

Supporting Information

Photo-cross-linking of DNA using 4-methylpyranocarbazole with thymine-base selectivity

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1. UPLC analysis of photo-cross-linking

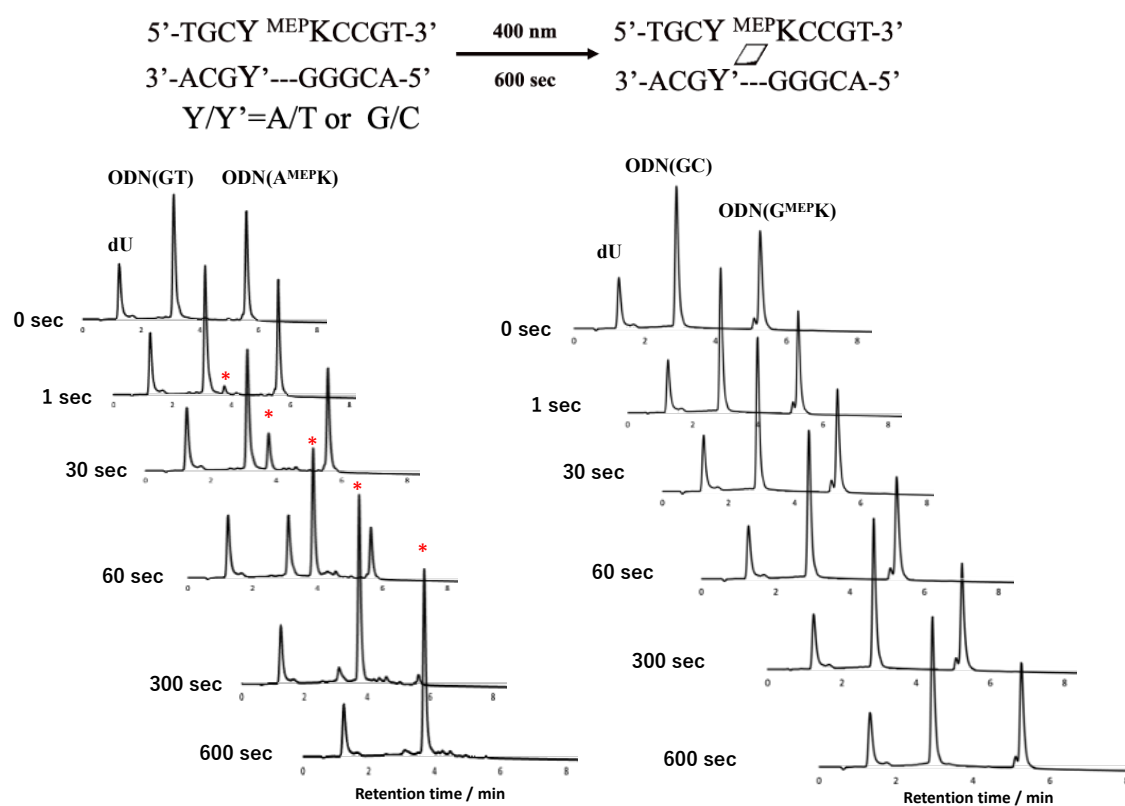


Figure S1. Photo-cross-linking using ^{MEP}K. 10 μM of ODNs in 50 mM Na-cacodylate buffer containing 100 mM NaCl was annealed and photoirradiated at 400 nm on ice.

2. MALDI-TOF-MS analysis of photo-cross-linked dsDNA

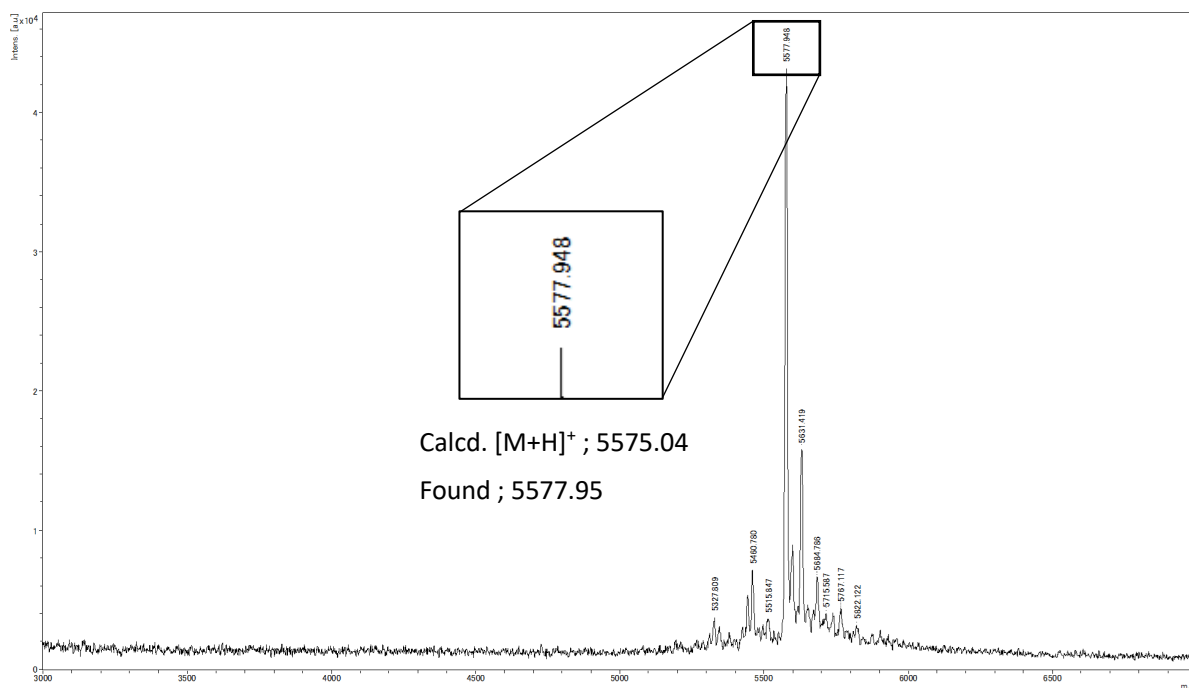


Figure S2. MALDI-TOF-MS analysis of photo-cross-linked dsDNA consisting of ODN(A^{MEP}K) and ODN (GT).

