

**Zinc(II) terpyridine complexes: substituent effect on
photoluminescence, antiproliferative activity and DNA interaction**

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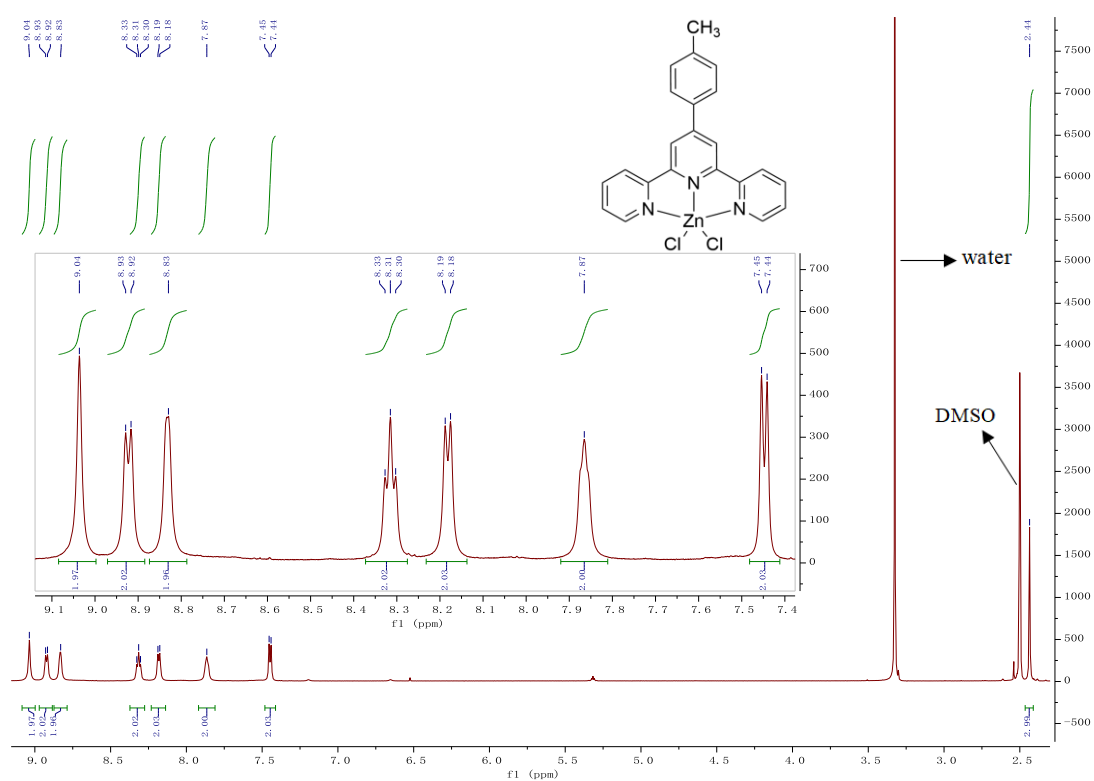


Figure S1 ^1H NMR spectrum of compound **2** in DMSO (600 MHz).

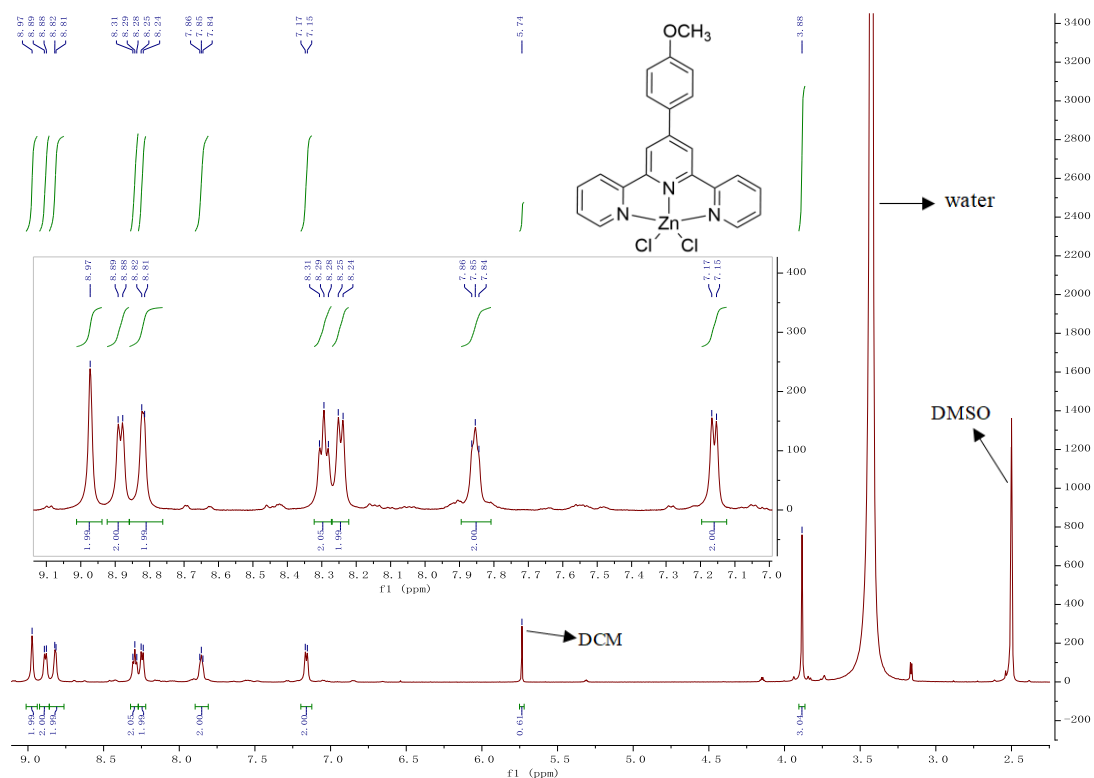


Figure S2 ^1H NMR spectrum of compound **3** in DMSO (600 MHz).

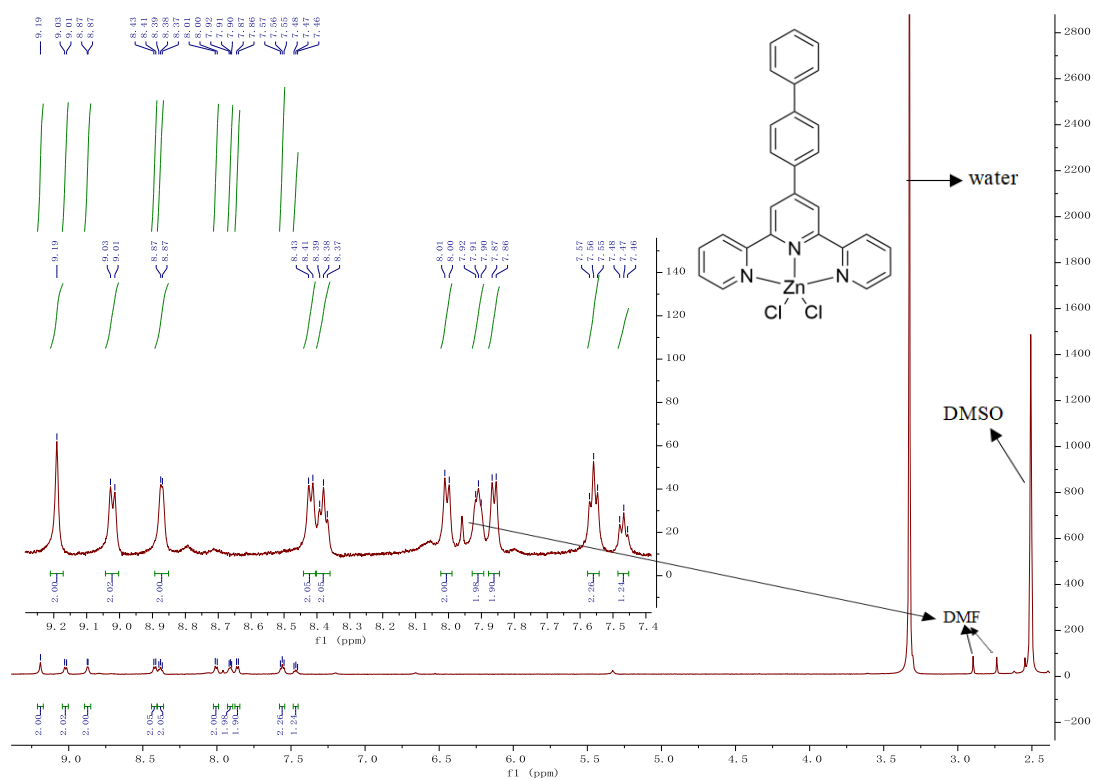


Figure S3 ^1H NMR spectrum of compound **4** in DMSO (600 MHz).

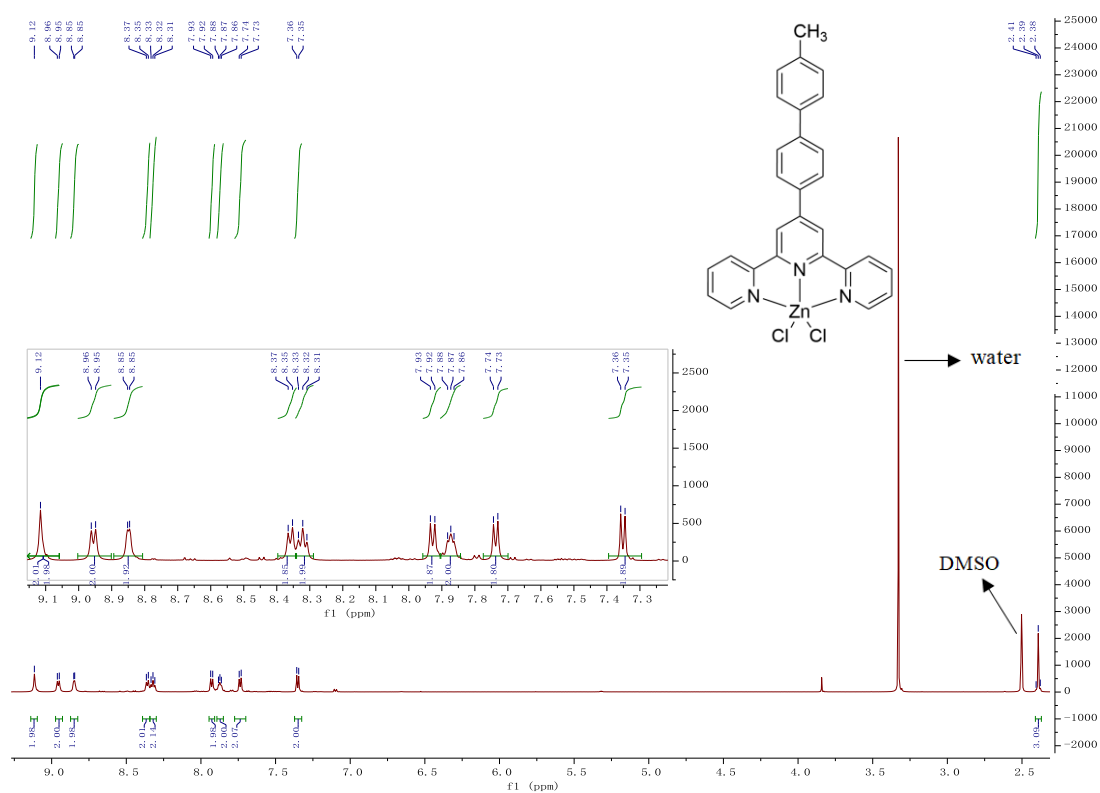


Figure S4 ^1H NMR spectrum of compound **5** in DMSO (600 MHz).

