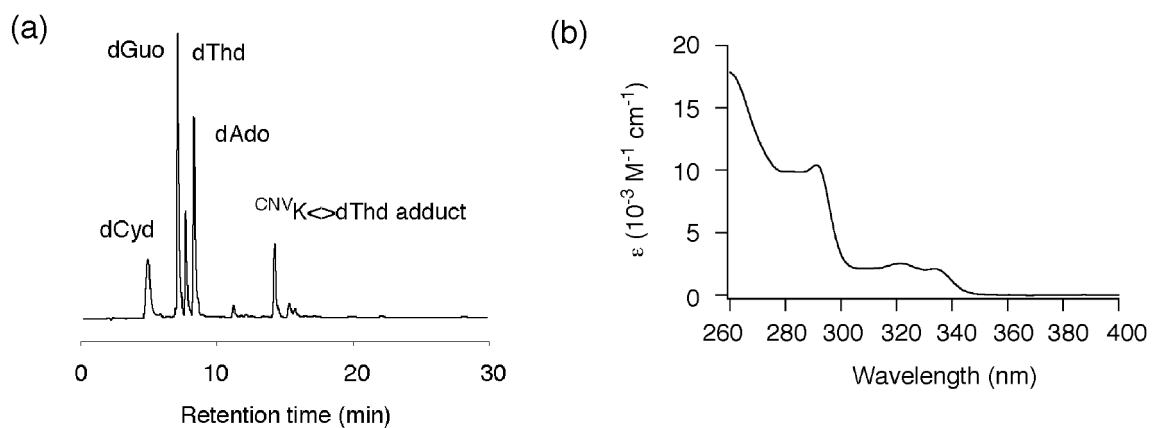


Figure S4. (a) HPLC analysis of products during enzymatic digestion process of ODN B, (b) UV spectrum of $\text{CNV K} \leftrightarrow \text{T}$ photoadduct.

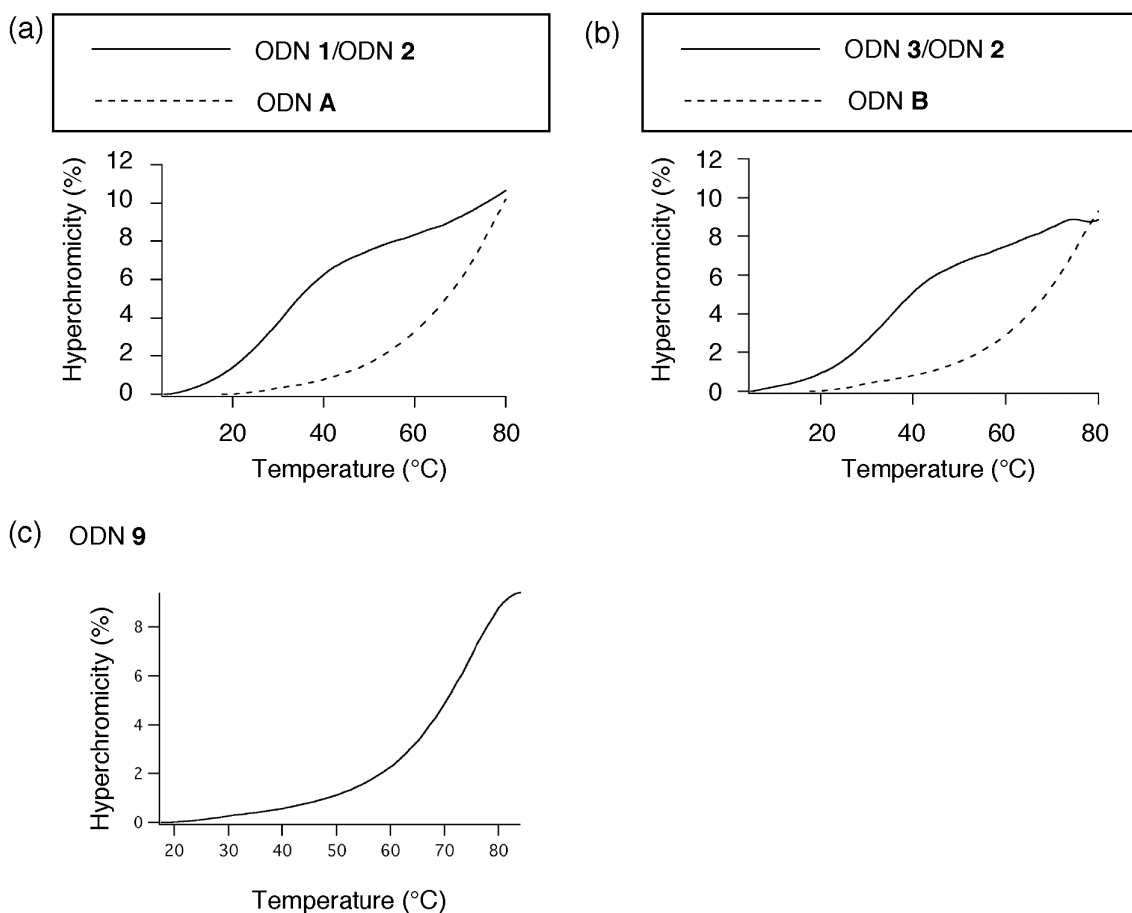


Figure S5. Melting curves: (a) the duplex ODN 1/ODN 2 and the end-capped ODN A; (b) the duplex ODN 3/ODN 2 and the end-capped ODN B; (c) ODN 9.