3. UV spectra of ^{MEP}K and ^{PCX} nucleoside

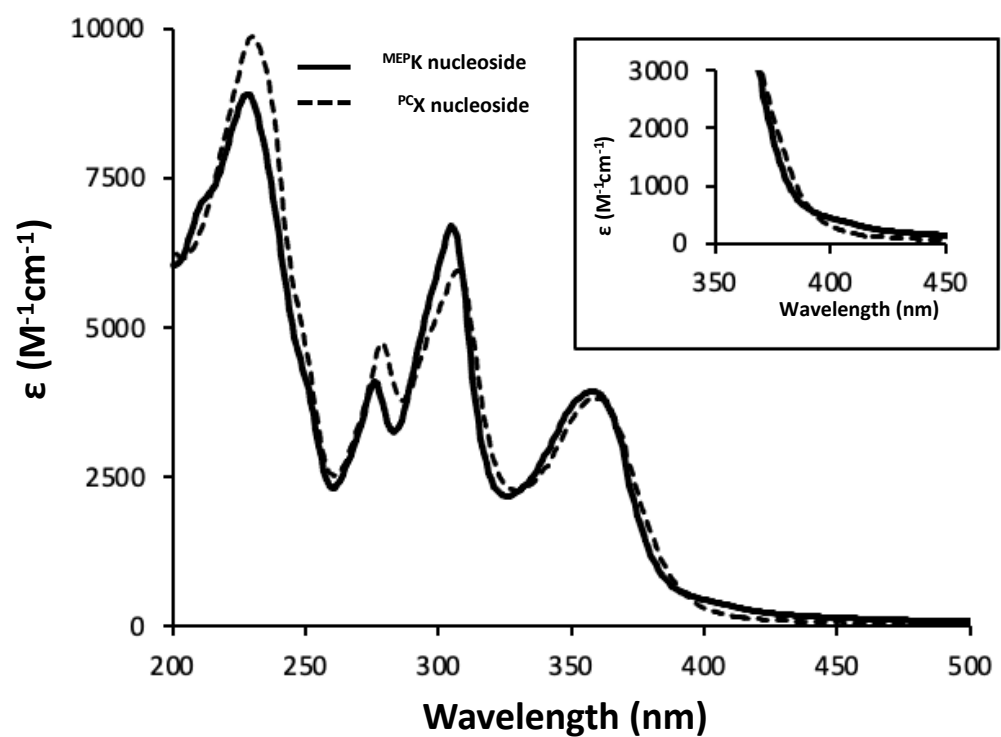
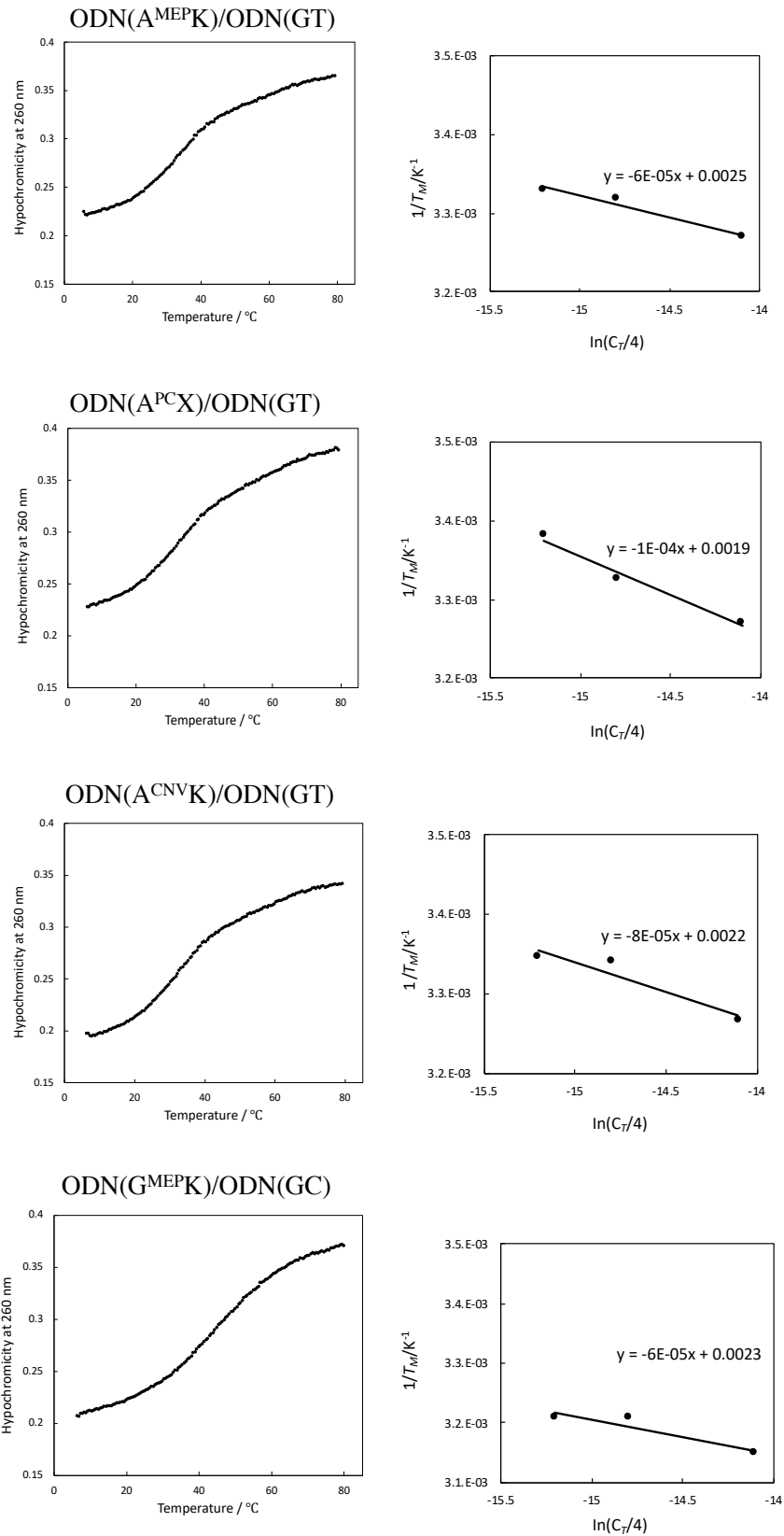


Figure S3. UV spectra of ^{MEP}K and ^{PCX} nucleoside

4. Melting temperature measurement of duplex DNA



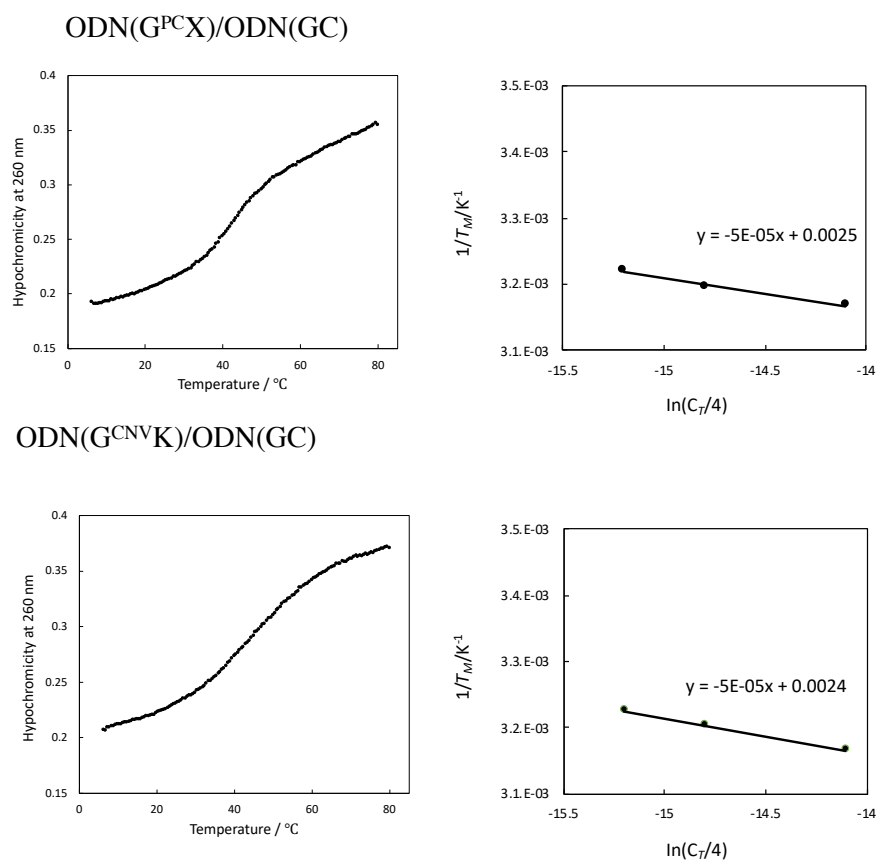


Figure S4. Melting curve and $1/T_m/\text{K}^{-1}$ vs $\ln(C_T/4)$ plot of DNA duplexes containing. Sample solutions were DNA duplexes in 50 mM Na-cacodylate buffer containing 100 mM NaCl. Absorbance was measured at 260 nm from 5 °C to 80 °C.

5. Circular Dichroism (CD) spectra of duplex DNA

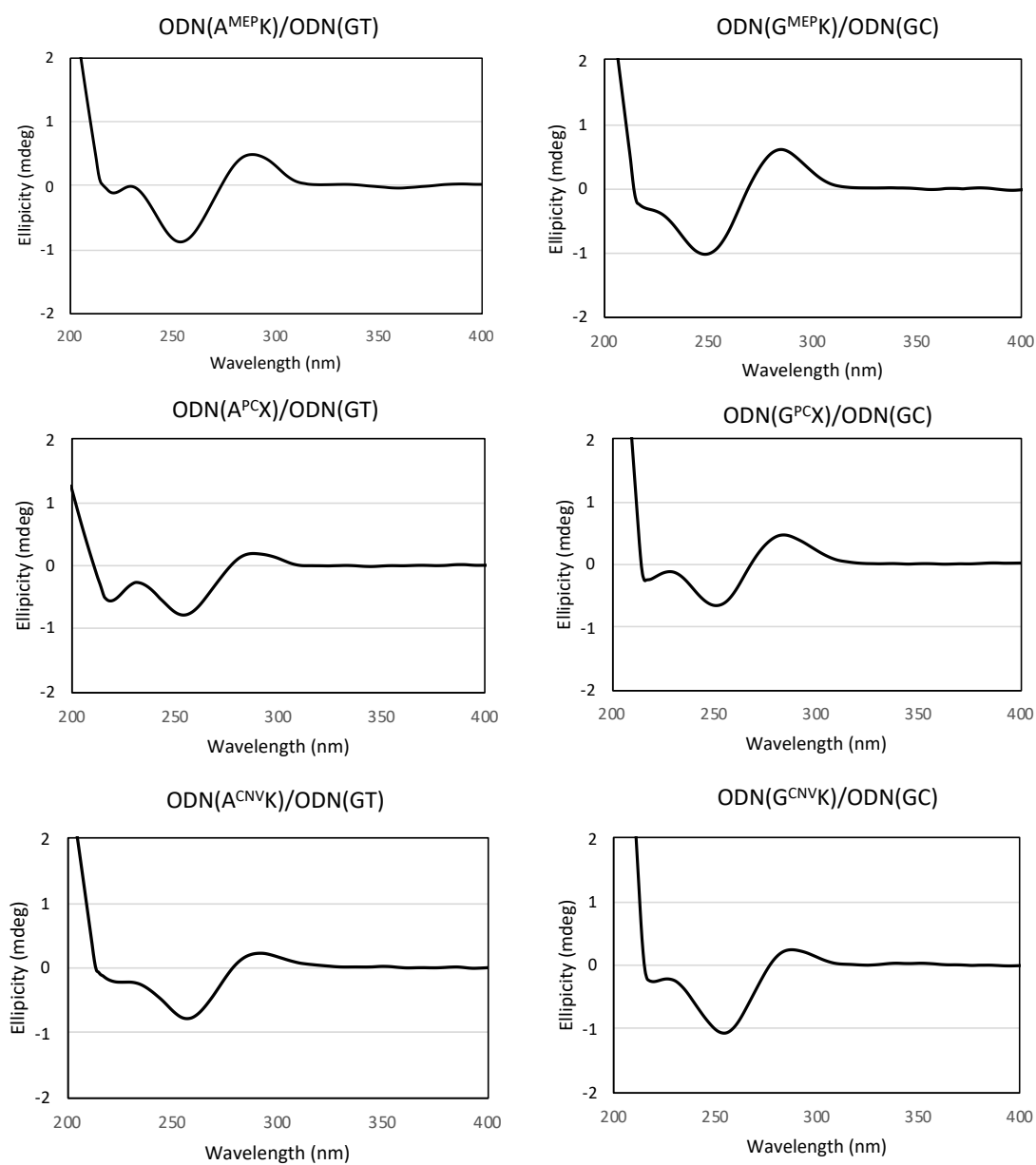


Figure S5. Circular dichroism spectra of duplexes DNA. [duplex]=10 μ M in 50 mM Na-Cacodylate buffer (pH 7.4) containing 100 mM NaCl.