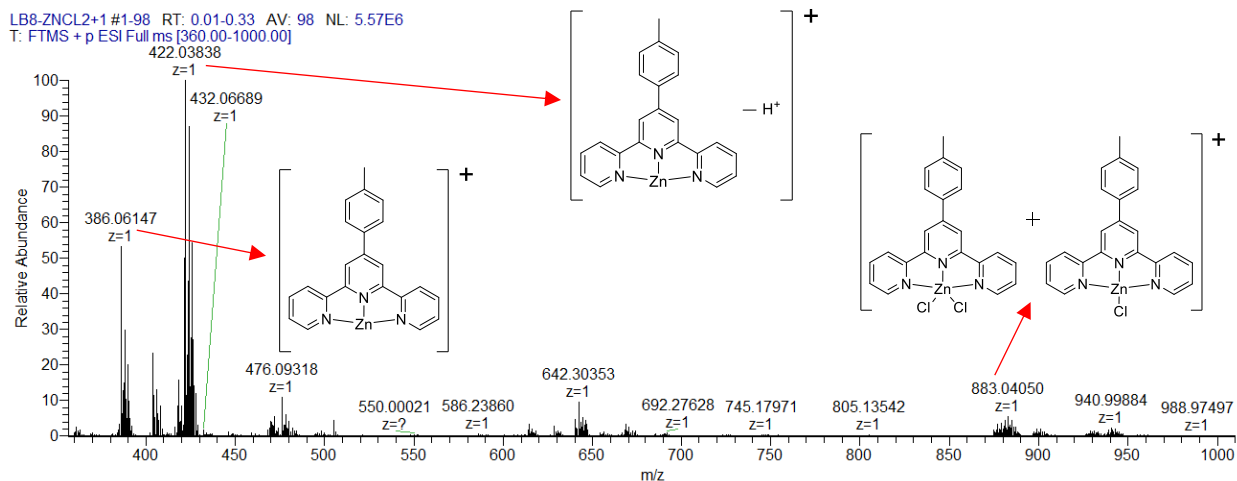


Figure S7 The ESI-MS spectrum of compound 2.

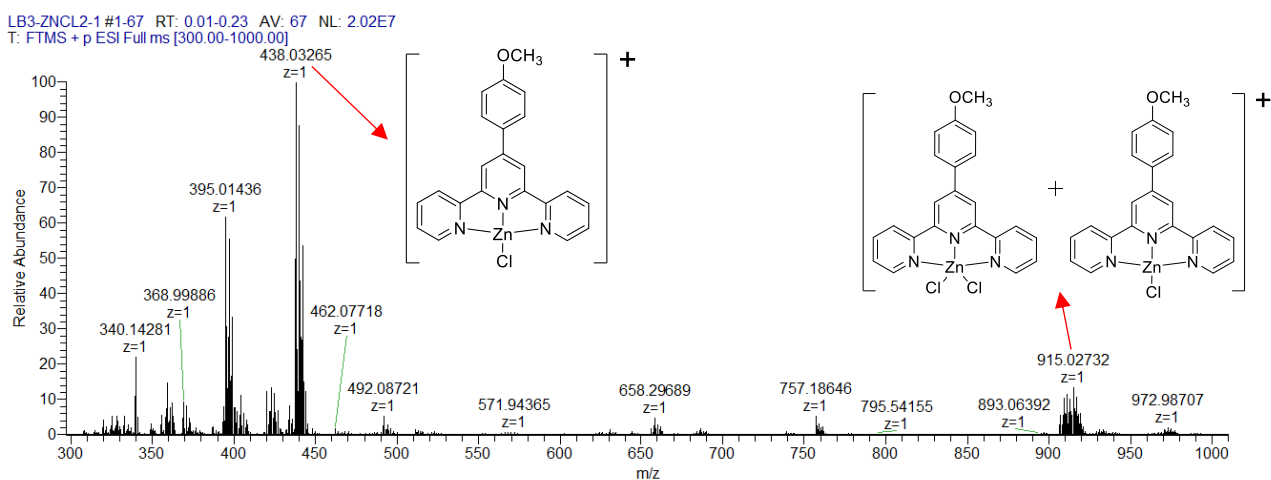


Figure S8 The ESI-MS spectrum of compound 3.

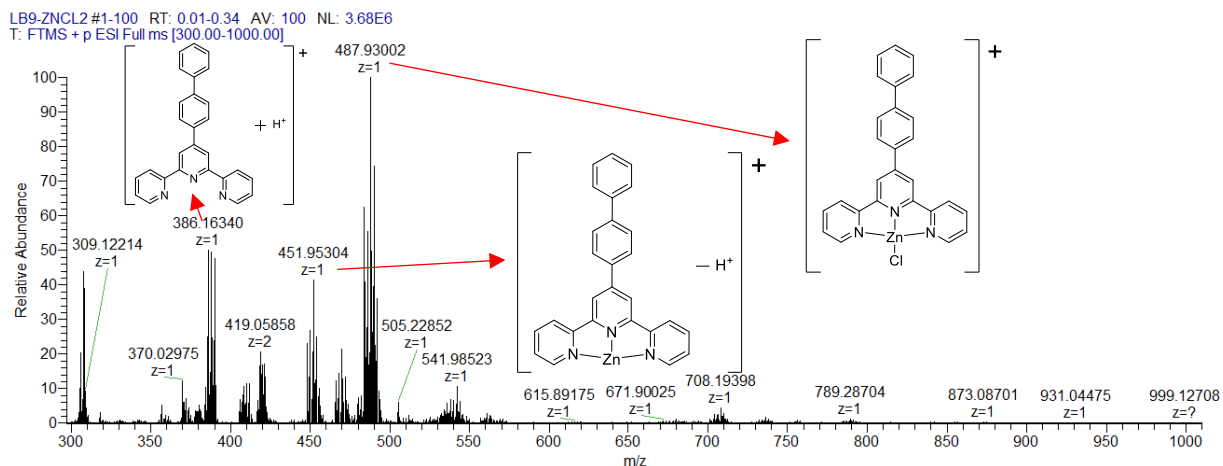


Figure S9 The ESI-MS spectrum of compound 4.

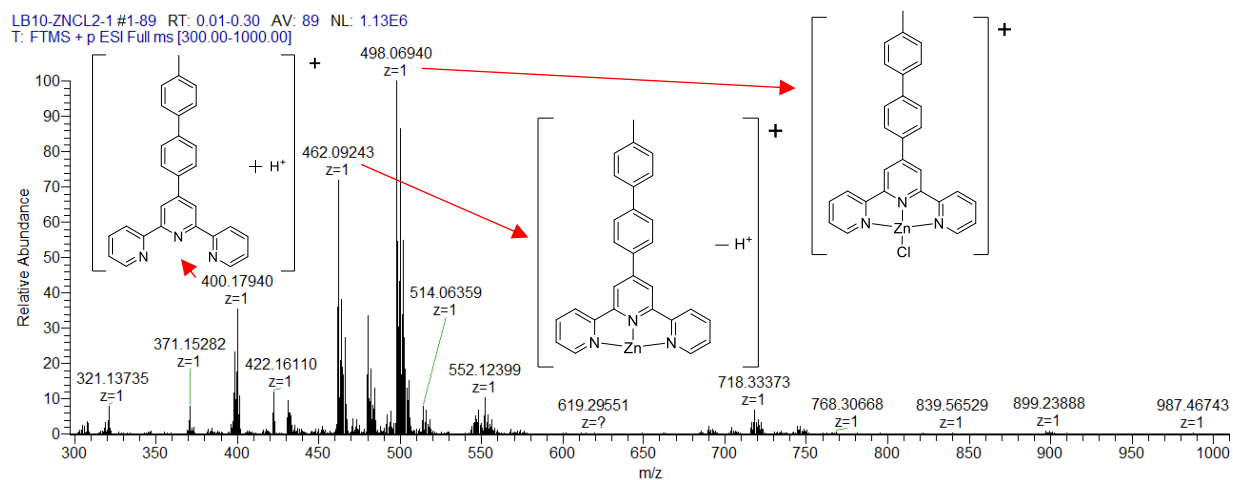


Figure S10 The ESI-MS spectrum of compound 5.

