Supplementary Materials

Figure S1. Spectrofluorimetric titration of 2 ($2.0 \times 10^{-3}$ M) with CT DNA of increasing volume (0–450 μL, only 0, 100, 200, 250, 350, 400 and 450 μL are shown for clarity) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

Figure S2. Spectrofluorimetric titration of 8a ($2.0 \times 10^{-3}$ M) with CT DNA of increasing volume (0–450 μL, only 0, 100, 200, 250, 350, 400 and 450 μL are shown for clarity) are shown for clarity in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

Figure S3. Spectrofluorimetric titration of 4b ($2.0 \times 10^{-3}$ M) with CT DNA of increasing volume (0–450 μL, only 0, 50, 100, 150, 200, 250, 350, 400 and 450 μL are shown for clarity) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.
**Figure S4.** Spectrofluorimetric titration of 4c (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL, only 0, 100, 150, 200, 250, 350, 400 and 450 μL are shown for clarity) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

**Figure S5.** Spectrofluorimetric titration of 4d (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

**Figure S6.** Spectrofluorimetric titration of 8e (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.
**Figure S7.** Spectrofluorimetric titration of 8f (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

**Figure S8.** Spectrofluorimetric titration of 8g (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.

**Figure S9.** Spectrofluorimetric titration of 8h (2.0 × 10⁻³ M) with CT DNA of increasing volume (0–450 μL, only 0, 50, 150, 200, 250, 350, 400 and 450 μL are shown for clarity) in 2.5 mL Tris-HCl buffer (pH 7.2) at room temperature, ex 325 nm.
**Figure S10.** Spectrofluorimetric titration of **8i** \((2.0 \times 10^{-3} \text{ M})\) with CT DNA of increasing volume \((0, 50, 60, 70, 80, 90, 100, 110, 120, 130 \mu\text{L})\) in 2.5 mL Tris-HCl buffer \((\text{pH 7.2})\) at room temperature, ex 325 nm.

**Figure S11.** Plot of \([\text{DNA}] \times 10^5\) vs. \((F_0/F-1)\) of compound **2**.

**Figure S12.** Plot of \([\text{DNA}] \times 10^5\) vs. \((F_0/F-1)\) of compound **8a**.
Figure S13. Plot of \([\text{DNA}] \times 10^5\) vs. \((F_0/F-1)\) of compound 8b.

Figure S14. Plot of \([\text{DNA}] \times 10^5\) vs. \((F_0/F-1)\) of compound 8c.

Figure S15. Plot of \([\text{DNA}] \times 10^5\) vs. \((F_0/F-1)\) of compound 8d.
Figure S16. Plot of [$\text{DNA}] \times 10^5$ vs. $(F_0/F-1)$ of compound 8e.

Figure S17. Plot of [$\text{DNA}] \times 10^5$ vs. $(F_0/F-1)$ of compound 8f.

Figure S18. Plot of [$\text{DNA}] \times 10^5$ vs. $(F_0/F-1)$ of compound 8g.
**Figure S19.** Plot of $[\text{DNA}] \times 10^5$ vs. $(F_0/F-1)$ of compound 8h.

**Figure S20.** Plot of $[\text{DNA}] \times 10^5$ vs. $(F_0/F-1)$ of compound 8i.

**Figure S21.** Plot of $\lg[\text{DNA}]$ vs. $\lg(F_0/F-1)$, $K_b = 4.56 \times 10^2$ M$^{-1}$ of compound 2.
Figure S22. Plot of $\lg[DNA]$ vs. $\lg(F_0/F-1)$, $K_b = 2.44 \times 10^2$ M$^{-1}$ of compound 8a.

Figure S23. Plot of $\lg[DNA]$ vs. $\lg(F_0/F-1)$, $K_b = 77.5$ M$^{-1}$ of compound 8b.

Figure S24. Plot of $\lg[DNA]$ vs. $\lg(F_0/F-1)$, $K_b = 1.30 \times 10^2$ M$^{-1}$ of compound 8c.
Figure S25. Plot of $\lg[\text{DNA}]$ vs. $\lg(F_0/F-1)$, $K_b = 5.91 \times 10^2 \text{ M}^{-1}$ of compound 8d.

Figure S26. Plot of $\lg[\text{DNA}]$ vs. $\lg(F_0/F-1)$, $K_b = 1.37 \times 10^2 \text{ M}^{-1}$ of compound 8e.