6. Molecular modeling of duplexes ODN

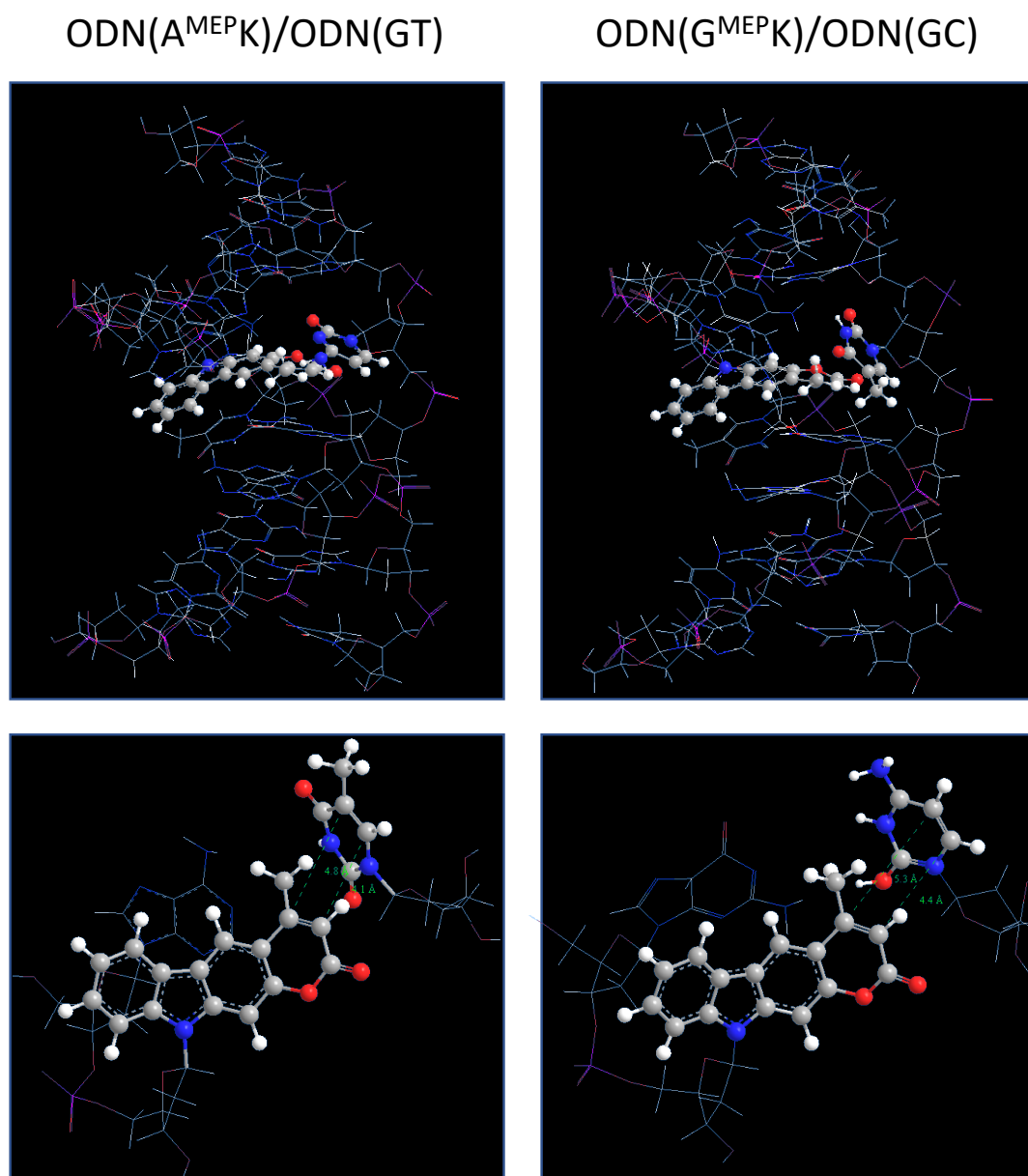


Figure S6. Molecular modeling of the ODN(A^{MEP}K)/ODN(GT) [left] and ODN(G^{MEP}K)/ODN(GC) [right] duplexes. Upper: side view of duplex; lower: top view of photo-cross-linking region.

7. UPLC analysis of photo-splitting

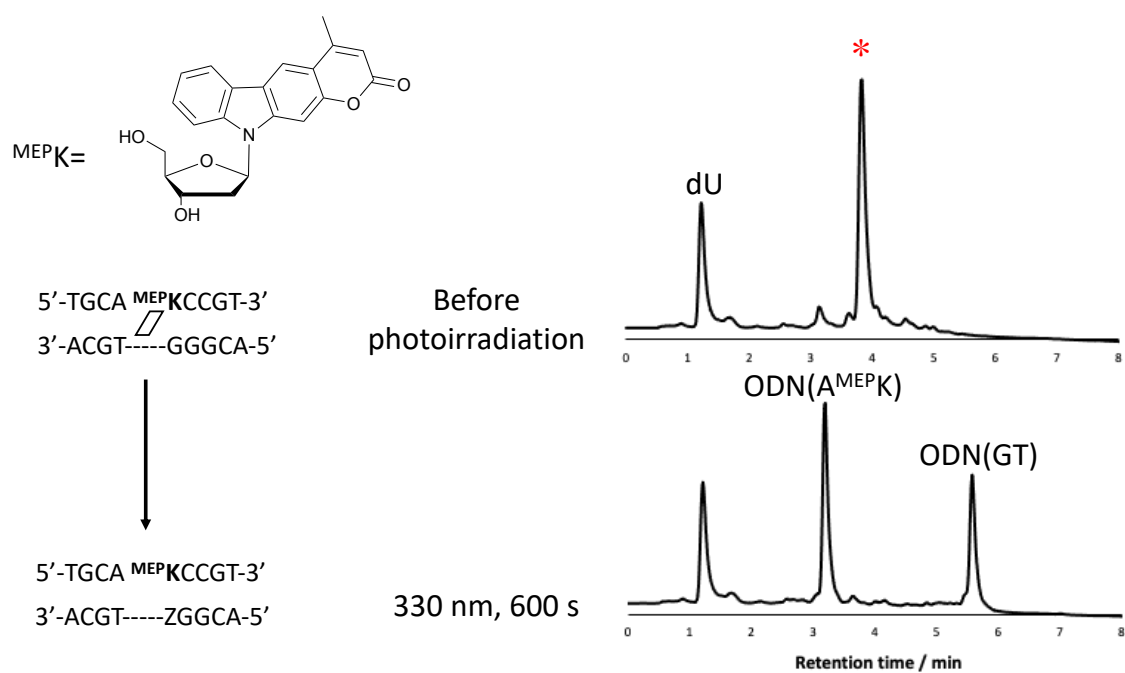


Figure S7. The photo-splitting of ^{MEPK}. The 10 μ M photoadduct in 50 mM Na-cacodylate buffer containing 100 mM NaCl was photoirradiated at 330 nm at 60 °C.