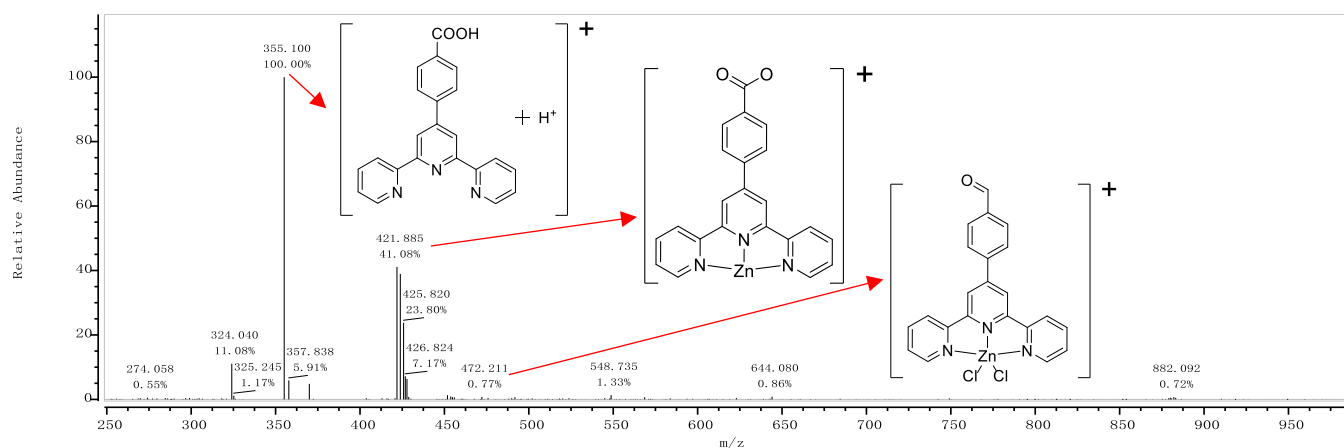


Figure S11 The ESI-MS spectrum of compound 9.

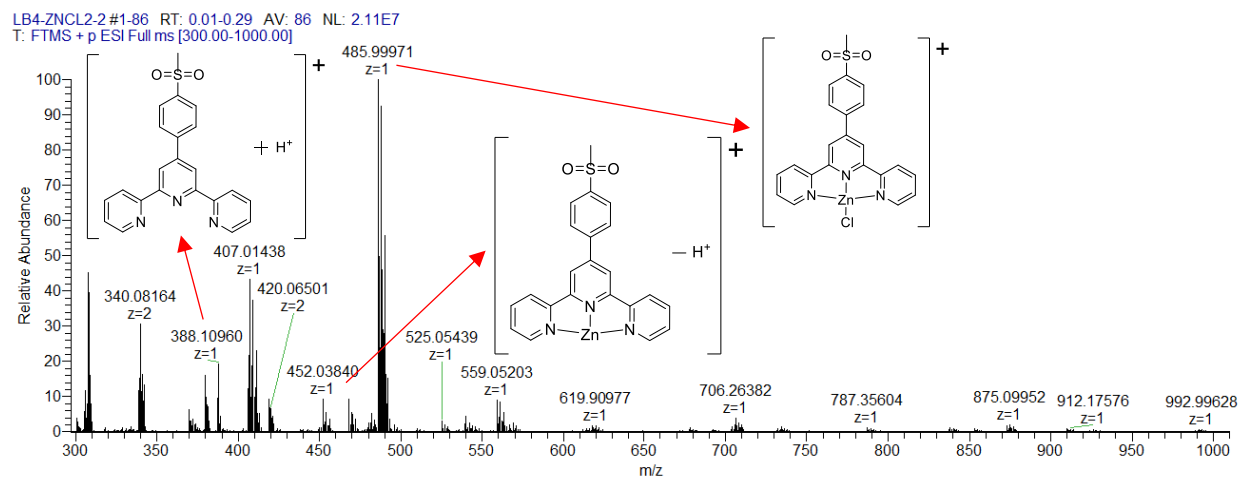


Figure S12 The ESI-MS spectrum of compound 10.

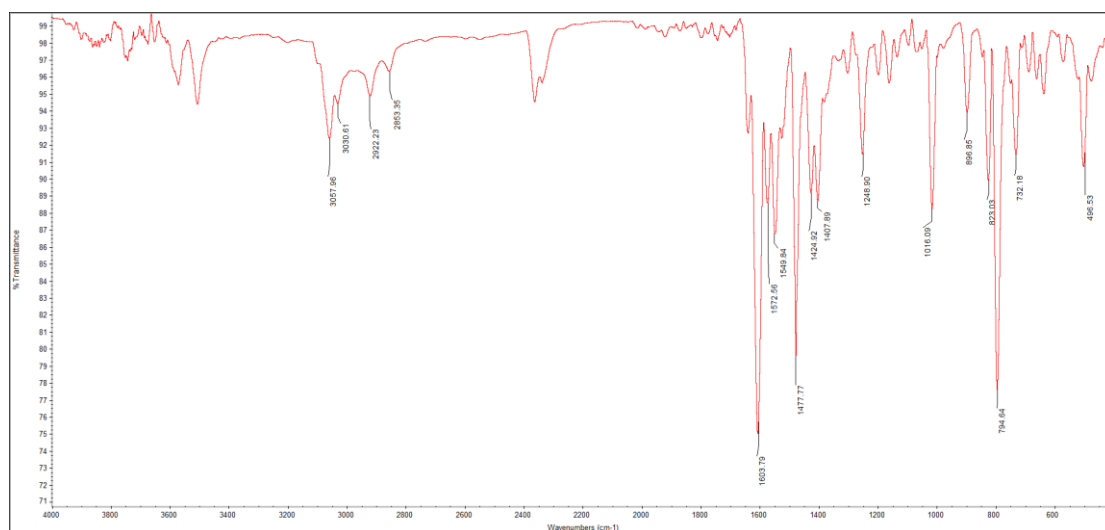


Figure S13 The IR spectrum of compound **2**.

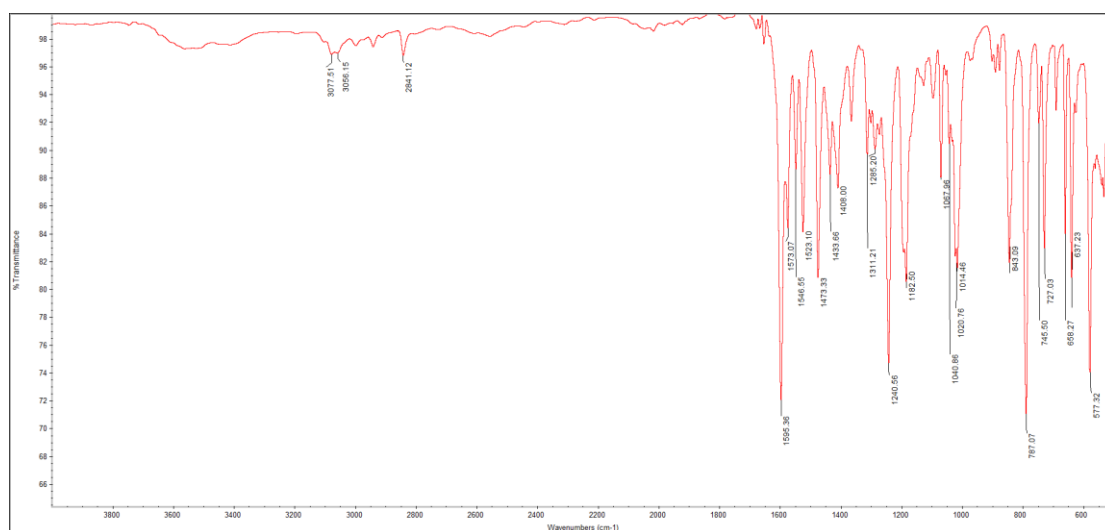


Figure S14 The IR spectrum of compound **3**.

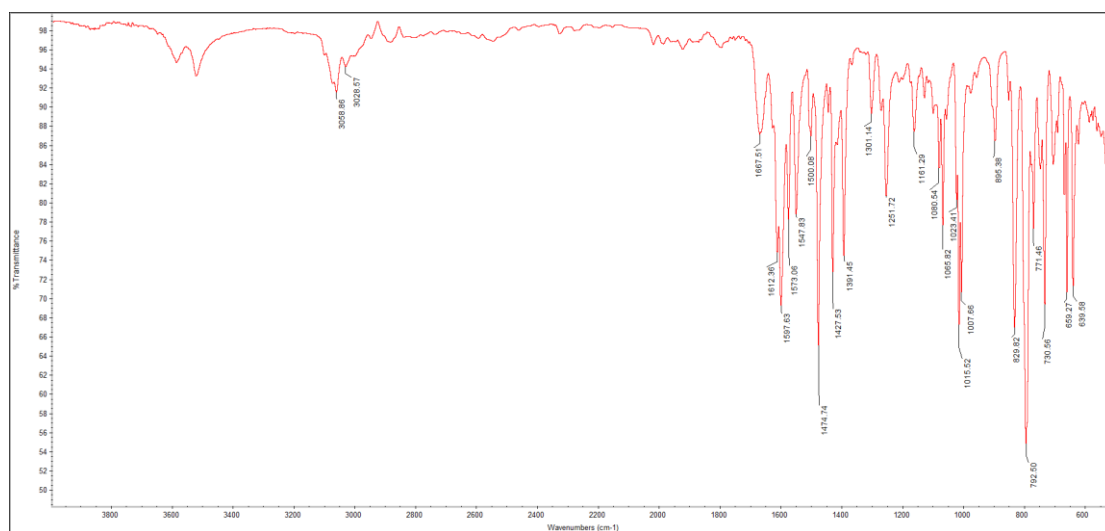


Figure S15 The IR spectrum of compound **4**.



Figure S16 The IR spectrum of compound **5**.

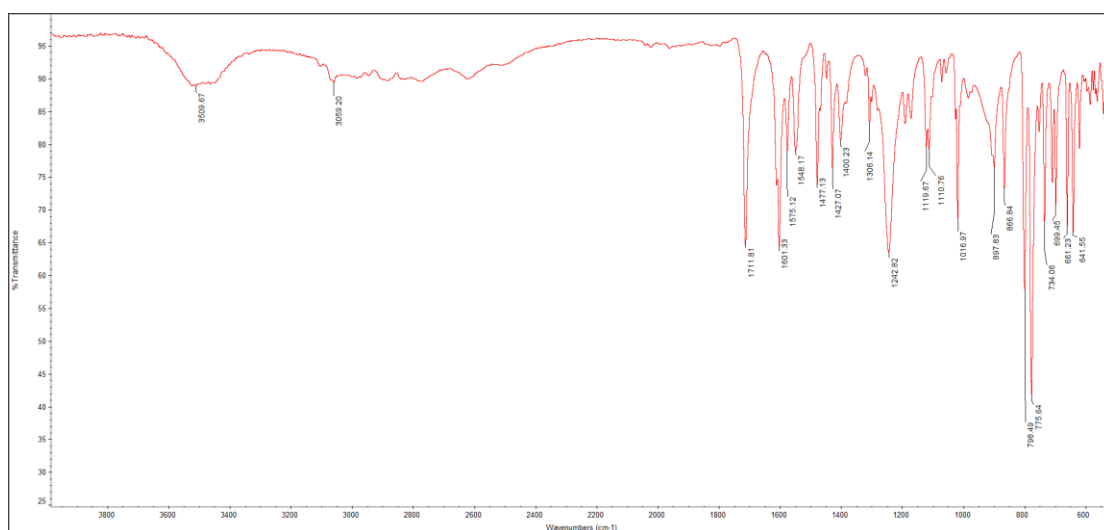


Figure S17 The IR spectrum of compound **9**.