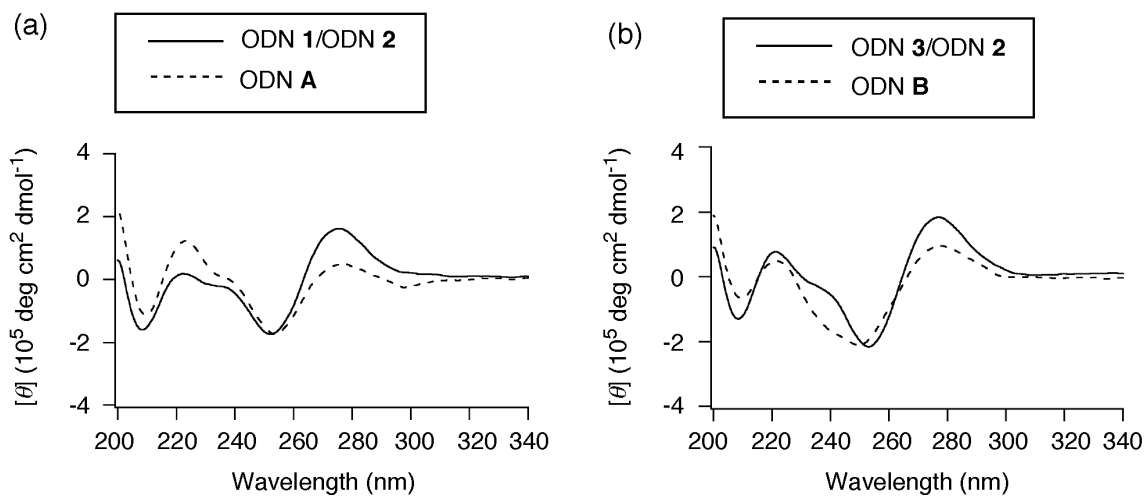


Figure S6. CD spectra: (a) the duplex ODN 1/ODN 2 and the end-capped ODN A; (b) the duplex ODN 3/ODN 2 and the end-capped ODN B.

Scheme S3. Photosplitting of the end-capped ODN.

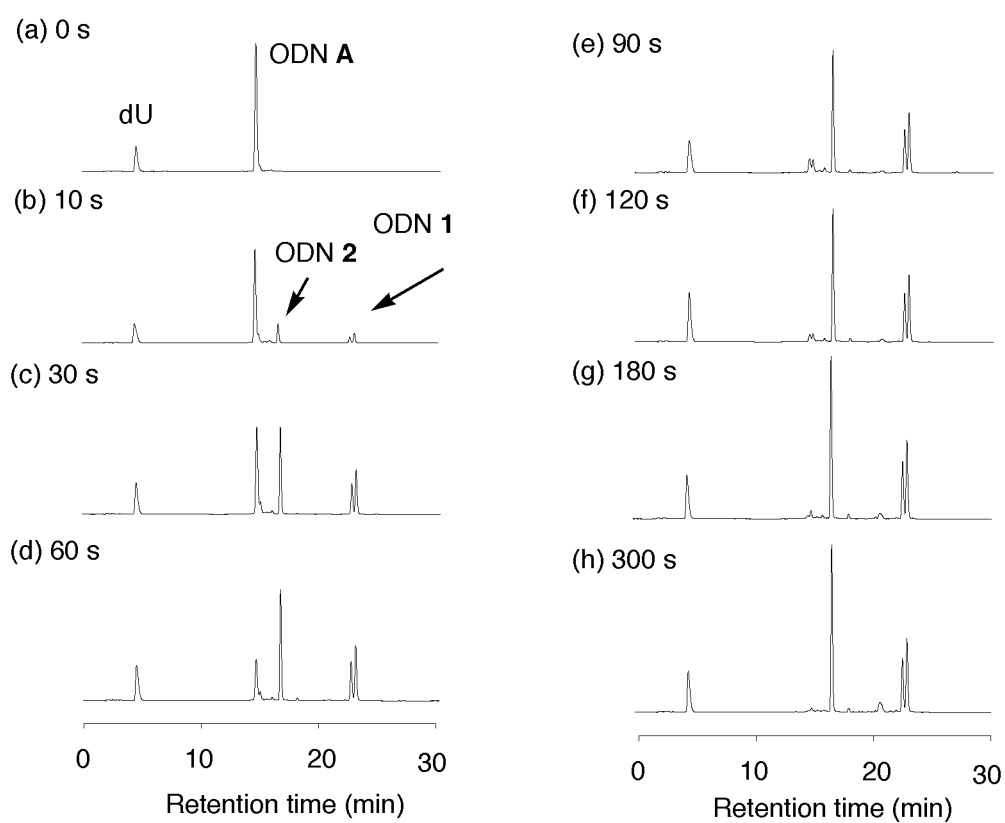
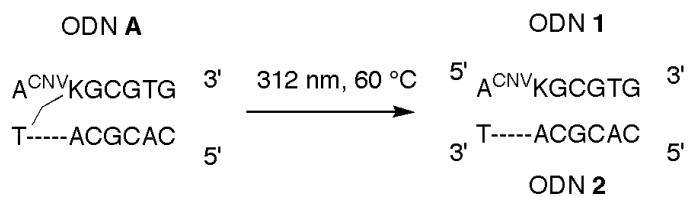


Figure S7. HPLC analysis of the photosplitting of ODN A. 2'-Deoxyuridine (dU) was used as an internal standard.

Scheme S4. Photoisomerization of ODN with ^{CNV}K.