8. MALDI-TOF-MS spectra of ODNs

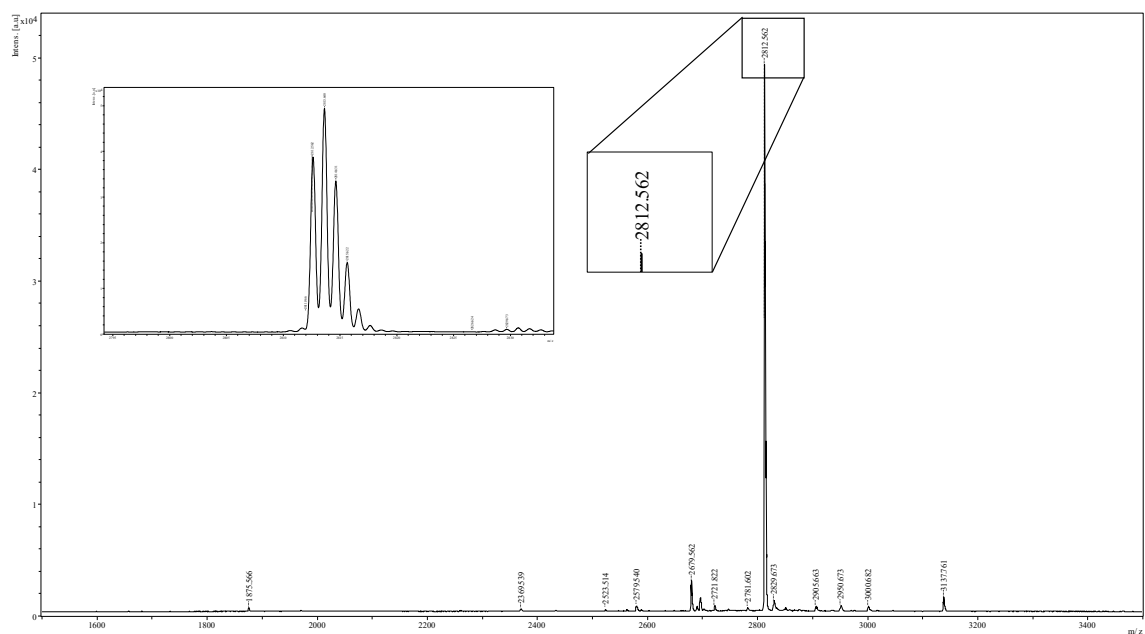


Figure S8. MALDI-TOF-MS analysis of ODN(A^{MEP}K)

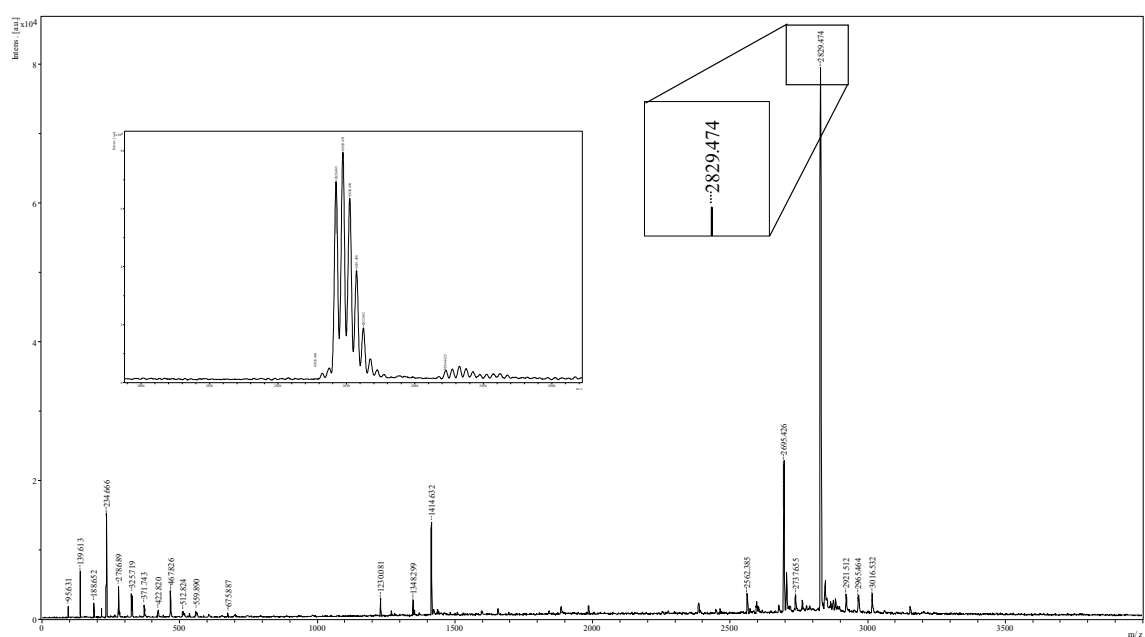


Figure S9. MALDI-TOF-MS analysis of ODN(G^{MEP}K)

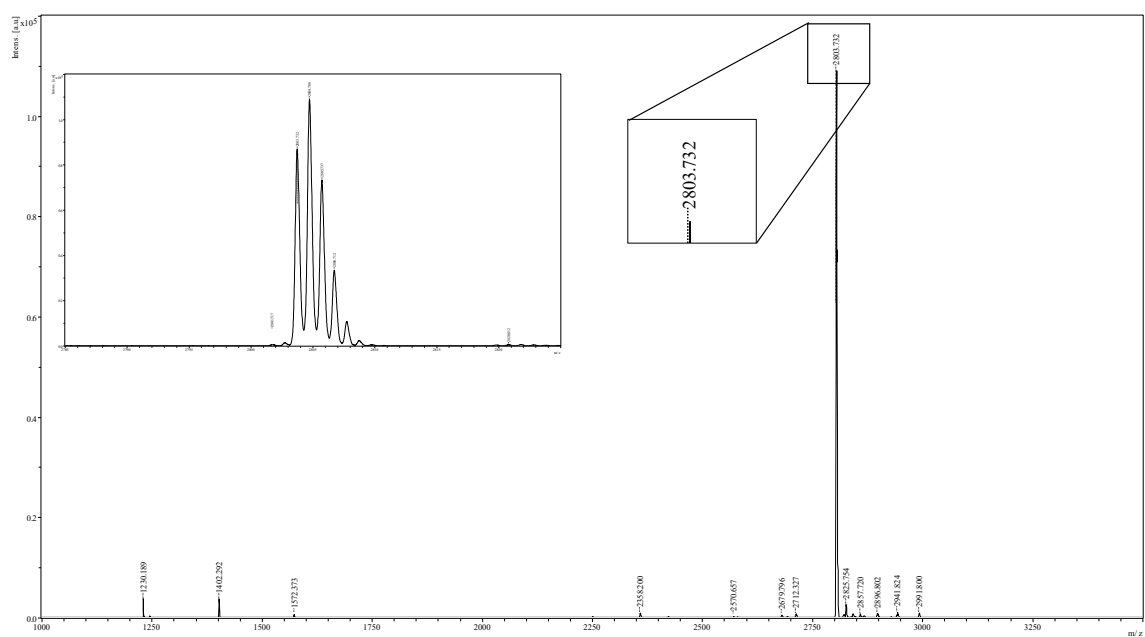


Figure S10. MALDI-TOF-MS analysis of ODN(T^{MEP}K)

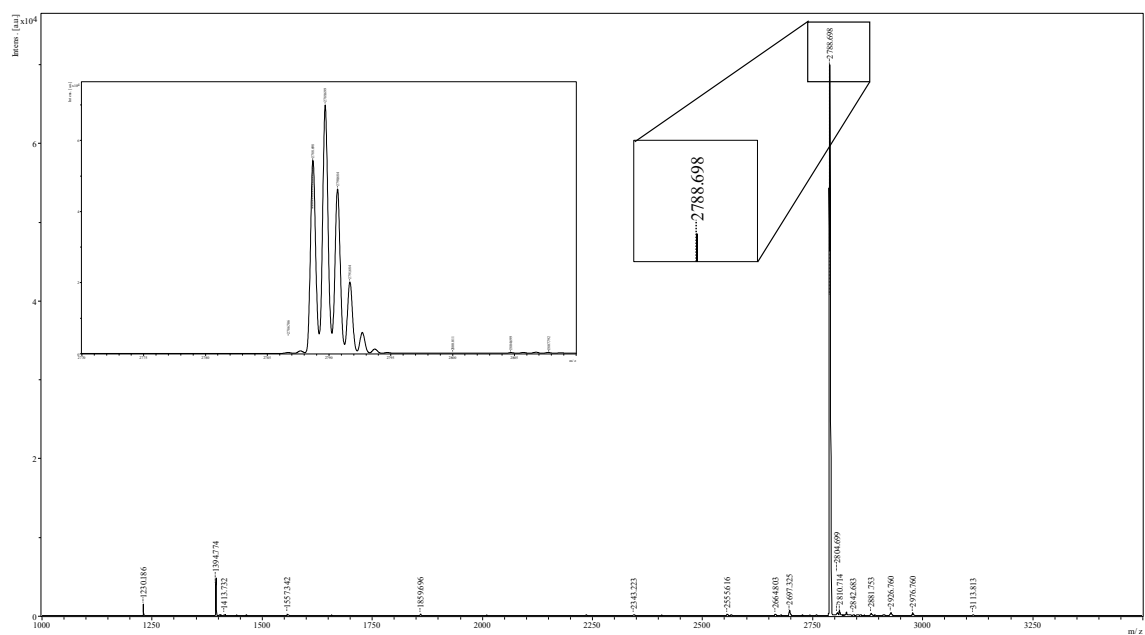


Figure S11. MALDI-TOF-MS analysis of ODN(C^{MEP}K)