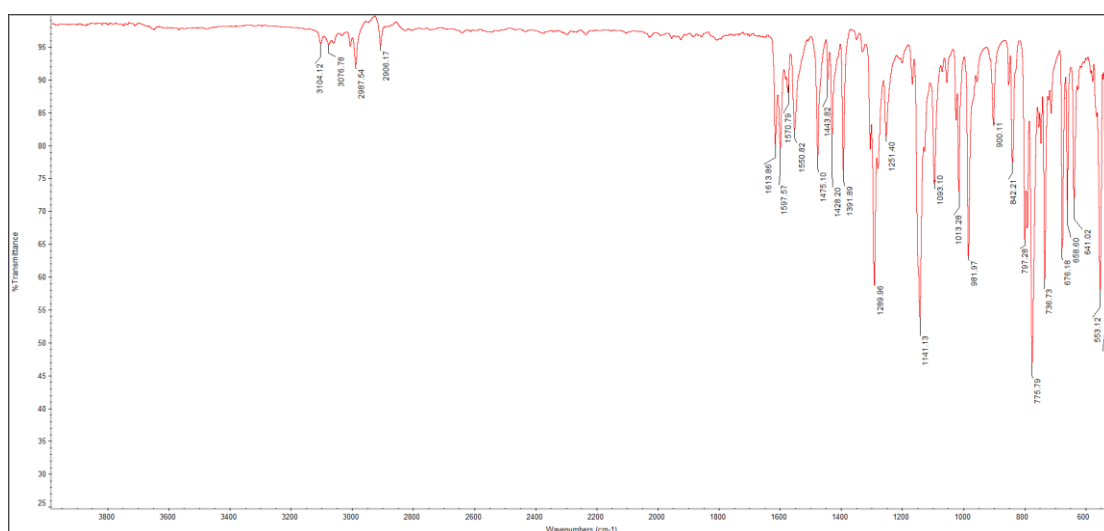


Figure S18 The IR spectrum of compound **10**.

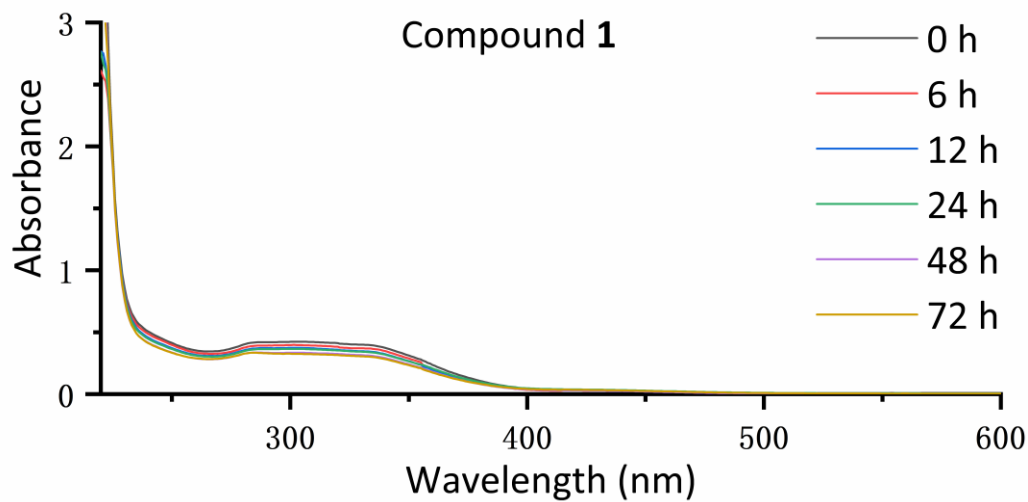


Figure S19 UV-vis spectra of compounds **1** for a period of 72 h.

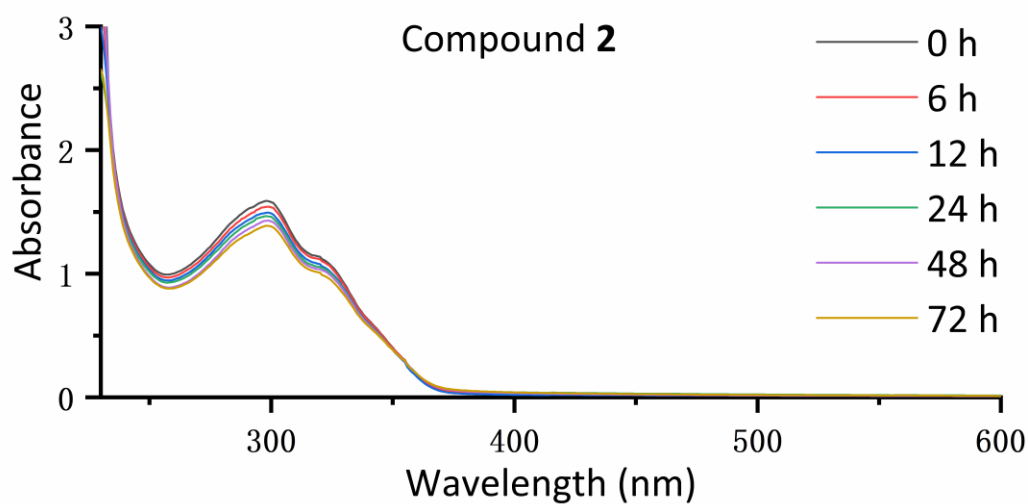


Figure S20 UV-vis spectra of compounds **2** for a period of 72 h.

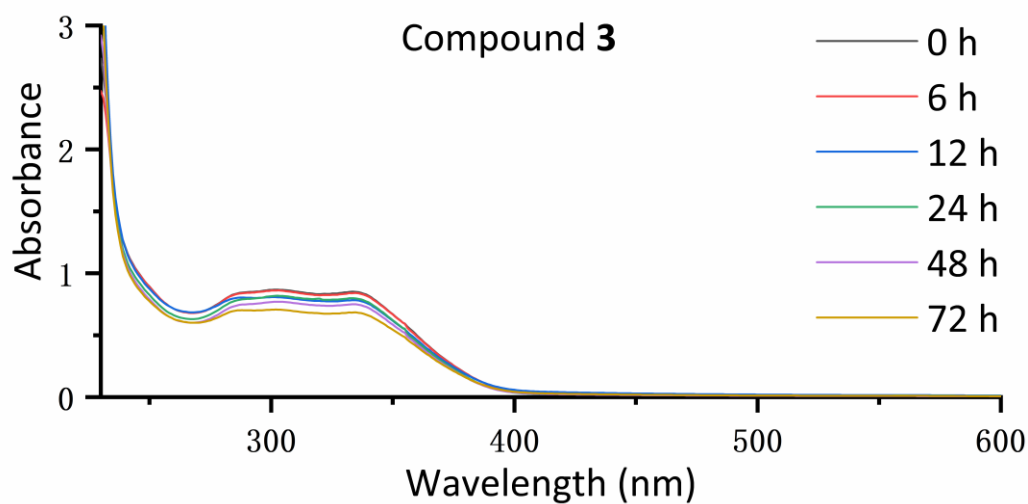


Figure S21 UV-vis spectra of compounds **3** for a period of 72 h.

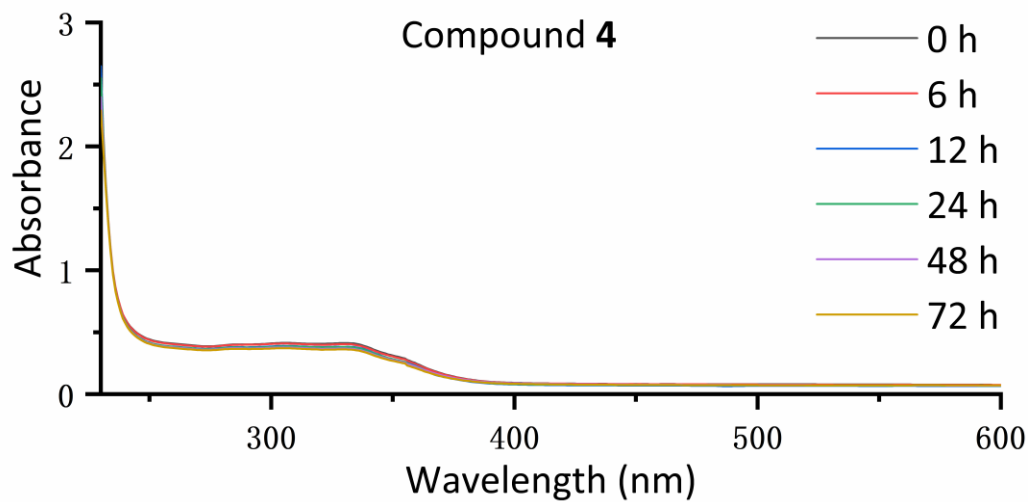


Figure S22 UV-vis spectra of compounds 4 for a period of 72 h.

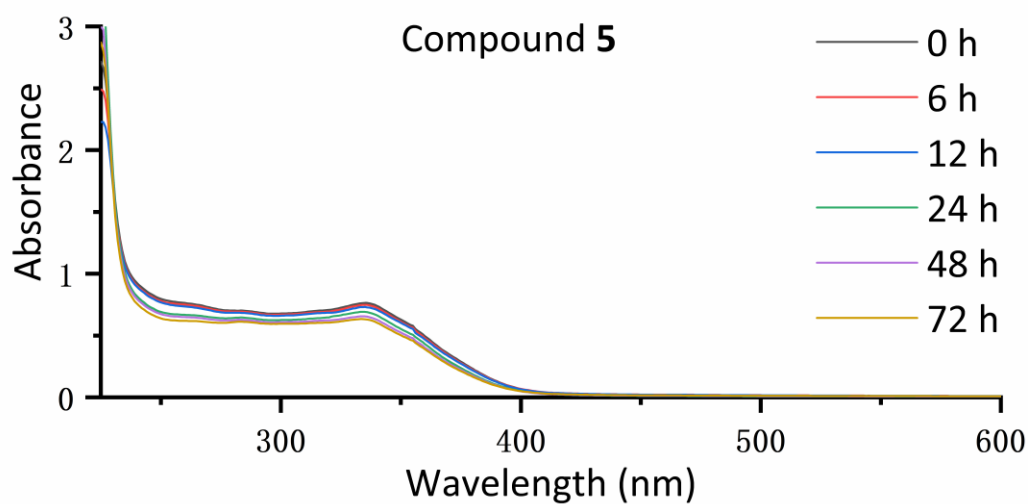


Figure S23 UV-vis spectra of compounds 5 for a period of 72 h.