Figure S27. Plot of $\lg[\text{DNA}]$ vs. $\lg(F_0/F-1)$, $K_b = 1.16 \times 10^4 \text{ M}^{-1}$ of compound 8f.
Figure S28. Plot of \( \text{lg}[\text{DNA}] \) vs. \( \text{lg}(F_0/F-1) \), \( K_b = 5.76 \times 10^2 \text{ M}^{-1} \) of compound 8g.

Figure S29. Plot of \( \text{lg}[\text{DNA}] \) vs. \( \text{lg}(F_0/F-1) \), \( K_b = 7.38 \times 10^5 \text{ M}^{-1} \) of compound 8h.

Figure S30. Plot of \( \text{lg}[\text{DNA}] \) vs. \( \text{lg}(F_0/F-1) \), \( K_b = 1.24 \times 10^4 \text{ M}^{-1} \) of compound 8i.
**Figure S31.** Emission spectra of DNA-GelRed (165 μM), in the presence of 0, 40, 80, 120, 160, 200, 240, 280, 320, 360 and 400 μM of compound 8f. Arrow indicates the changes in the emission intensity as a function of compound concentration. Inset: SterneVolmer plot of the fluorescence titration data corresponding to the compound 8f.

**Figure S32.** Emission spectra of DNA-GelRed (165 μM), in the presence of 0, 15, 30, 45, 60, 75, 90, 105 and 120 μM of compound 8h. Arrow indicates the changes in the emission intensity as a function of compound concentration. Inset: SterneVolmer plot of the fluorescence titration data corresponding to the compound 8h.

**Figure S33.** CD spectra of CT-DNA (3 mL solution, 1.5 × 10⁻⁴ M) in the absence and presence of compound 8f (1.5 × 10⁻⁵ M).
Figure S34. CD spectra of CT-DNA (3 mL solution, $1.5 \times 10^{-4}$ M) in the absence and presence of compound 8h ($1.5 \times 10^{-5}$ M).

$^1$H-NMR (500 MHz, CDCl$_3$) for compound 3: $\delta$ 7.42 (d, $J = 8.8$ Hz, 1H), 6.75 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.70 (d, $J = 2.5$ Hz, 1H), 6.09 (d, $J = 1.1$ Hz, 1H), 4.27 (t, $J = 6.3$ Hz, 2H), 2.76 (t, $J = 6.3$ Hz, 2H), 2.34 (d, $J = 1.1$ Hz, 3H).

Figure S35. Spectrum of compound 3.
$^1$H-NMR (500 MHz, CDCl$_3$) for compound 8a: $\delta$ 7.53–7.49 (m, 2H), 7.42 (d, $J = 8.8$ Hz, 1H), 7.29 (qd, $J = 7.9$, 1.3 Hz, 3H), 6.75 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.70 (d, $J = 2.5$ Hz, 1H), 6.09 (d, $J = 1.1$ Hz, 1H), 5.61 (dd, $J = 21.0$, 9.7 Hz, 1H), 4.30–4.23 (m, 2H), 4.18–3.59 (m, 4H), 2.76 (t, $J = 6.3$ Hz, 2H), 2.34 (d, $J = 1.1$ Hz, 3H), 1.31 (t, $J = 7.1$ Hz, 3H), 1.05 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) $\delta$ (ppm) 21.49 (s). HRMS for C$_{24}$H$_{29}$NO$_7$P ([M + H]$^+$): calcd 474.16816: found 474.16656.

Figure S36. Spectrum of compound 8a.
$^1$H-NMR (500 MHz, CDCl₃) for compound 8b: δ (ppm) 8.30 (d, $J = 7.4$ Hz, 1H), 7.46 (ddd, $J = 8.6$, 5.1, 2.0 Hz, 2H), 7.41 (d, $J = 8.8$ Hz, 1H), 6.97 (t, $J = 8.6$ Hz, 2H), 6.73 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.70 (d, $J = 2.4$ Hz, 1H), 6.08 (d, $J = 1.1$ Hz, 1H), 5.56 (dd, $J = 21.0$, 9.6 Hz, 1H), 4.25 (ddd, $J = 15.5$, 9.3, 3.1 Hz, 2H), 4.18–3.65 (m, 4H), 2.74 (t, $J = 6.2$ Hz, 2H), 2.34 (d, $J = 1.1$ Hz, 3H), 1.29 (t, $J = 7.1$ Hz, 3H), 1.07 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl₃) δ (ppm) 21.20 (d, $J = 4.3$ Hz). HRMS for C$_{24}$H$_{28}$NO$_7$ FP ([M + H]$^+$): calcd 492.15874; found 492.15732.