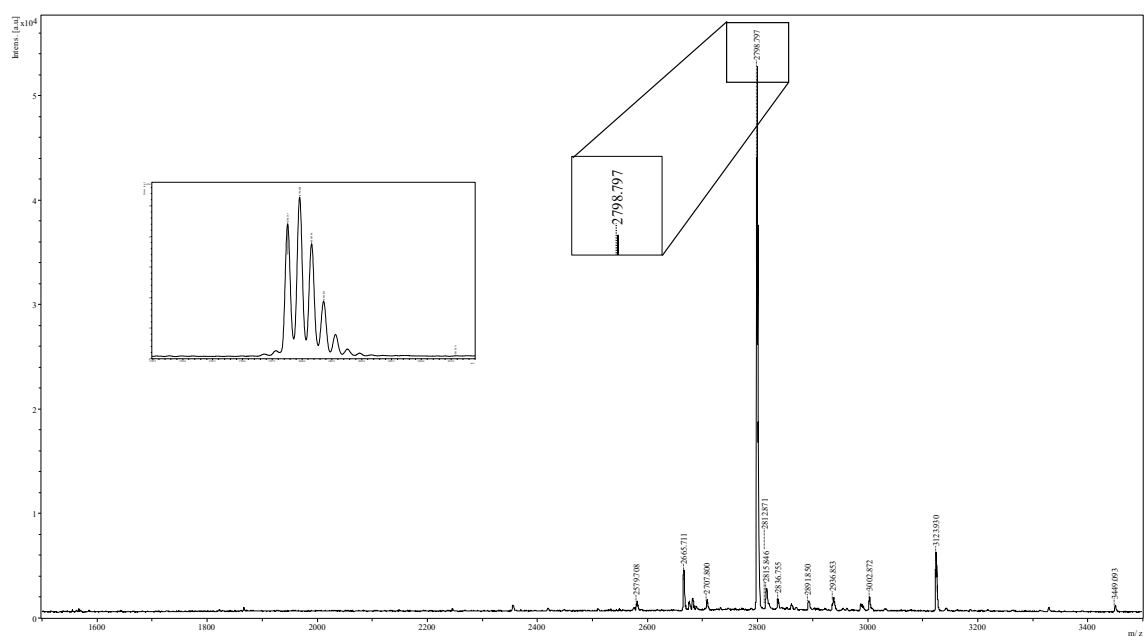


Figure S12. MALDI-TOF-MS analysis of ODN(A^{PC}X)

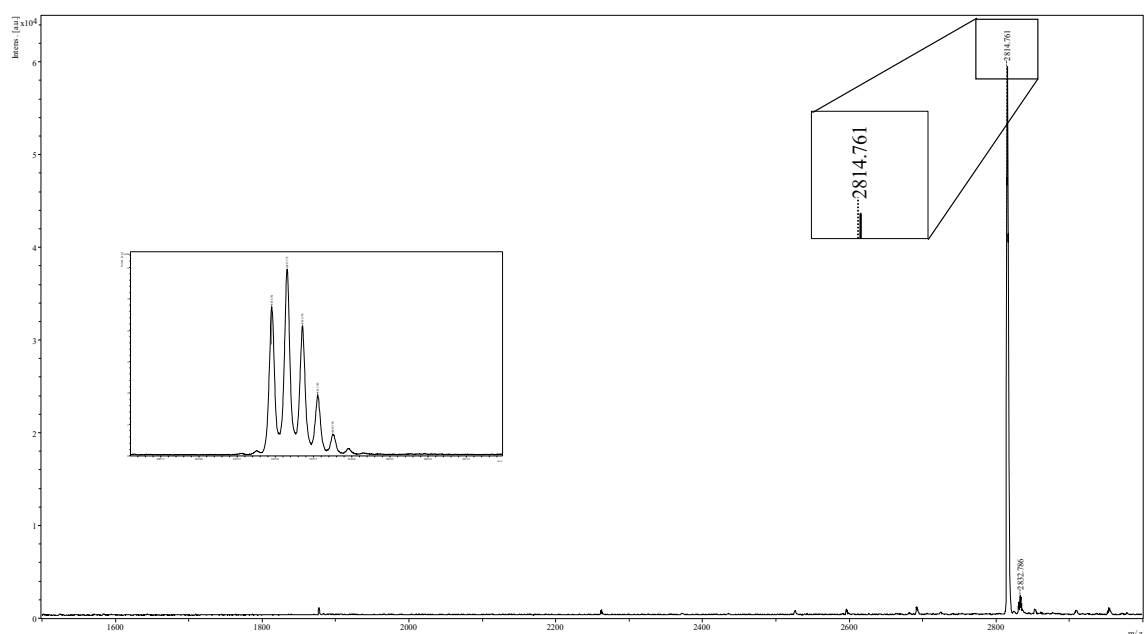
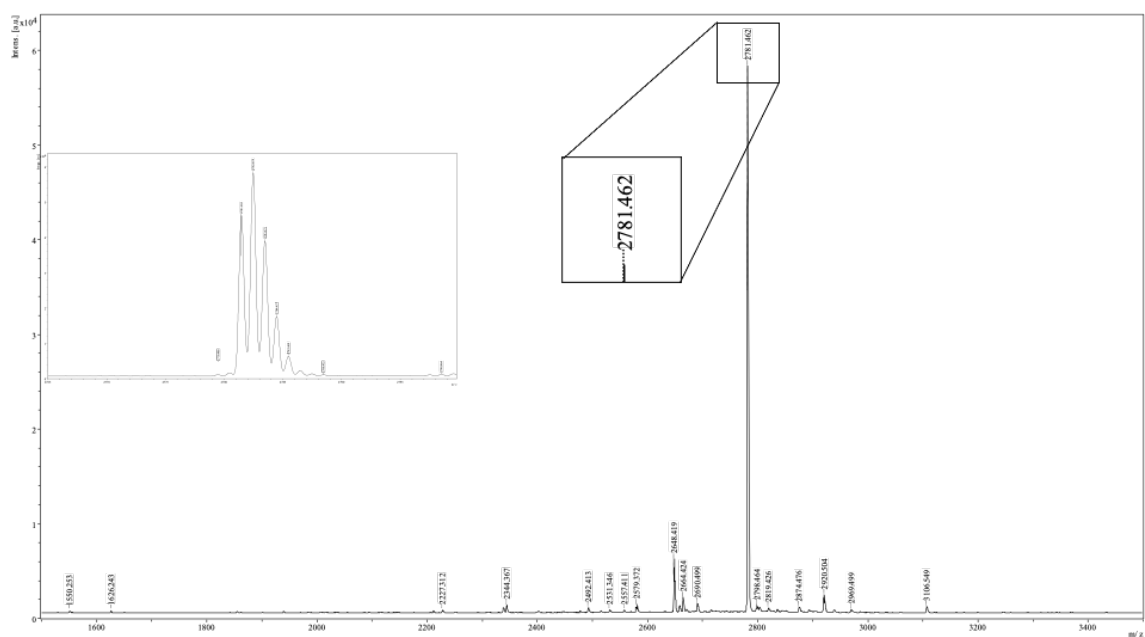


Figure S13. MALDI-TOF-MS analysis of ODN(G^{PC}X)



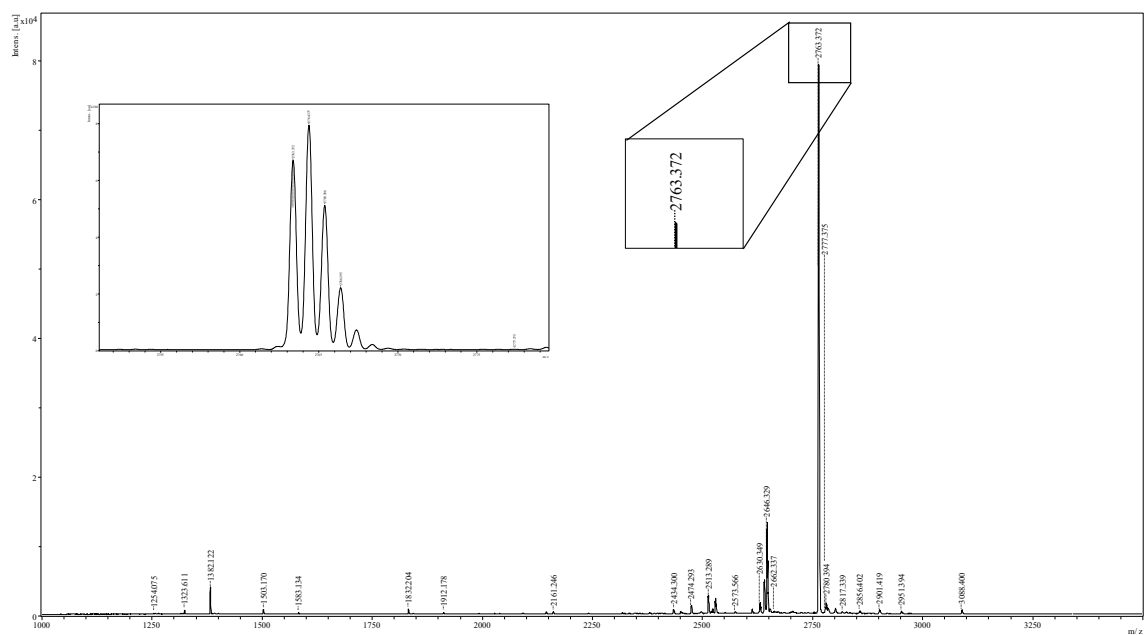


Figure S16. MALDI-TOF-MS analysis of ODN(GT)