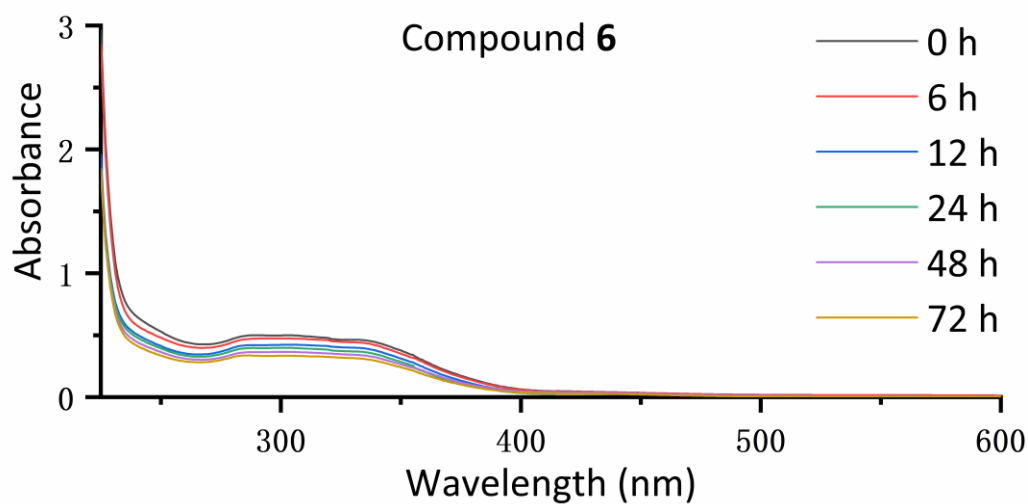


Figure S24 UV-vis spectra of compounds 6 for a period of 72 h.

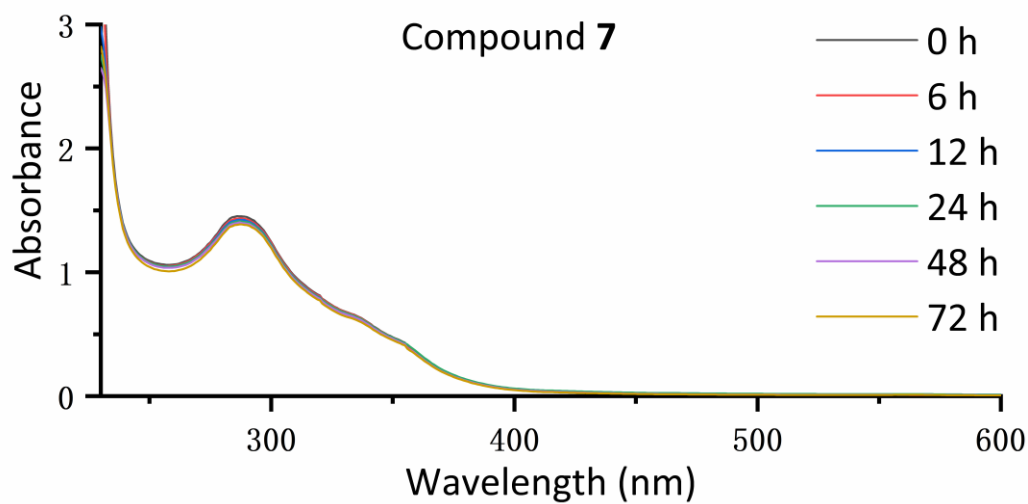


Figure S25 UV-vis spectra of compounds 7 for a period of 72 h.

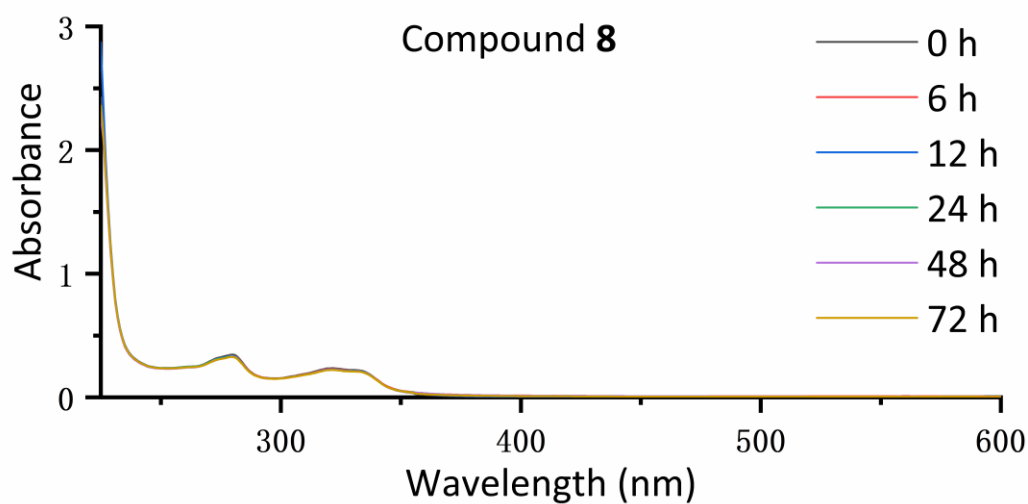


Figure S26 UV-vis spectra of compounds 8 for a period of 72 h.

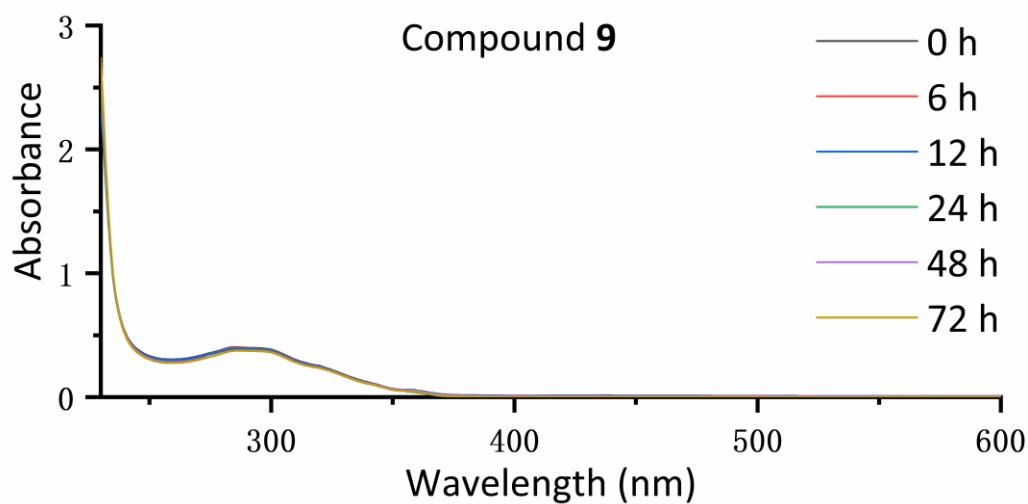


Figure S27 UV-vis spectra of compounds 9 for a period of 72 h.