Figure S37. Spectrum of compound 8b.
$^1$H-NMR (500 MHz, CDCl$_3$) for compound 8c: $\delta$ (ppm) 8.01 (s, 1H), 7.47 (d, $J = 8.8$ Hz, 1H), 7.42–7.21 (m, 4H), 6.81 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.75 (d, $J = 2.4$ Hz, 1H), 6.22–6.16 (m, 1H), 6.14 (s, 1H), 4.36–4.30 (m, 2H), 4.30–3.64 (m, 4H), 2.79 (td, $J = 6.1$, 2.6 Hz, 2H), 2.39 (d, $J = 0.8$ Hz, 3H), 1.36 (t, $J = 7.1$ Hz, 3H), 1.06 (t, $J = 7.0$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) $\delta$ (ppm) 20.72(s). HRMS for C$_{24}$H$_{28}$NO$_7$ PCl ([M + H]$^+$): calcd 508.12919; found 508.12781.

Figure S38. Spectrum of compound 8c.
\(^1\)H-NMR (500 MHz, CDCl\(_3\)) for compound 8d: \(\delta\) (ppm) 8.21 (s, 1H), 7.46 (dd, \(J = 8.5\), 2.2 Hz, 1H), 7.42 (d, \(J = 8.3\) Hz, 2H), 7.29 (dd, \(J = 8.3\), 1.6 Hz, 2H), 6.78 (d, \(J = 2.5\) Hz, 1H), 6.76 (s, 1H), 6.13 (d, \(J = 1.0\) Hz, 1H), 5.58 (dd, \(J = 21.3, 9.5\) Hz, 1H), 4.40–4.23 (m, 2H), 4.21–3.72 (m, 4H), 2.78 (t, \(J = 6.0\) Hz, 2H), 2.38 (d, \(J = 1.0\) Hz, 3H), 1.32 (t, \(J = 7.0\) Hz, 3H), 1.12 (dd, \(J = 7.7, 6.4\) Hz, 3H). \(^{31}\)P-NMR (202 MHz, CDCl\(_3\)) \(\delta\) (ppm) 21.21 (s). HRMS for C\(_{24}\)H\(_{28}\)NO\(_7\) PCl ([M + H]\(^+\)): calcd 508.12919; found 508.12775.

**Figure S39.** Spectrum of compound 8d.
$^1$H-NMR (500 MHz, CDCl$_3$) for compound 8e: $\delta$ (ppm) 8.67 (s, 1H), 7.75 (d, $J = 7.8$ Hz, 1H), 7.53 (d, $J = 8.0$ Hz, 1H), 7.40 (dd, $J = 8.8$, 1.2 Hz, 1H), 7.27 (dd, $J = 12.7$, 5.2 Hz, 1H), 7.12 (dd, $J = 11.0$, 4.3 Hz, 1H), 6.73 (d, $J = 8.8$, 2.4 Hz, 1H), 6.67 (d, $J = 2.3$ Hz, 1H), 6.20 (dd, $J = 21.0$, 9.3 Hz, 1H), 6.07 (s, 1H), 4.34–4.23 (m, 2H), 4.24–3.58 (m, 4H), 2.77 (q, $J = 6.1$ Hz, 2H), 2.33 (s, 3H), 1.34 (t, $J = 7.1$ Hz, 3H), 1.02 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) $\delta$ (ppm) 20.85 (s). HRMS for C$_{24}$H$_{28}$NO$_7$PBr ([M + H$^+$]): calcd 552.07868; found 552.07666.

Figure S40. Spectrum of compound 8e.
$^1$H-NMR (500 MHz, CDCl$_3$) for compound 8f: $\delta$ (ppm) 8.36 (d, $J = 5.7$ Hz, 1H), 7.67 (d, $J = 1.5$ Hz, 1H), 7.44 (dd, $J = 15.1$, 8.4 Hz, 2H), 7.20 (t, $J = 7.8$ Hz, 1H), 6.79 (dd, $J = 8.8$, 2.4 Hz, 1H), 6.74 (d, $J = 2.4$ Hz, 1H), 6.13 (d, $J = 0.7$ Hz, 1H), 5.58 (dd, $J = 21.3$, 9.5 Hz, 1H), 4.30 (dq, $J = 9.3$, 6.4 Hz, 2H), 4.26–3.73 (m, 4H), 2.79 (t, $J = 6.1$ Hz, 2H), 2.38 (d, $J = 0.5$ Hz, 3H), 1.33 (t, $J = 7.1$ Hz, 3H), 1.12 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) $\delta$ (ppm) 21.71 (s). HRMS for C$_{24}$H$_{28}$NO$_7$PBr ([M + H]$^+$): calcd 552.07868; found 552.07642.