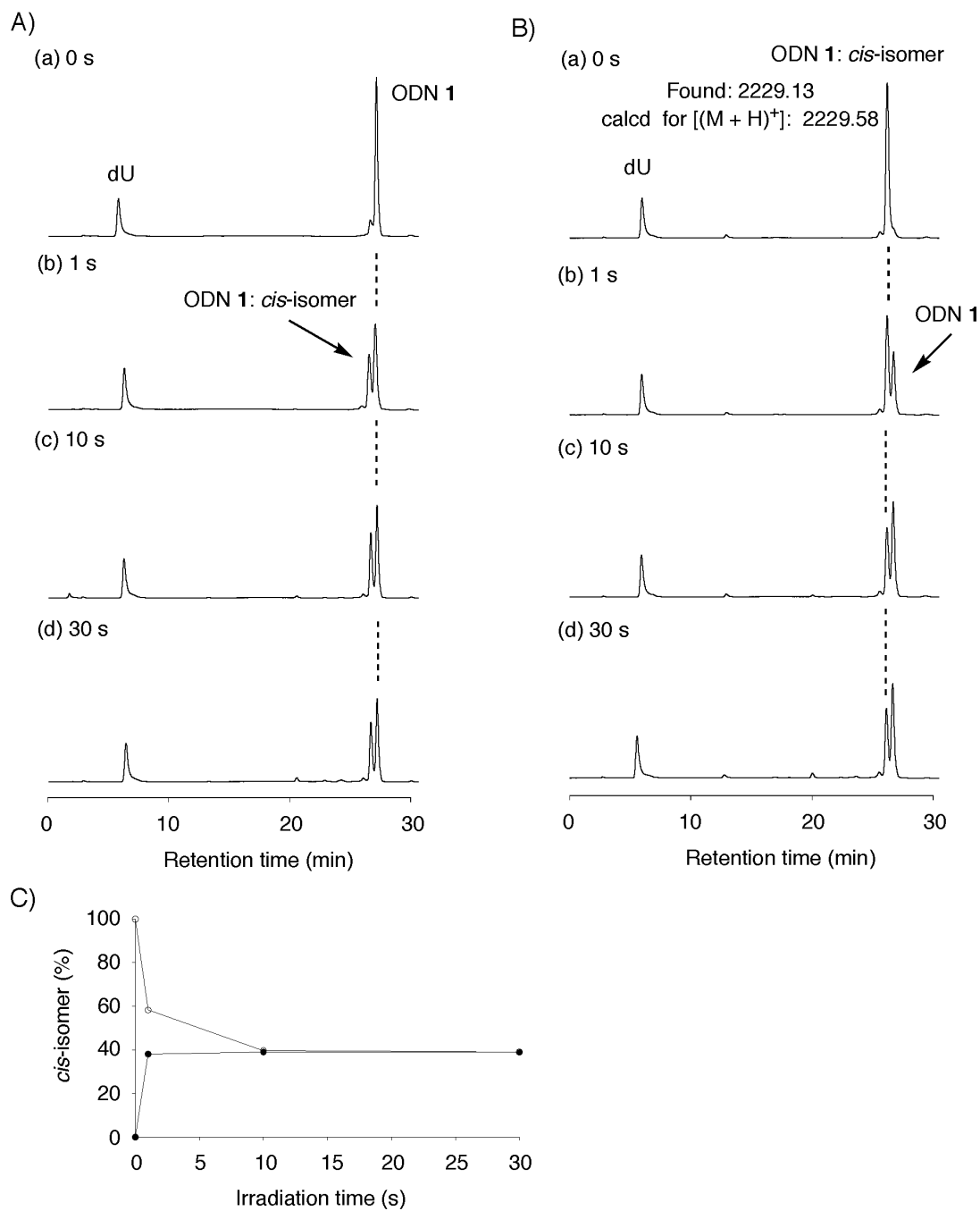
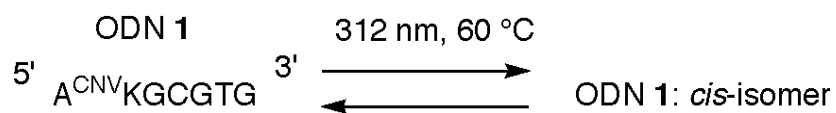


Figure S8. HPLC analysis of A) ODN 1 and B) ODN 1(*cis*-isomer). 2'-Deoxyuridine (dU) was used as an internal standard. C) Plot of %*cis* vs. irradiation time: ODN 1 (filled symbols) and ODN 1(*cis*-imer) (open symbols).

Scheme S5. Photosplitting of the end-capped ODN.

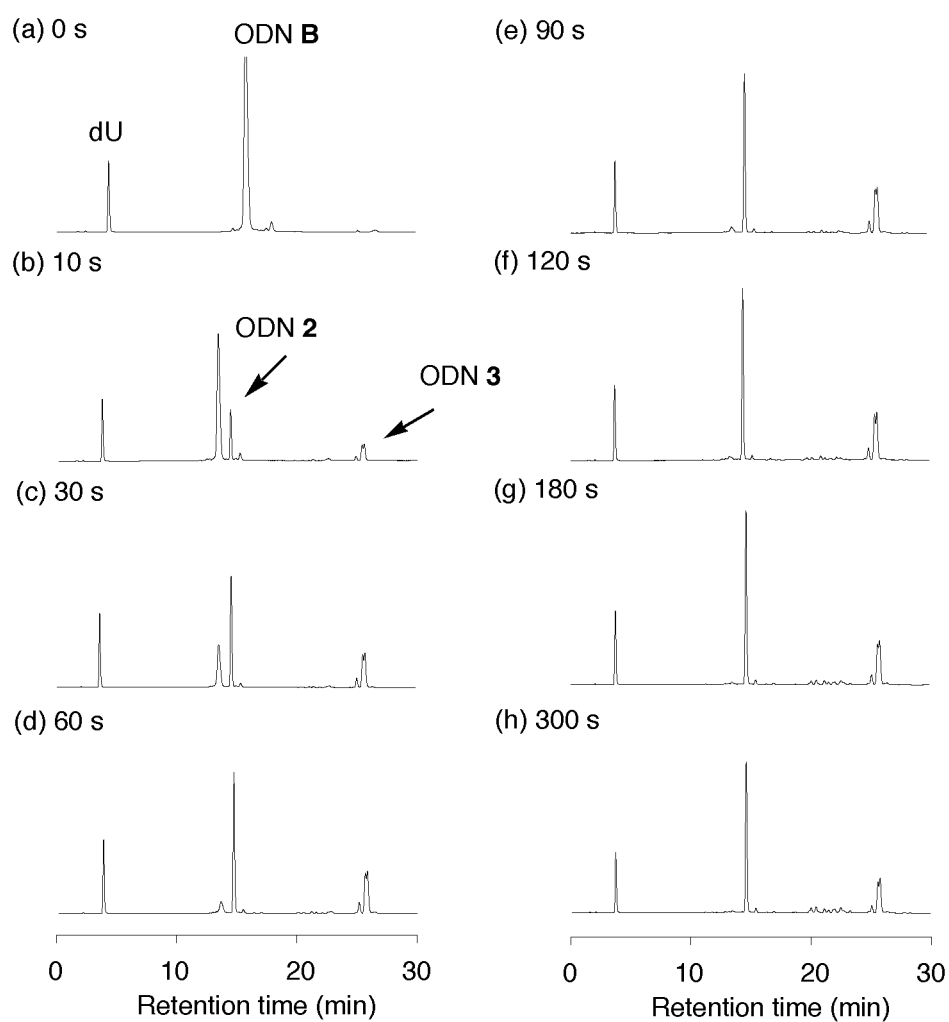
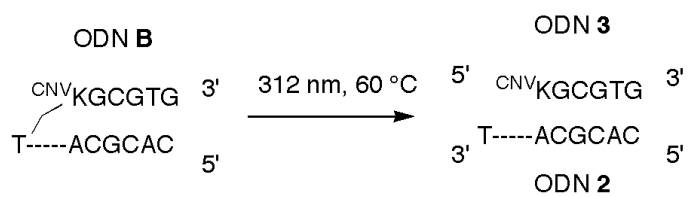