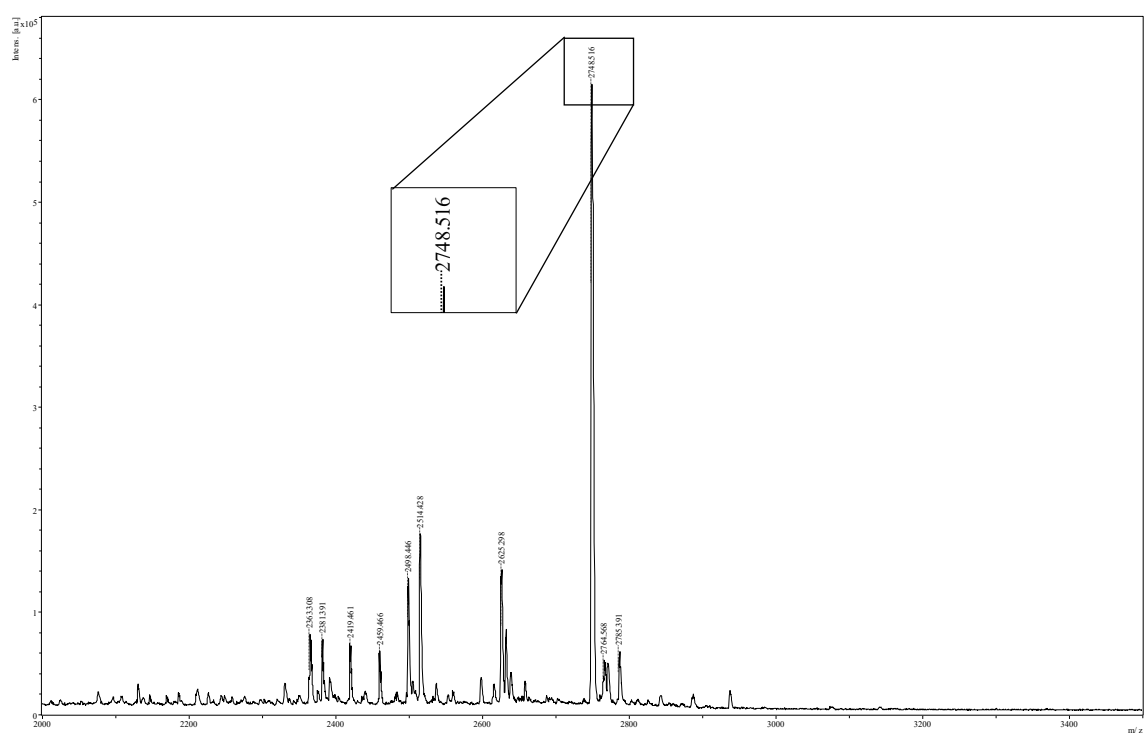


Figure S17. MALDI-TOF-MS analysis of ODN(GC)

9. NMR spectra and ESI-FT-ICR MS analysis of synthesized compound

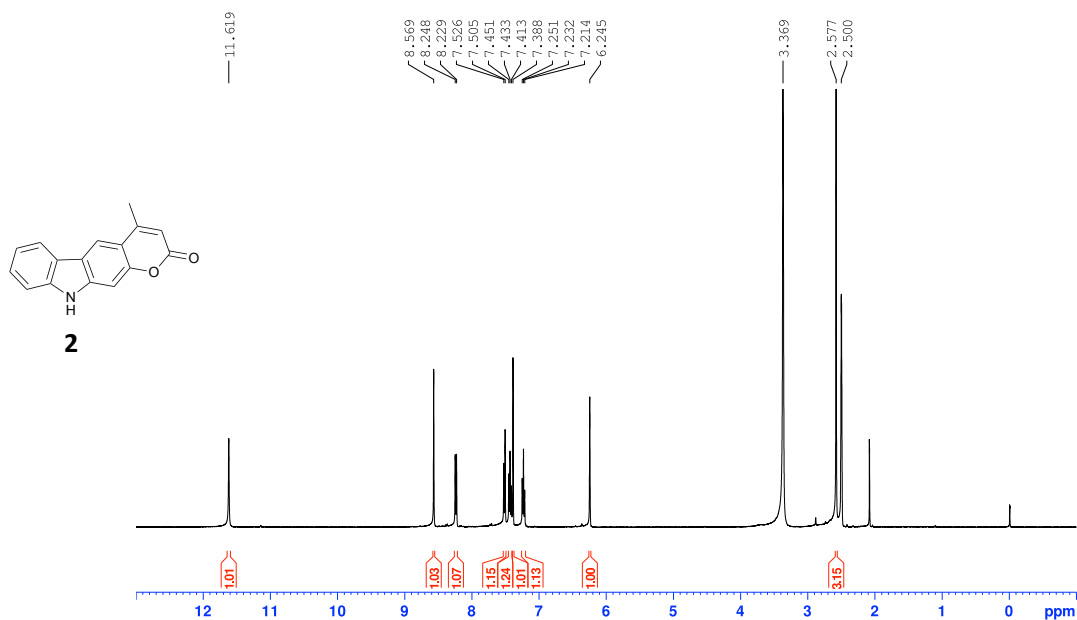


Figure S18. ¹H-NMR spectra of 4-methylpyrano[2,3-b]carbazol-2(10H)-one (2)

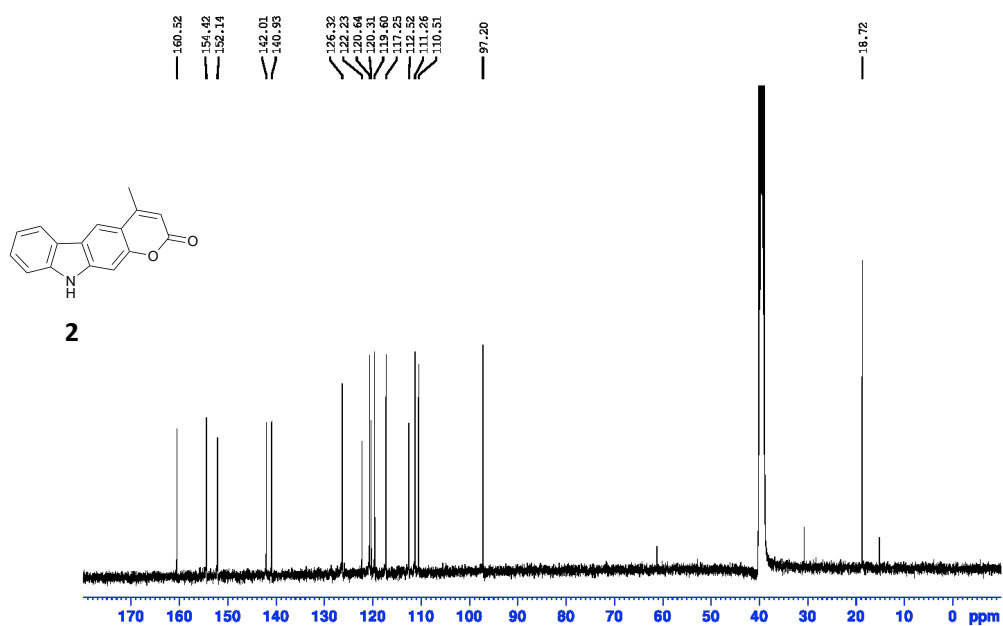


Figure S19. ¹³C-NMR spectra of 4-methylpyrano[2,3-b]carbazol-2(10H)-one (2)

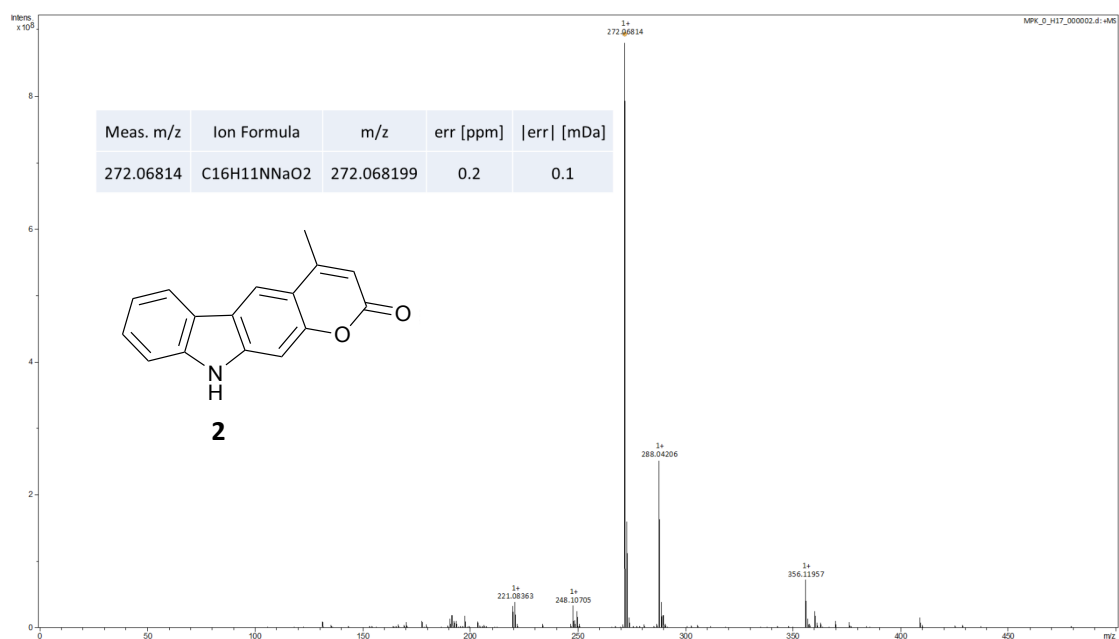


Figure S20. ESI-FT-ICR MS analysis of 4-methylpyrano[2,3-b]carbazol-2(10H)-one (**2**)