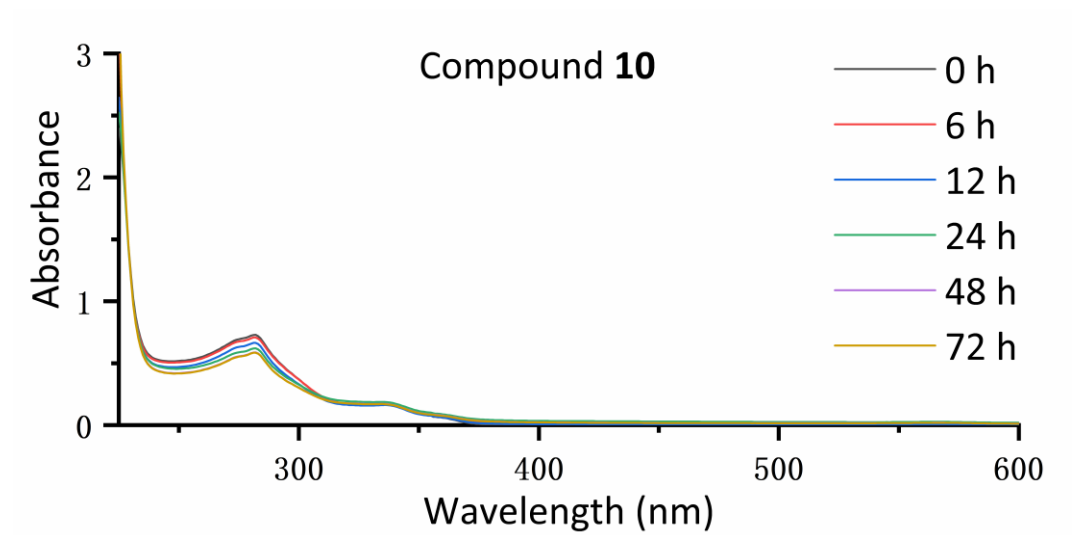
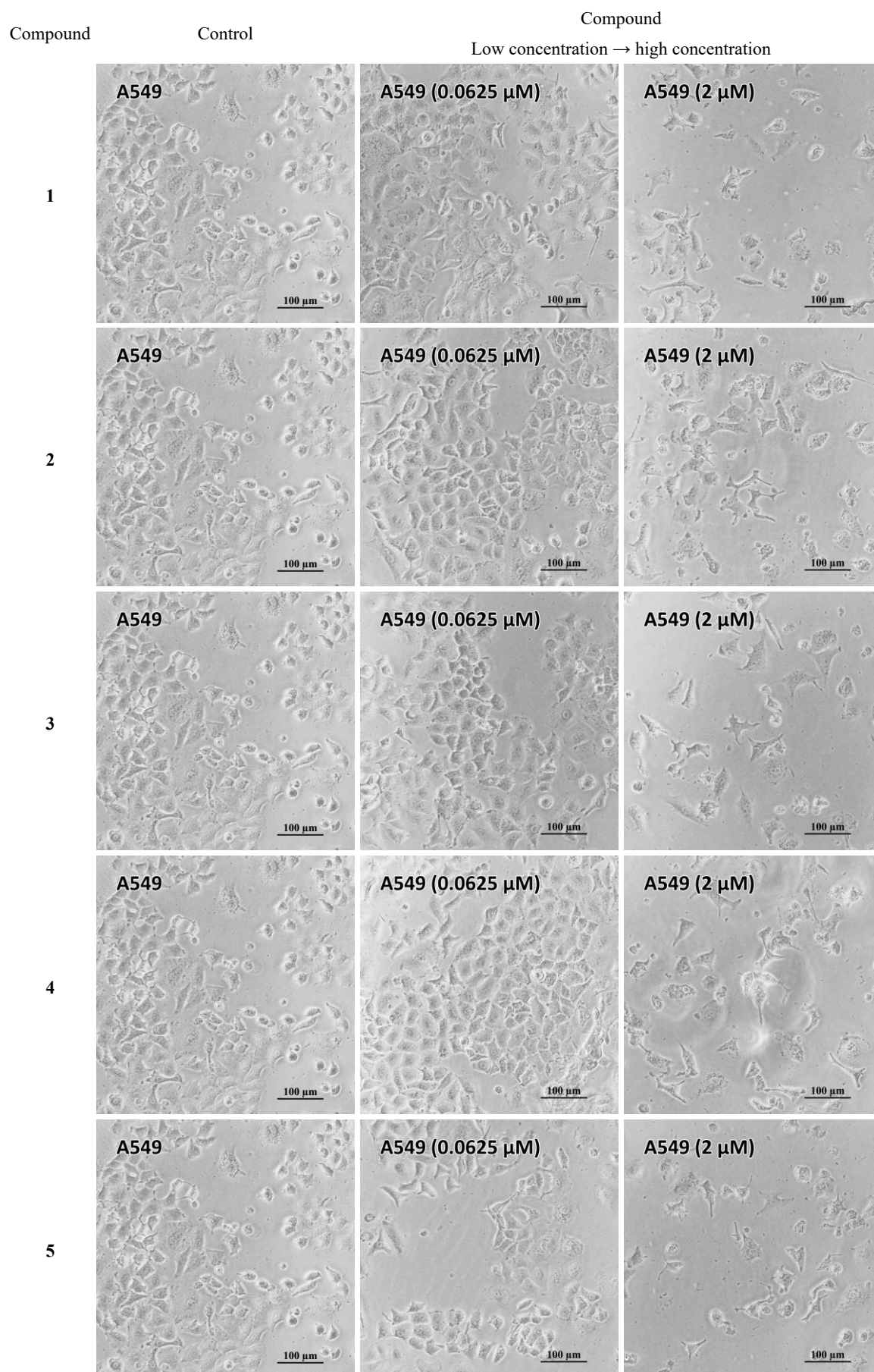


Figure S28 UV-vis spectra of compounds **10** for a period of 72 h.



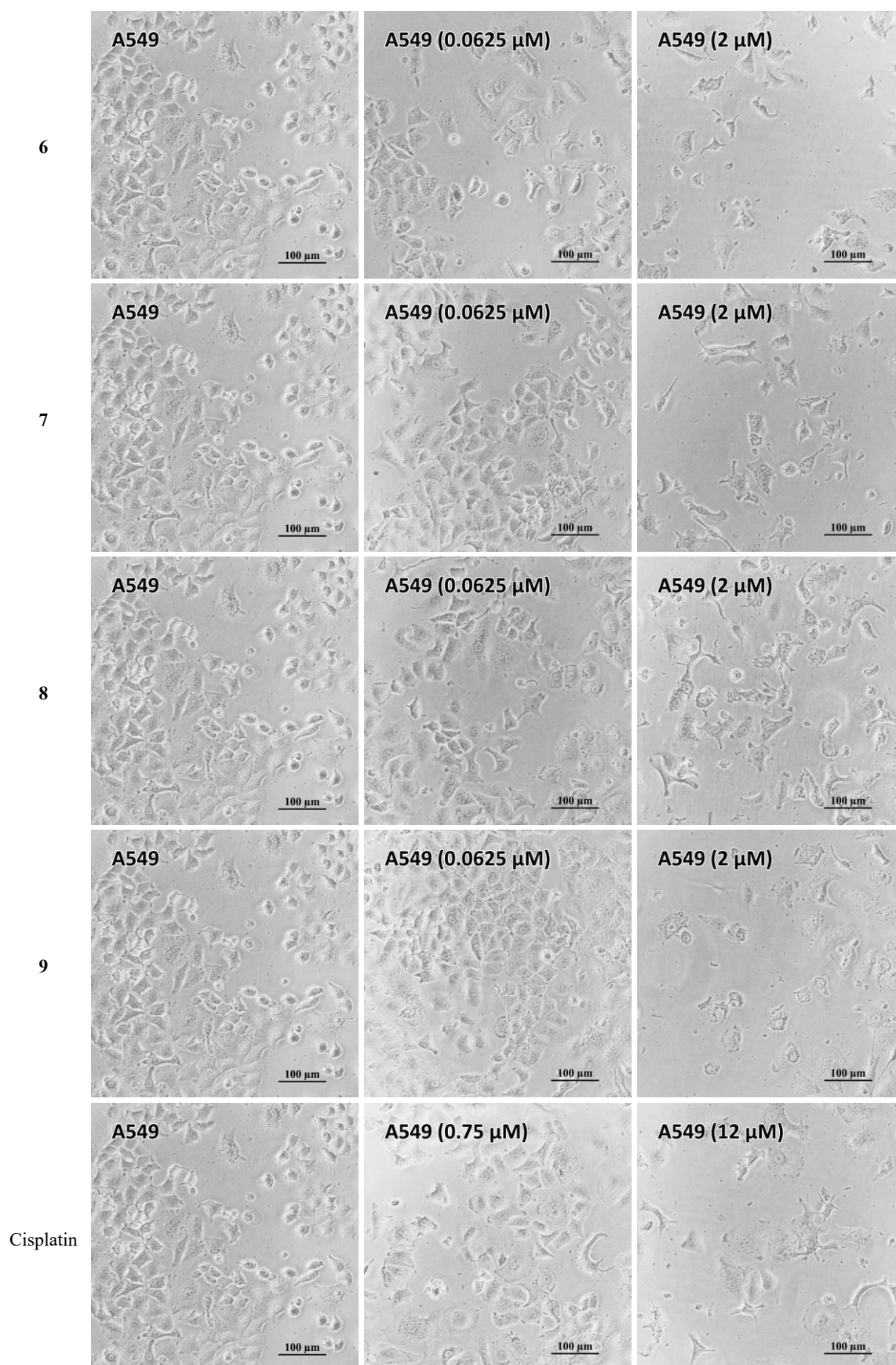
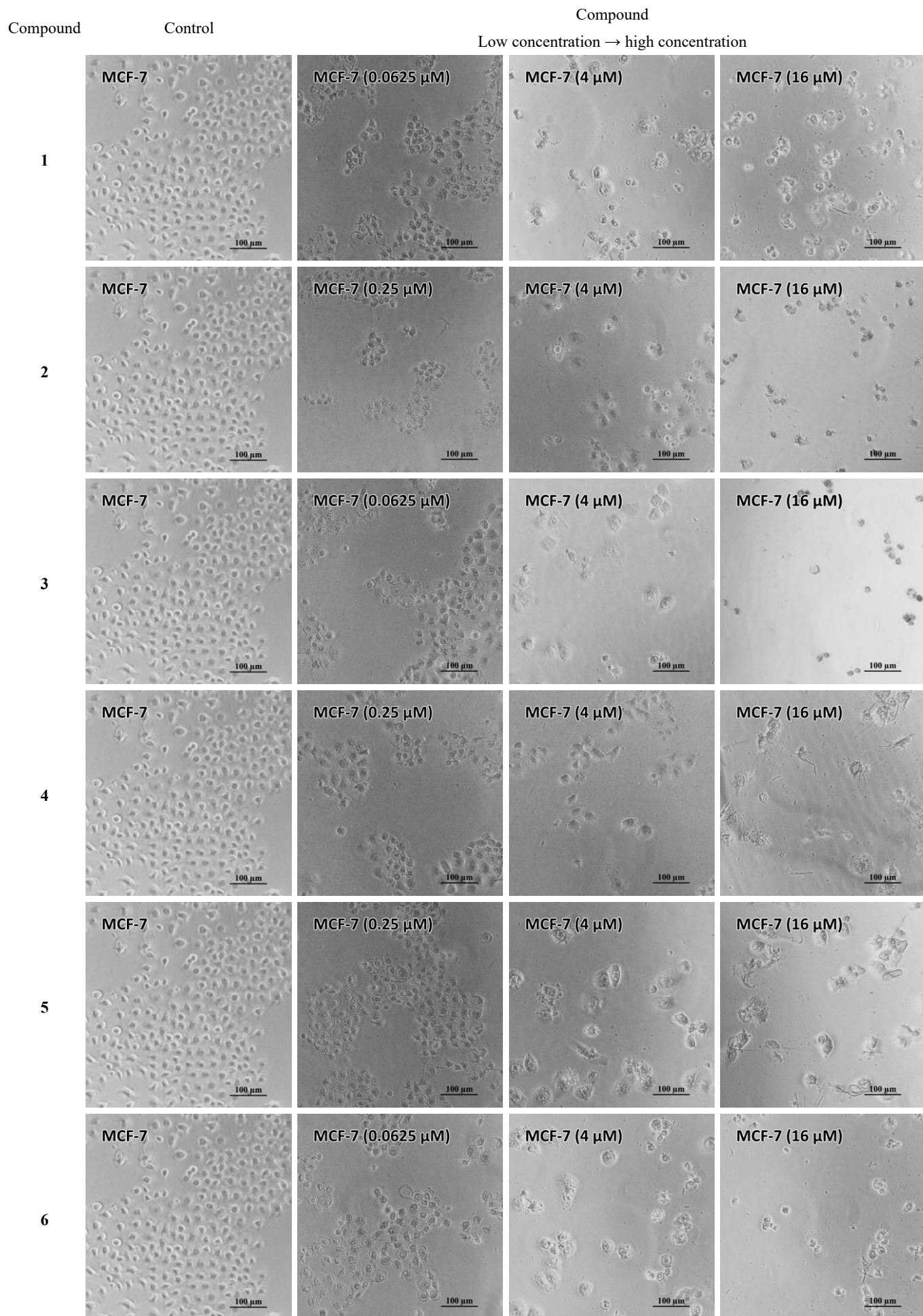


Figure S29 The microscopic photographs of the A549 cancer cell treated with increased concentrations of the compounds 1–9 and cisplatin at magnification of 200 \times .