Figure S9. HPLC analysis of the photosplitting of ODN B. 2'-Deoxyuridine (dU) was used as an internal standard.

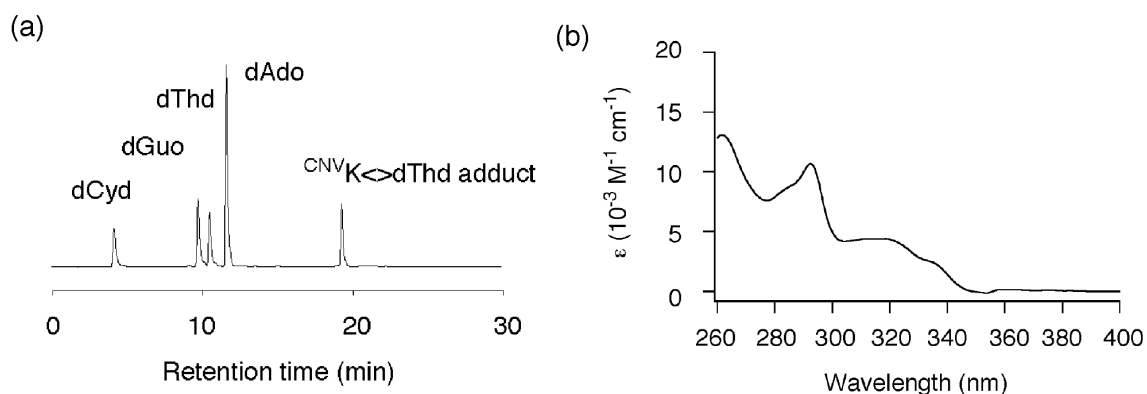


Figure S12. (a) HPLC analysis of products during enzymatic digestion process of ODN C, (b) UV spectrum of ^{CNV}K \leftrightarrow T photoadduct.

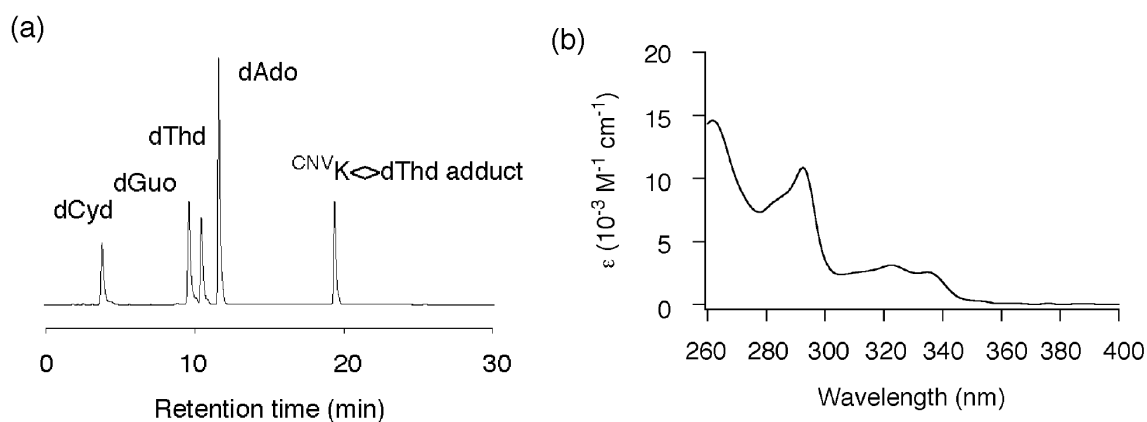


Figure S13. (a) HPLC analysis of products during enzymatic digestion process of ODN D, (b) UV spectrum of ^{CNV}K \leftrightarrow T photoadduct.