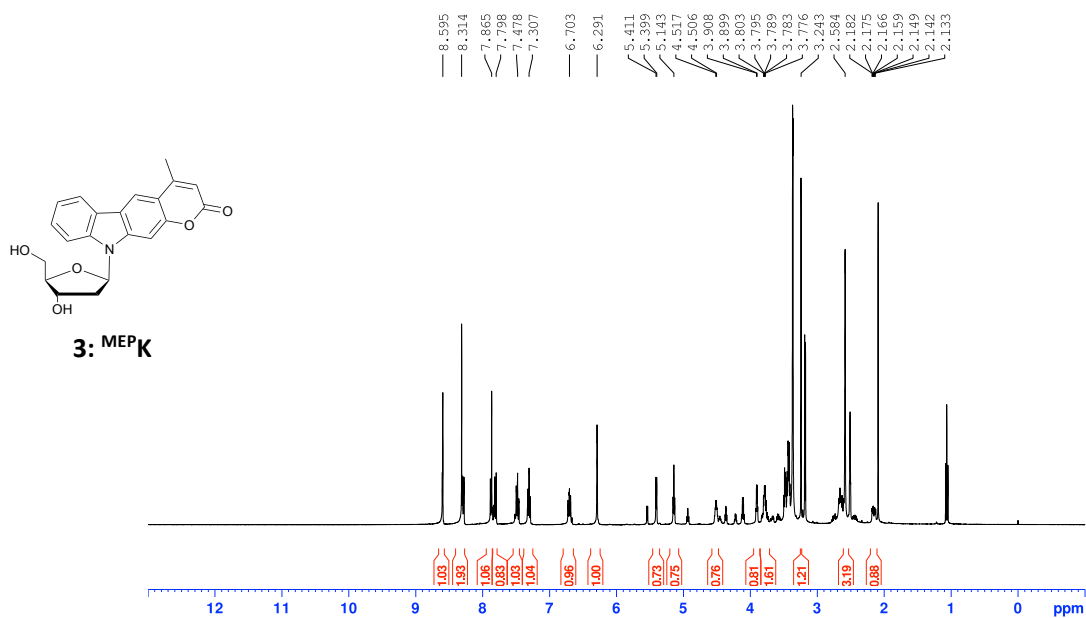


Figure S21. ¹H-NMR spectra of 10-(2-Deoxy-β-D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**3**): Me₂SO

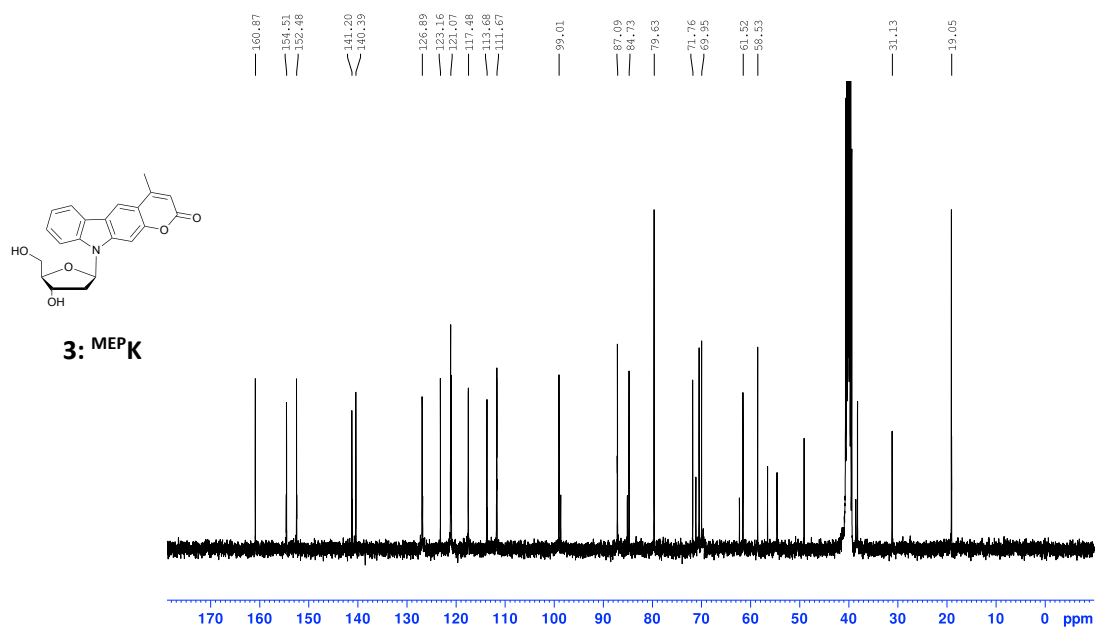


Figure S22. ¹³C-NMR spectra of 10-(2-Deoxy-β-D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**3**): ^{MEPK}

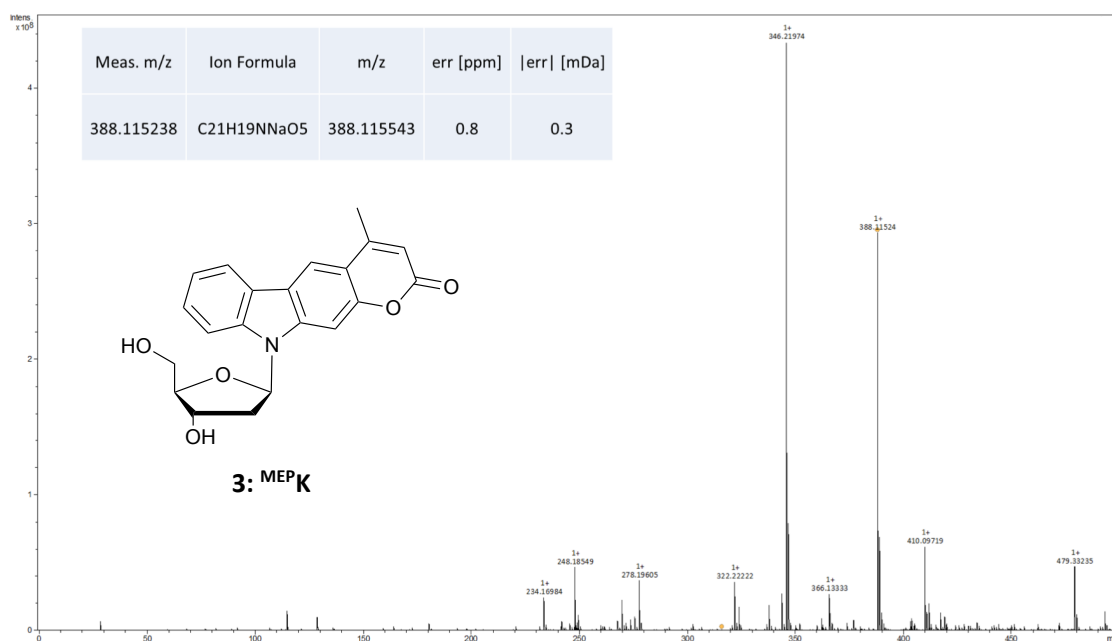


Figure S23. ESI-FT-ICR MS analysis of 10-(2-Deoxy-β-D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**3**): ^{MEPK}