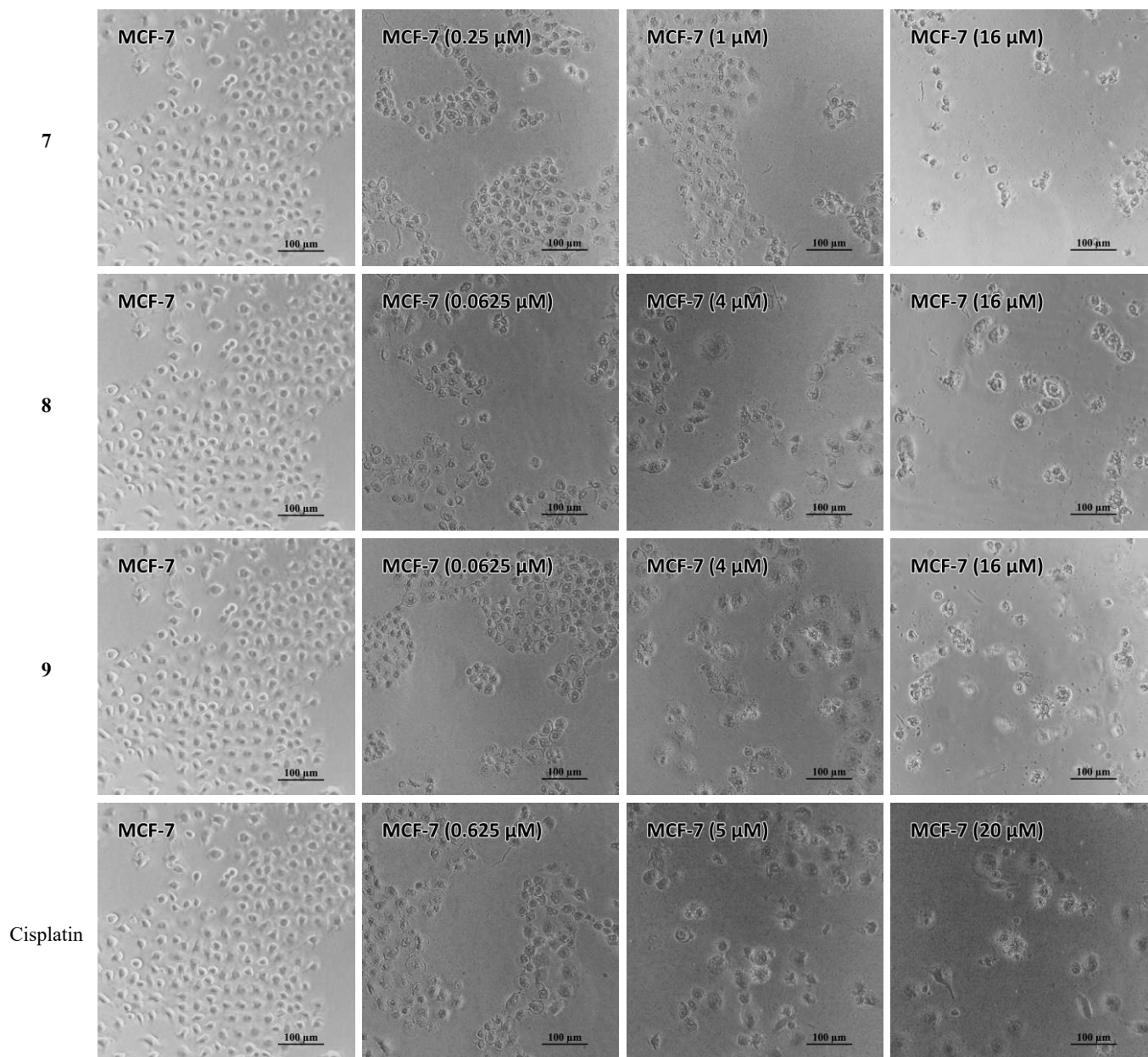
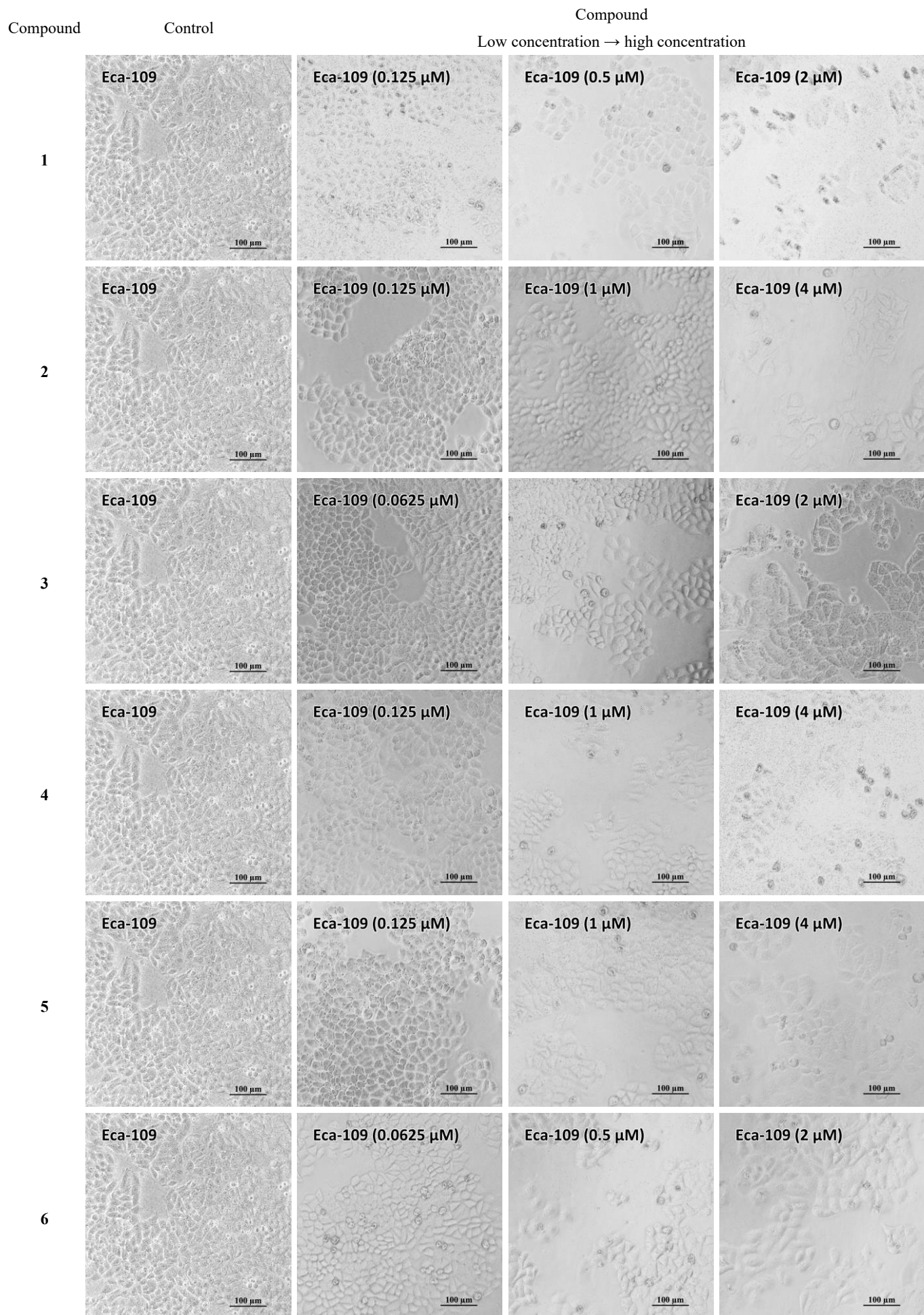


Figure S30 The microscopic photographs of the MCF-7 cancer cell treated with increased concentrations of the compounds **1–9** and cisplatin at magnification of 200 \times .