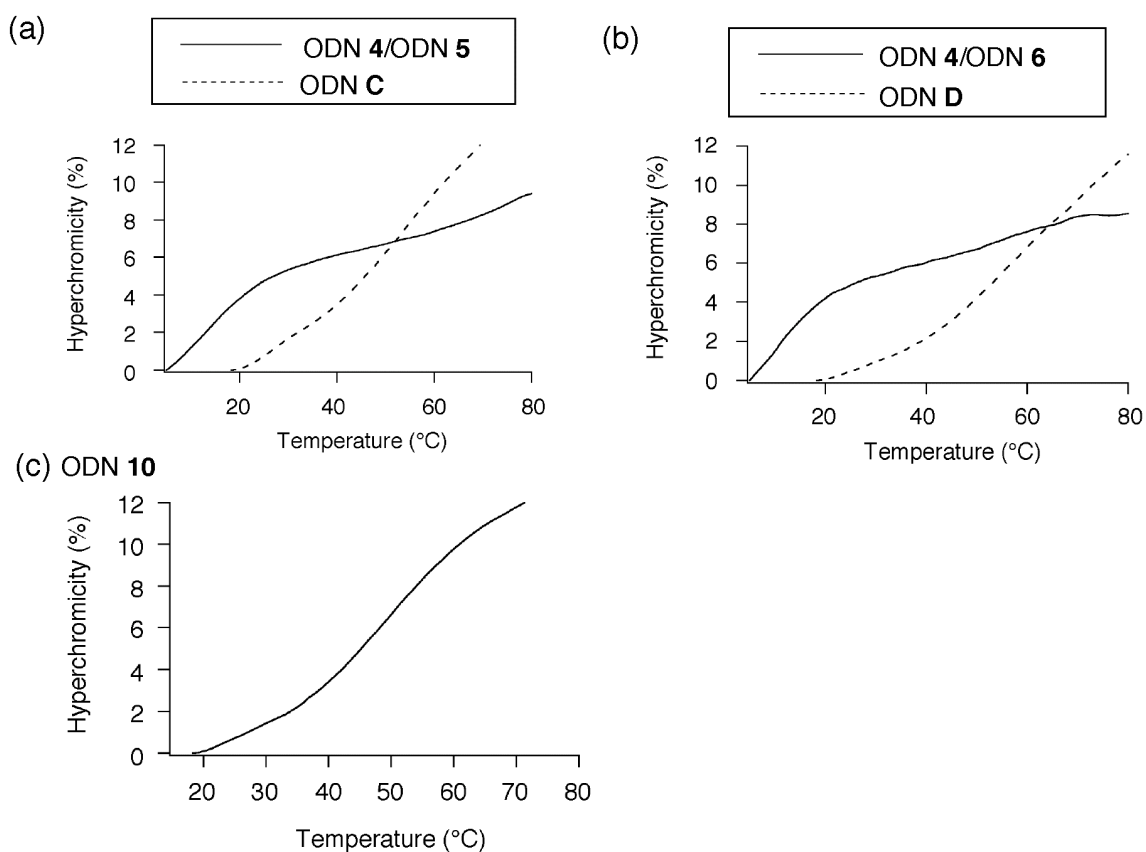


Figure S14. Melting curves: (a) the duplex ODN 4/ODN 5 and the end-capped ODN C; (b) the duplex ODN 4/ODN 6 and the end-capped ODN D; (c) ODN 10.

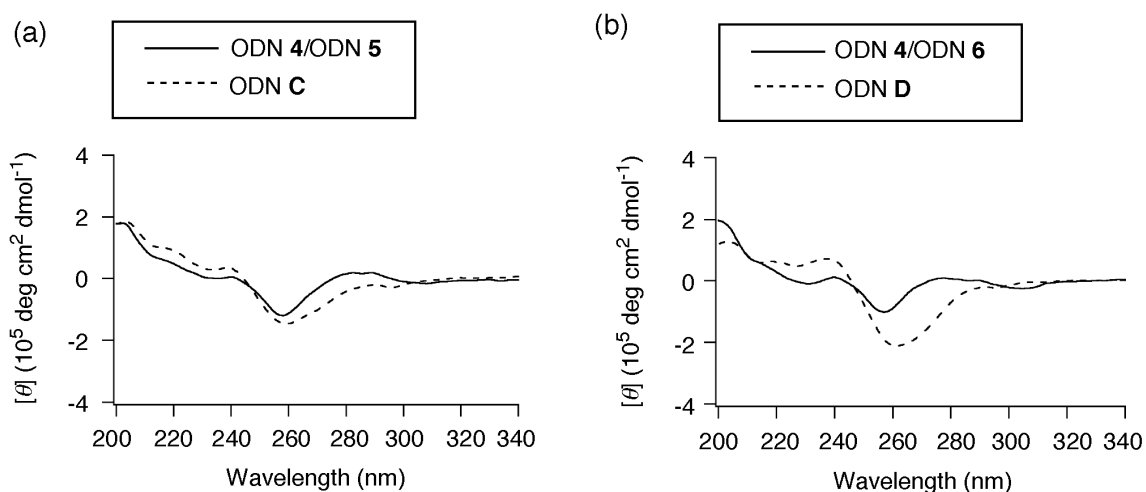


Figure S15. CD spectra: (a) the duplex ODN 4/ODN 5 and the end-capped ODN C; (b) the duplex ODN 4/ODN 6 and the end-capped ODN D.

Scheme S8. Photosplitting of the end-capped ODN.