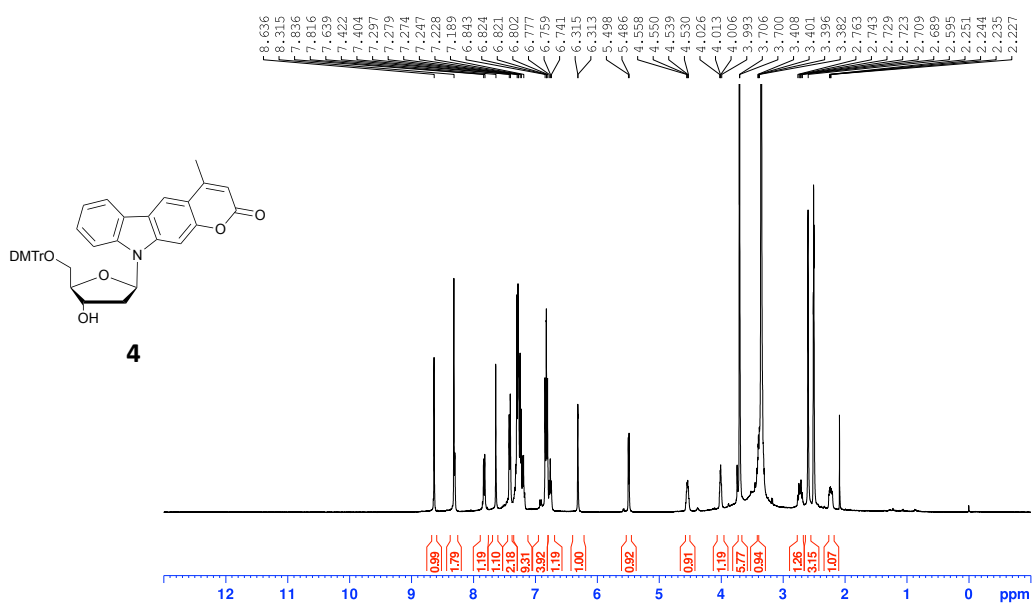


Figure S24. ¹H-NMR spectra of 5'-O-(Dimethoxytrityl)-10-(2-Deoxy-β-D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**4**)

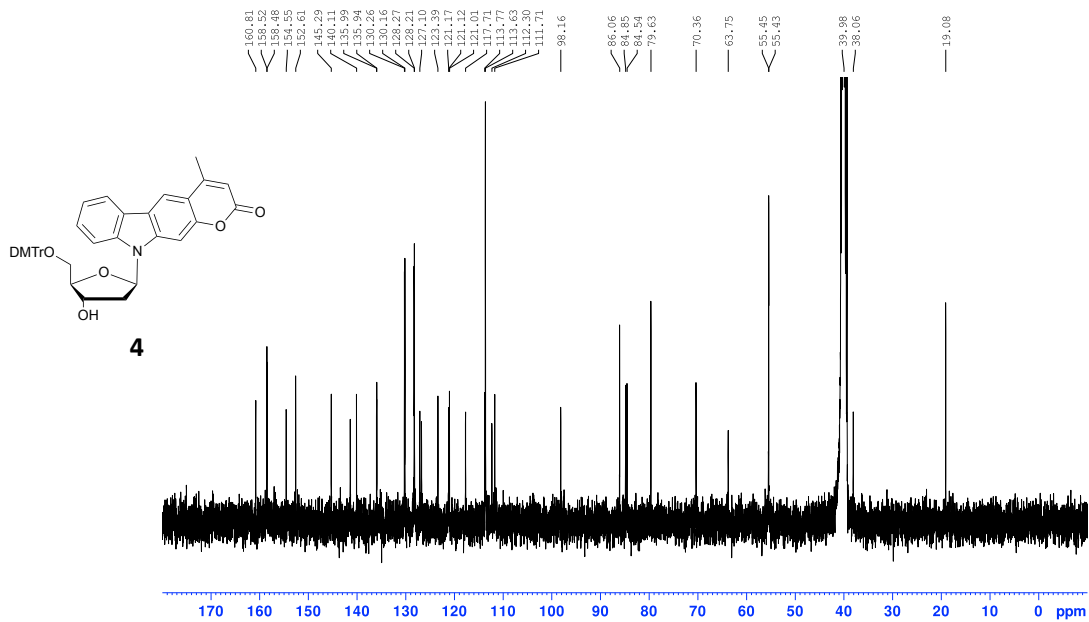


Figure S25. ¹³C-NMR spectra of 5'-O-(Dimethoxytrityl)-10-(2-Deoxy-β-D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**4**)

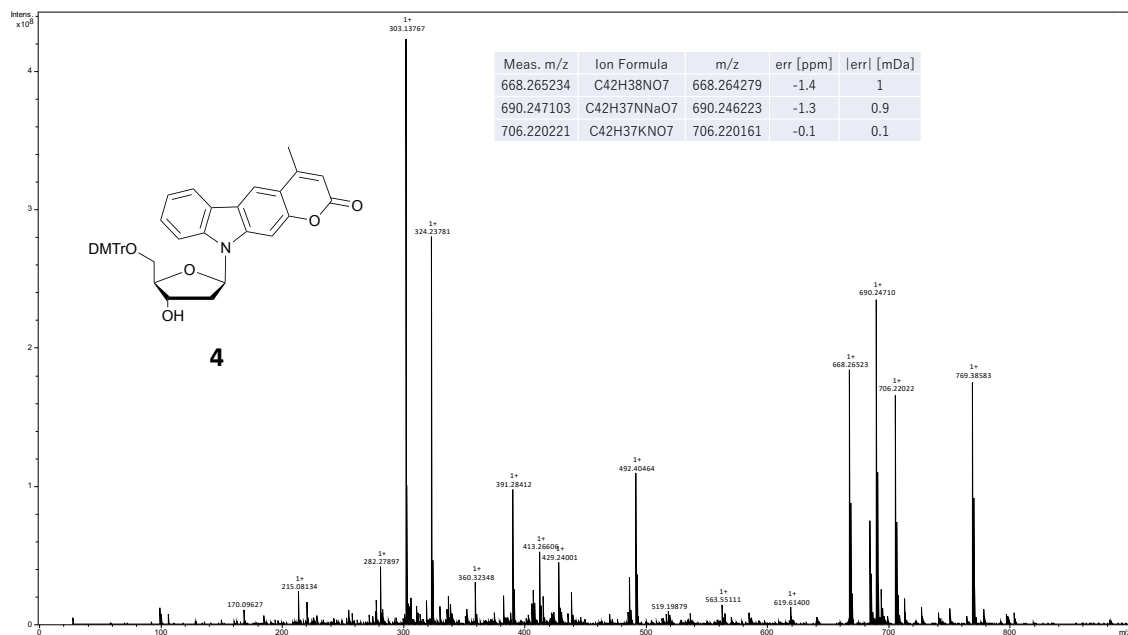


Figure S26. ESI-FT-ICR MS analysis of 5'-O-(Dimethoxytrityl)-10-(2-Deoxy- β -D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one (**4**)

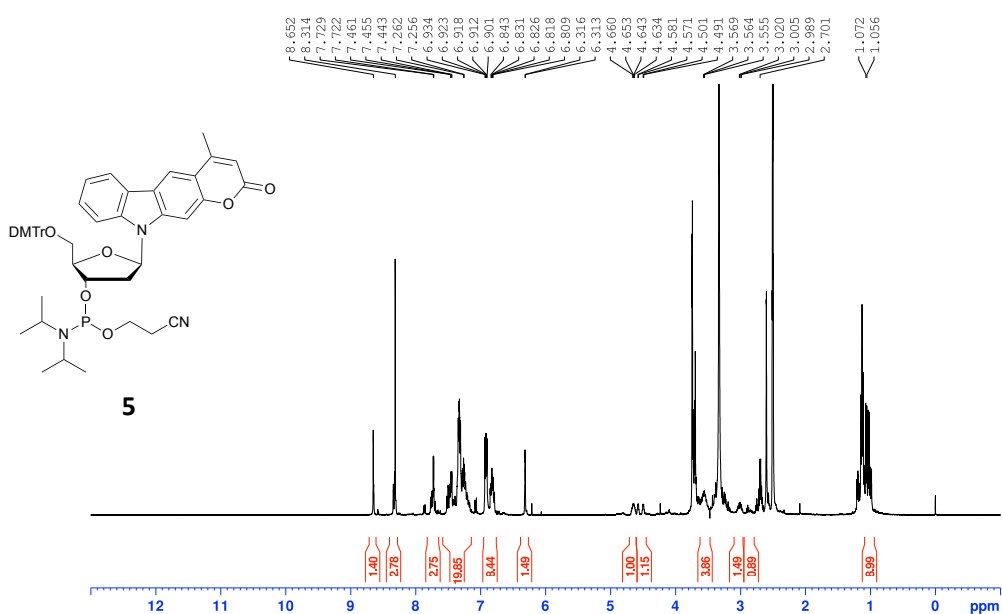
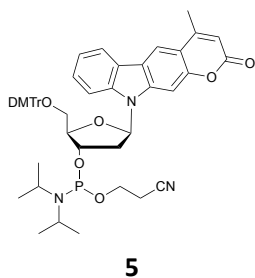
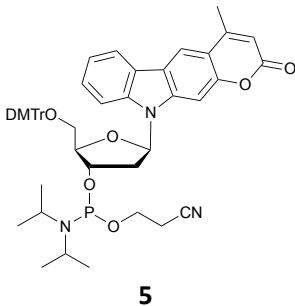


Figure S27. ^1H -NMR spectra of 5'-O-(Dimethoxytrityl)-10-(2-Deoxy- β -D-ribofuranosyl)-4-methylpyrano[2,3-b]carbazol-2(10H)-one 3'-O-(2-cyanoethyl-*N,N'*-diisopropyl)phosphoramidite (**5**)



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