Figure S41. Spectrum of compound 8f.
$^1$H-NMR (500 MHz, CDCl$_3$) for compound 8g: $\delta$ (ppm) 8.23 (dd, $J$ = 9.5, 4.1 Hz, 1H), 7.43 (d, $J$ = 8.1 Hz, 2H), 7.41 (s, 1H), 7.33 (dd, $J$ = 8.5, 2.0 Hz, 2H), 6.75 dd, $J$ = 8.8, 2.4 Hz, 1H), 6.73 (d, $J$ = 2.3 Hz, 1H), 6.10 (d, $J$ = 1.2 Hz, 1H), 5.54 (dd, $J$ = 21.3, 9.5 Hz, 1H), 4.32–4.21 (m, 2H), 4.19–3.70 (m, 4H), 2.75 (t, $J$ = 6.1 Hz, 2H), 2.35 (d, $J$ = 1.2 Hz, 3H), 1.29 (t, $J$ = 7.1 Hz, 3H), 1.09 (t, $J$ = 7.1 Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) $\delta$ (ppm) 20.87 (s). HRMS for C$_{24}$H$_{28}$NO$_7$PBr ([M + H]$^+$): calcd 552.07868; found 552.07629.

Figure S42. Spectrum of compound 8g.
$^1$H-NMR (500 MHz, CDCl₃) for complex 8h: δ (ppm) 8.08 (dd, $J = 9.7$, 2.9 Hz, 1H), 7.57–7.45 (m, 1H), 7.39 (d, $J = 8.8$ Hz, 1H), 7.24–7.18 (m, 1H), 6.91–6.81 (m, 2H), 6.74 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.68 (d, $J = 2.5$ Hz, 1H), 6.14–6.08 (m, 1H), 6.06 (d, $J = 1.2$ Hz, 1H), 4.30–4.20 (m, 2H), 4.19–3.70 (m, 4H), 3.82 (s, 3H), 2.73 (dd, $J = 10.4$, 6.1 Hz, 2H), 2.32 (d, $J = 1.0$ Hz, 3H), 1.28 (t, $J = 7.1$ Hz, 3H), 0.98 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl₃) δ (ppm) 22.05 (s). HRMS for C₂₅H₃₁NO₈ P ([M + H]$^+$): calcd 504.17873; found 504.17688.

Figure S43. Spectrum of compound 8h.
$^1$H-NMR (500 MHz, CDCl₃) for complex 8i: δ (ppm) 8.46 (s, 1H), 7.98 (s, 1H), 7.79–7.71 (m, 3H), 7.63 (dd, $J = 8.5$, 1.4 Hz, 1H), 7.47–7.39 (m, 2H), 7.32–7.27 (m, 1H), 6.67 (d, $J = 1.3$ Hz, 1H), 6.65 (t, $J = 1.9$ Hz, 1H), 6.07 (s, 1H), 5.80 (dd, $J = 21.0$, 9.6 Hz, 1H), 4.27–3.59 (m, 6H) 2.76 (t, $J = 6.3$ Hz, 2H), 2.29 (s, 3H), 1.34 (t, $J = 7.1$ Hz, 3H), 1.02 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl₃) δ (ppm) 21.44 (s). HRMS for C₂₈H₃₁NO₇P([M + H]⁺): calcd 524.18381; found 524.18213.

Figure S44. Spectrum of compound 8i.
$^1$H-NMR (500 MHz, CDCl$_3$) for complex 8j: $^1$H-NMR (500 MHz, CDCl$_3$) δ (ppm) 8.45 (dd, $J = 9.6$, 3.4 Hz, 1H), 7.62–7.45 (m, 2H), 7.42 (d, $J = 8.8$ Hz, 1H), 7.29 (dd, $J = 7.9$, 4.1 Hz, 3H), 6.75 (dd, $J = 8.8$, 2.5 Hz, 1H), 6.70 (d, $J = 2.5$ Hz, 1H), 6.09 (d, $J = 1.1$ Hz, 1H), 4.34–4.22 (m, 2H), 4.22–3.67 (m, 4H), 2.78 (td, $J = 6.2$, 2.7 Hz, 2H), 2.34 (d, $J = 1.0$ Hz, 3H), 2.10 (d, $J = 16.1$ Hz, 1H), 1.31 (t, $J = 7.1$ Hz, 3H), 1.09 (t, $J = 7.1$ Hz, 3H). $^{31}$P-NMR (202 MHz, CDCl$_3$) δ (ppm) 21.33 (s). HRMS for C$_{25}$H$_{31}$NO$_7$P ([M + H]$^+$): calcd 488.18381; found 488.18231.

Figure S45. Spectrum of compound 8j.