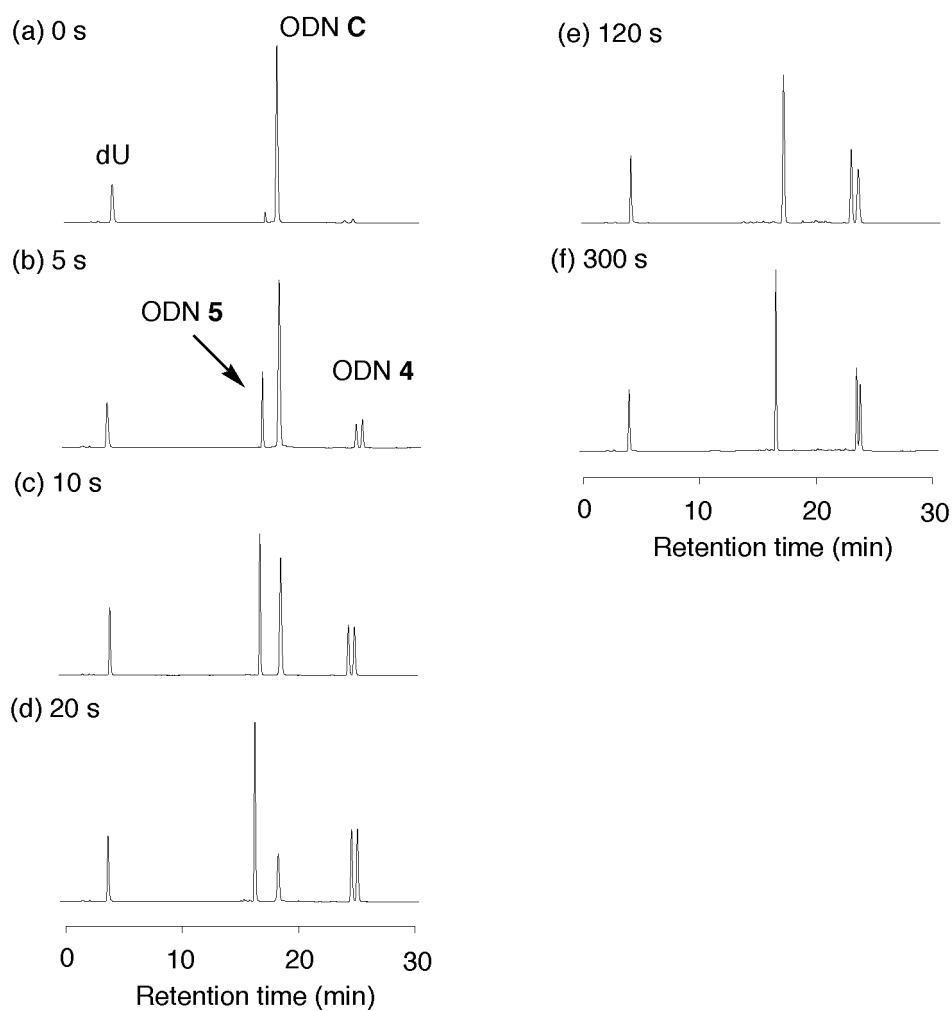
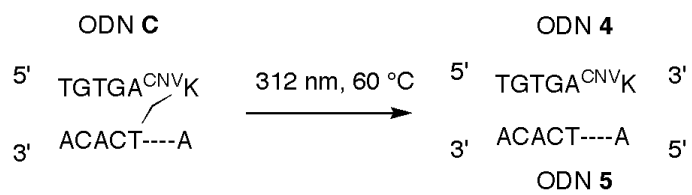


Figure S16. HPLC analysis of the photosplitting of ODN C. 2'-Deoxyuridine (dU) was used as an internal standard.

Scheme S9. Photoisomerization of ODN with ^{CNV}K.

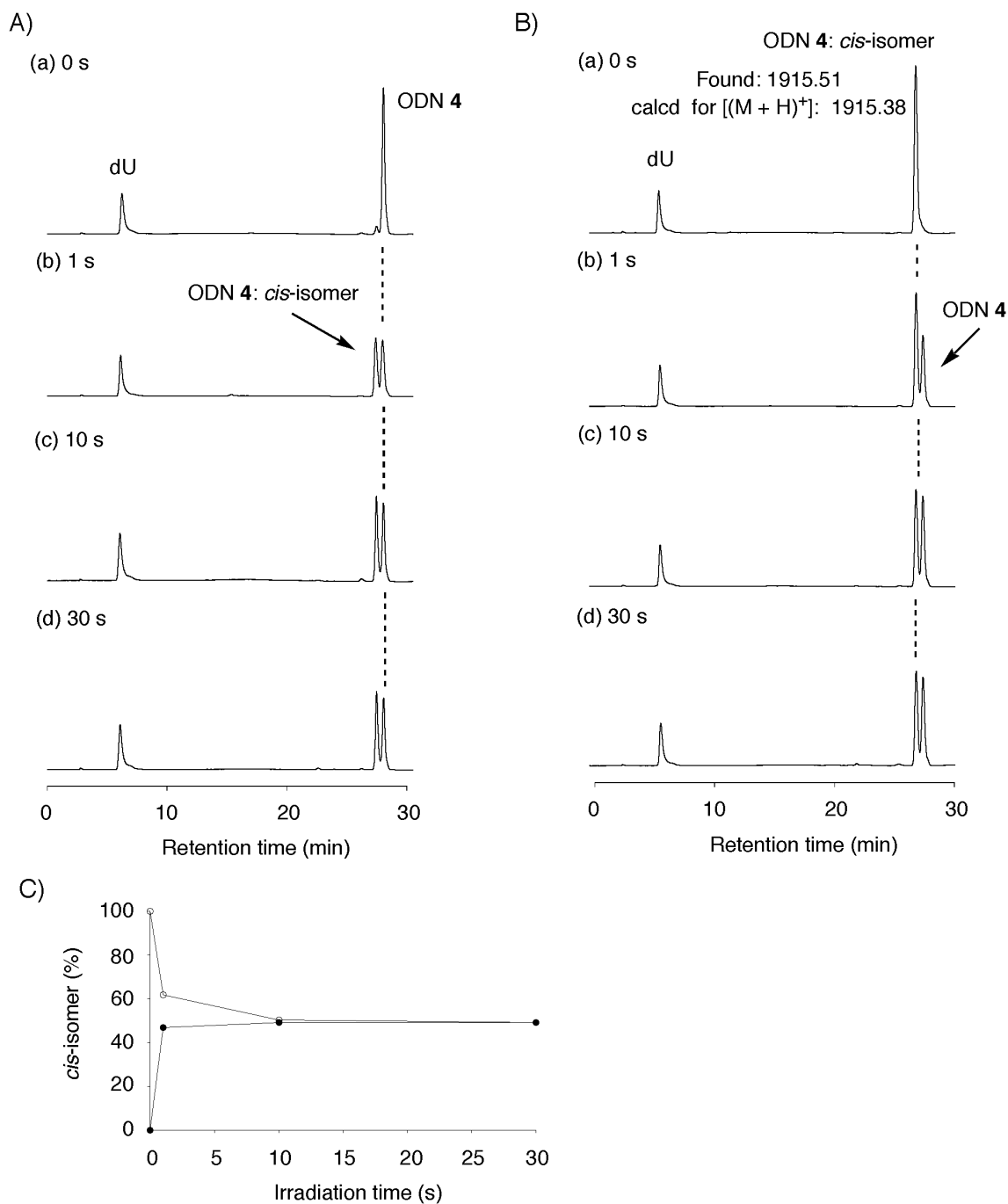
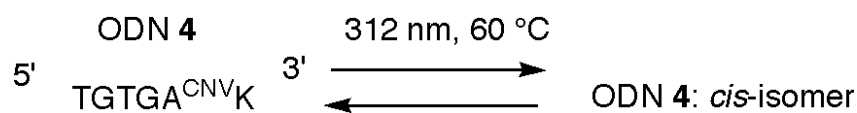


Figure S17. HPLC analysis of A) ODN 4 and B) ODN 4(*cis*-isomer). 2'-Deoxyuridine (dU) was used as an internal standard. C) Plot of %*cis* vs. irradiation time: ODN 4 (filled symbols) and ODN 4(*cis*-imer) (open symbols).

Scheme S10. Photosplitting of the end-capped ODN.

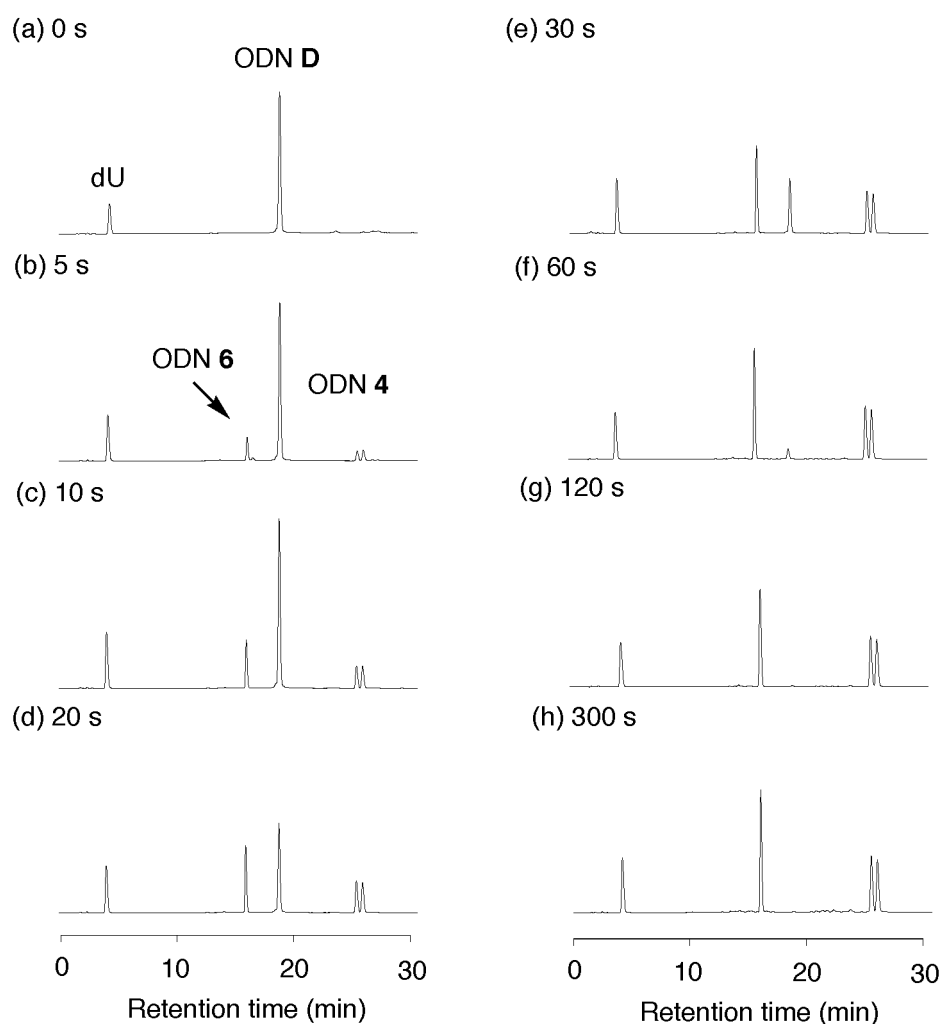
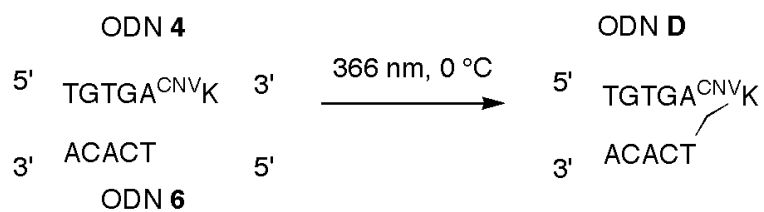
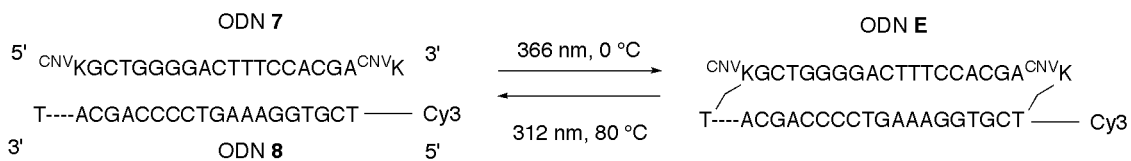
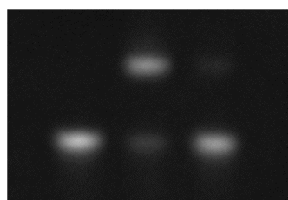


Figure S18. HPLC analysis of the photosplitting of ODN D. 2'-Deoxyuridine (dU) was used as an internal standard.

Scheme S11. Photochemical doubly end capping of ODNs with ^{CNV}K.



366 nm	-	+	+
312 nm	-	-	+



1 2 3

Figure S19. 16% PAGE of photoreversible end capping of Cy3-labeled ODN. Lane 1: duplex ODN 7/ODN 8 labeled with Cy3; lane 2: 366 nm irradiation of lane 1 for 40 s, 92% yield; lane 3: 312 nm irradiation of lane 2 for 90 s, 83% yield.

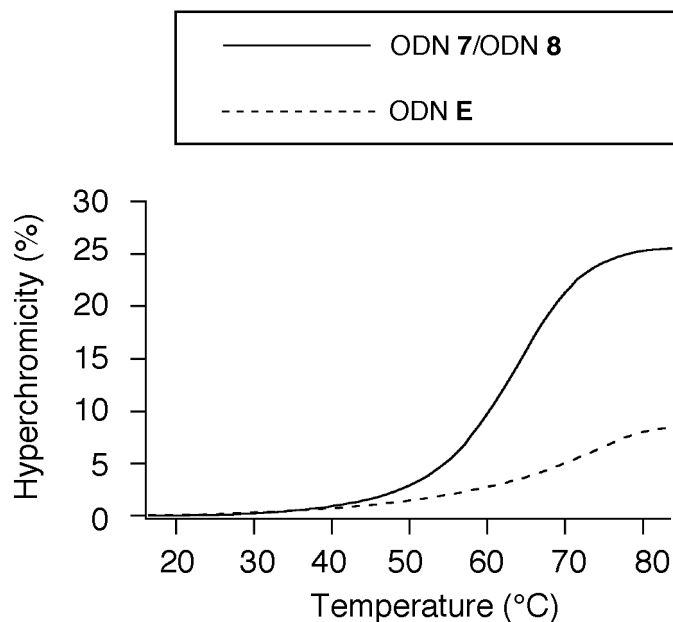


Figure S20. Melting curves: the duplex ODN 7/ODN 8 and the end-capped ODN E. T_m values of the duplex ODN 7/ODN 8 and the end-capped ODN E were measured in 50 mM sodium cacodylate buffer (pH 7.0) and 5 mM sodium chloride.

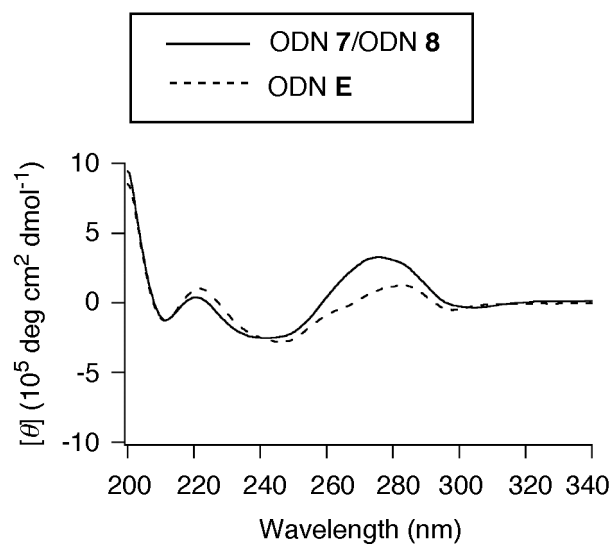


Figure S21. CD spectra: the duplex ODN 7/ODN 8 and the end-capped ODN E.

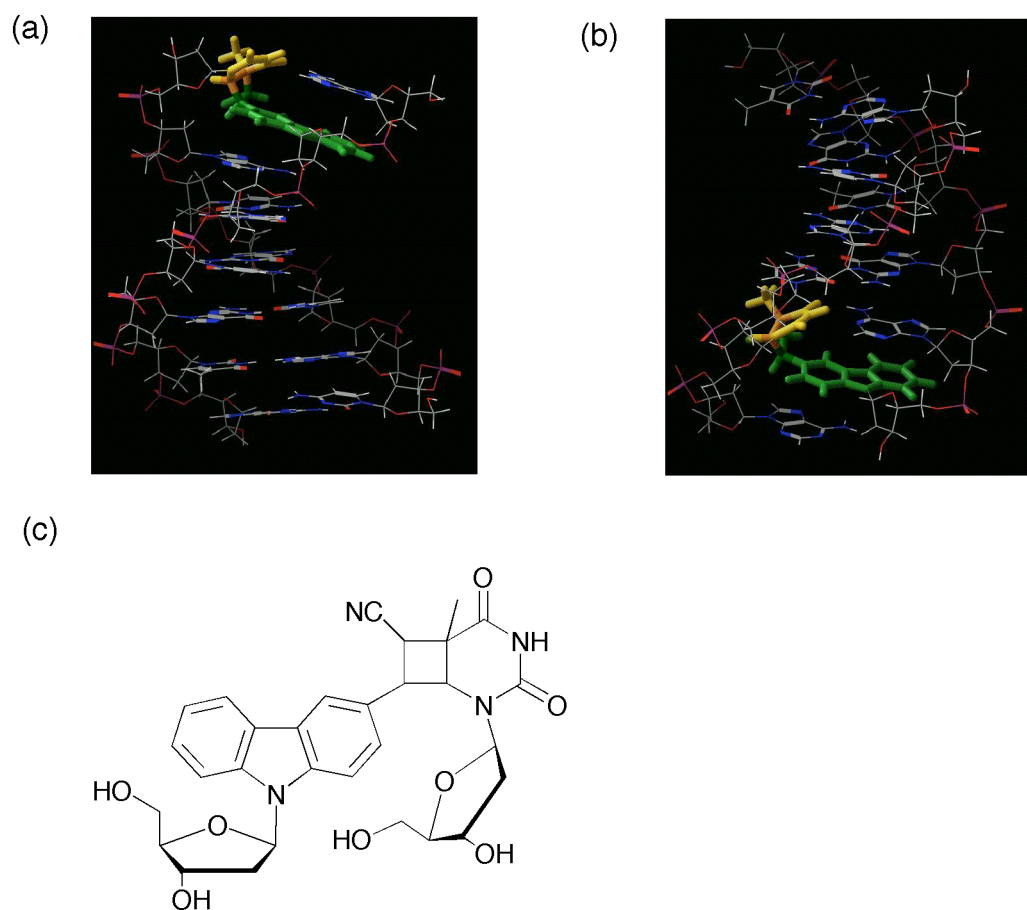


Figure S22. (a) Molecular modeling of stacked geometry in the end capped ODN **A**. (b) Molecular modeling of stacked geometry in the end capped ODN **C**. Yellow, and green molecules are T, and ^{CNV}K, respectively. (c) Proposed structure of ^{CNV}K \leftrightarrow T photoadduct.