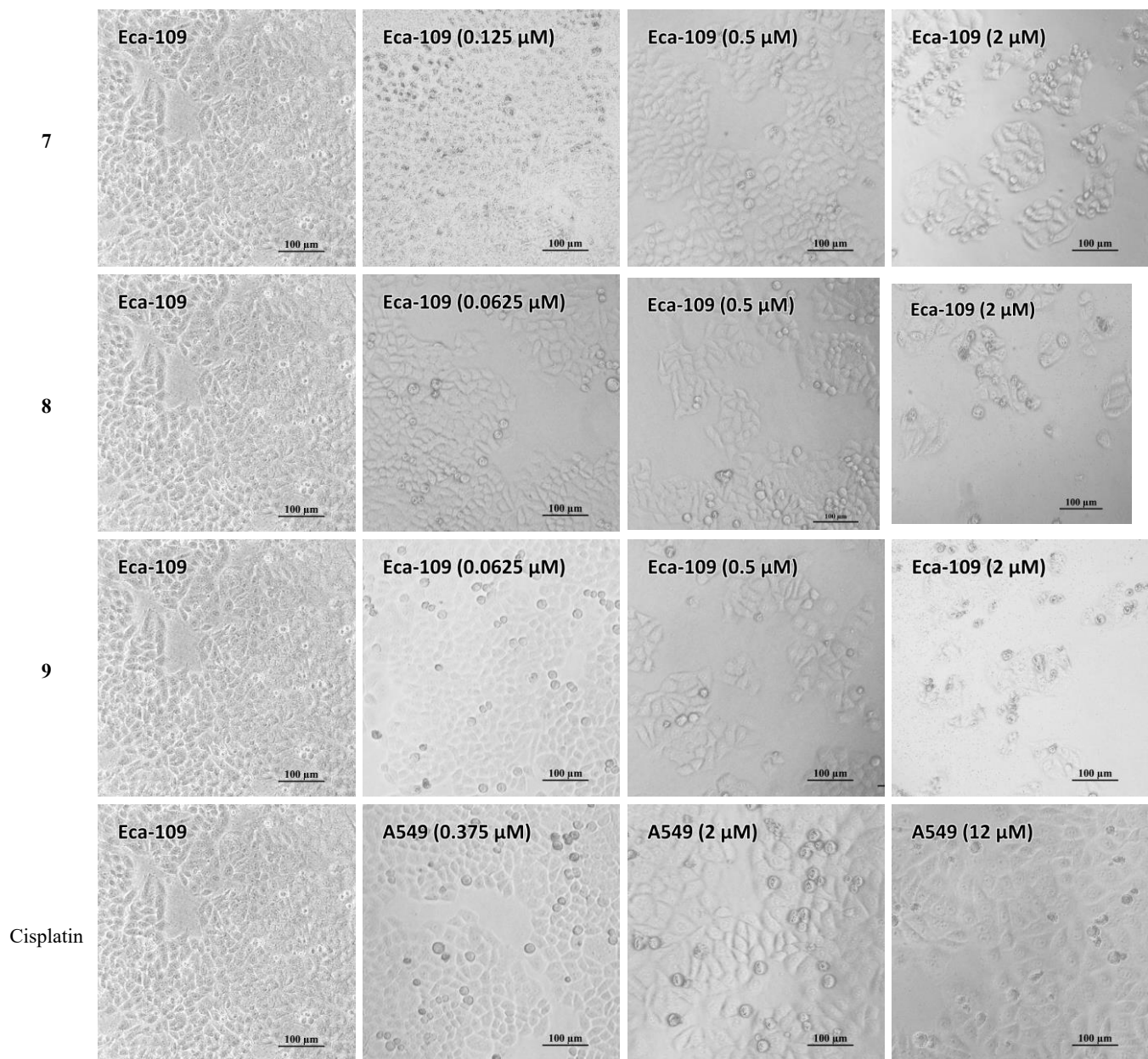


Figure S31 The microscopic photographs of the Eca-109 cancer cell treated with increased concentrations of the compounds **1–9** and cisplatin at magnification of 200 \times .

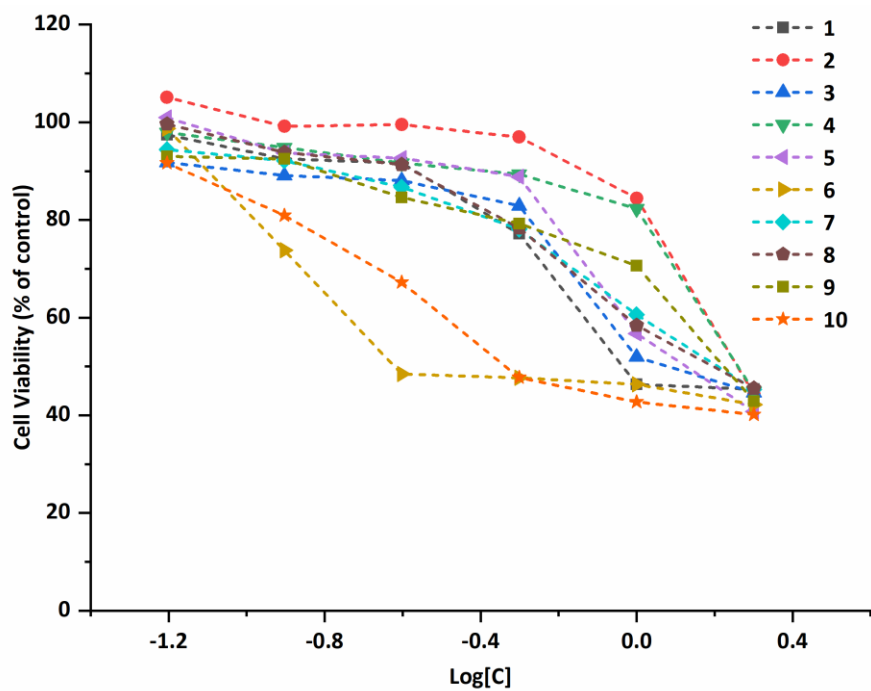


Figure S32 The plots of the cell viability vs. the concentration of compounds **1–10** against Bel-7402 cell line.

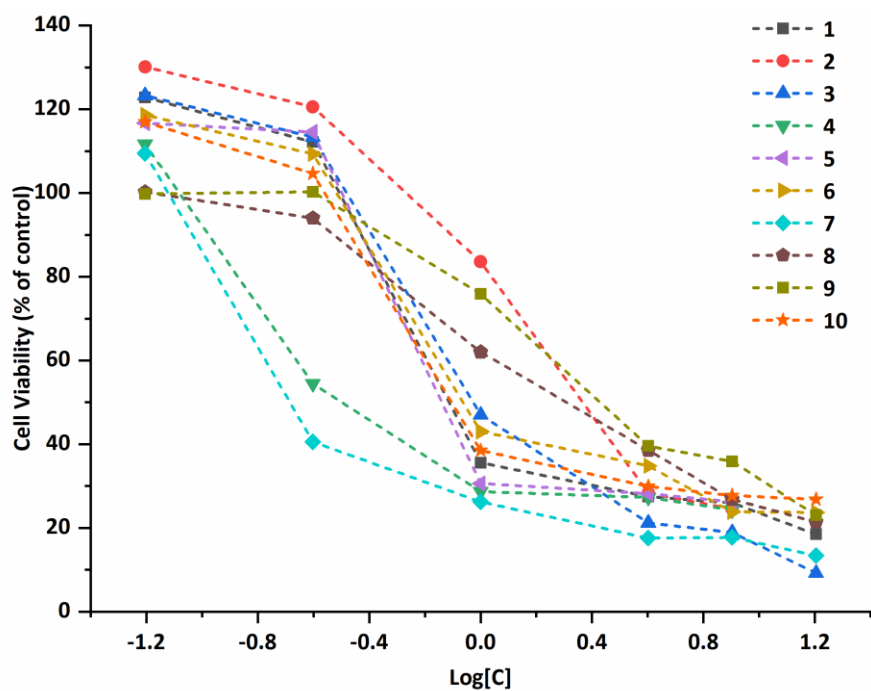


Figure S33 The plots of the cell viability vs. the concentration of compounds **1–10** against MCF-7 cell line.

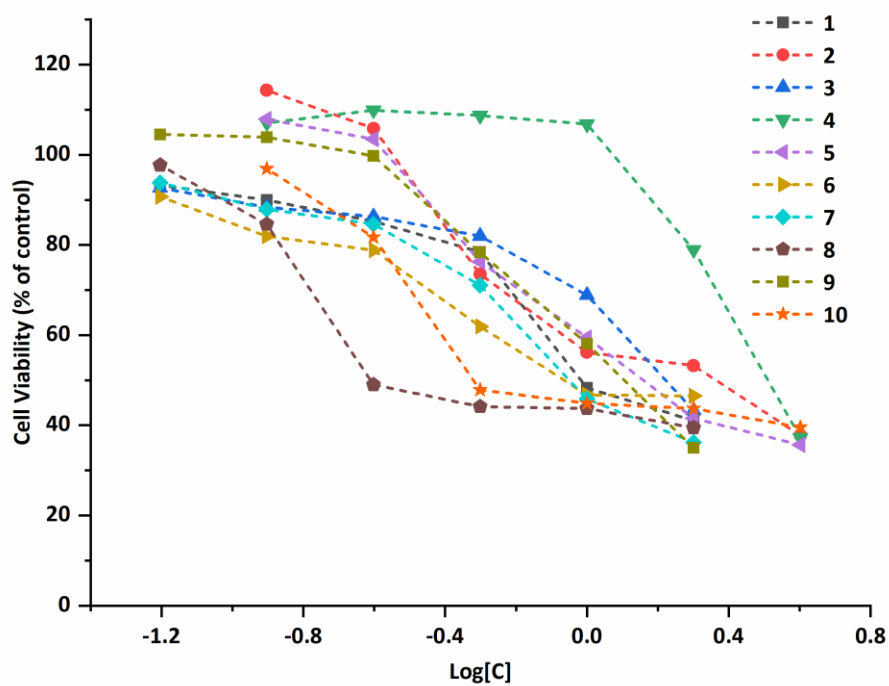


Figure S34 The plots of the cell viability vs. the concentration of compounds **1–10** against Eca-109 cell line.

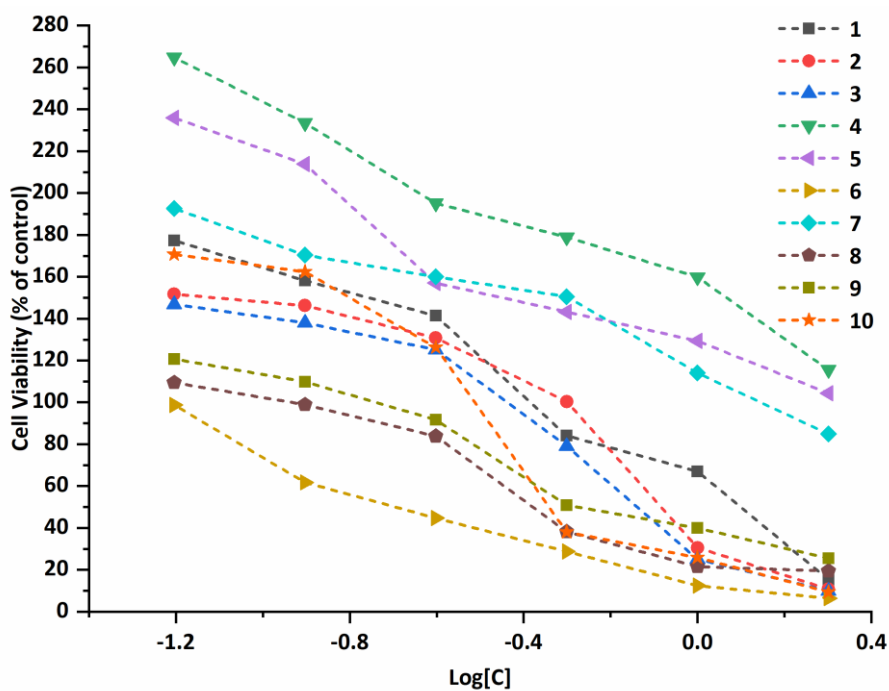
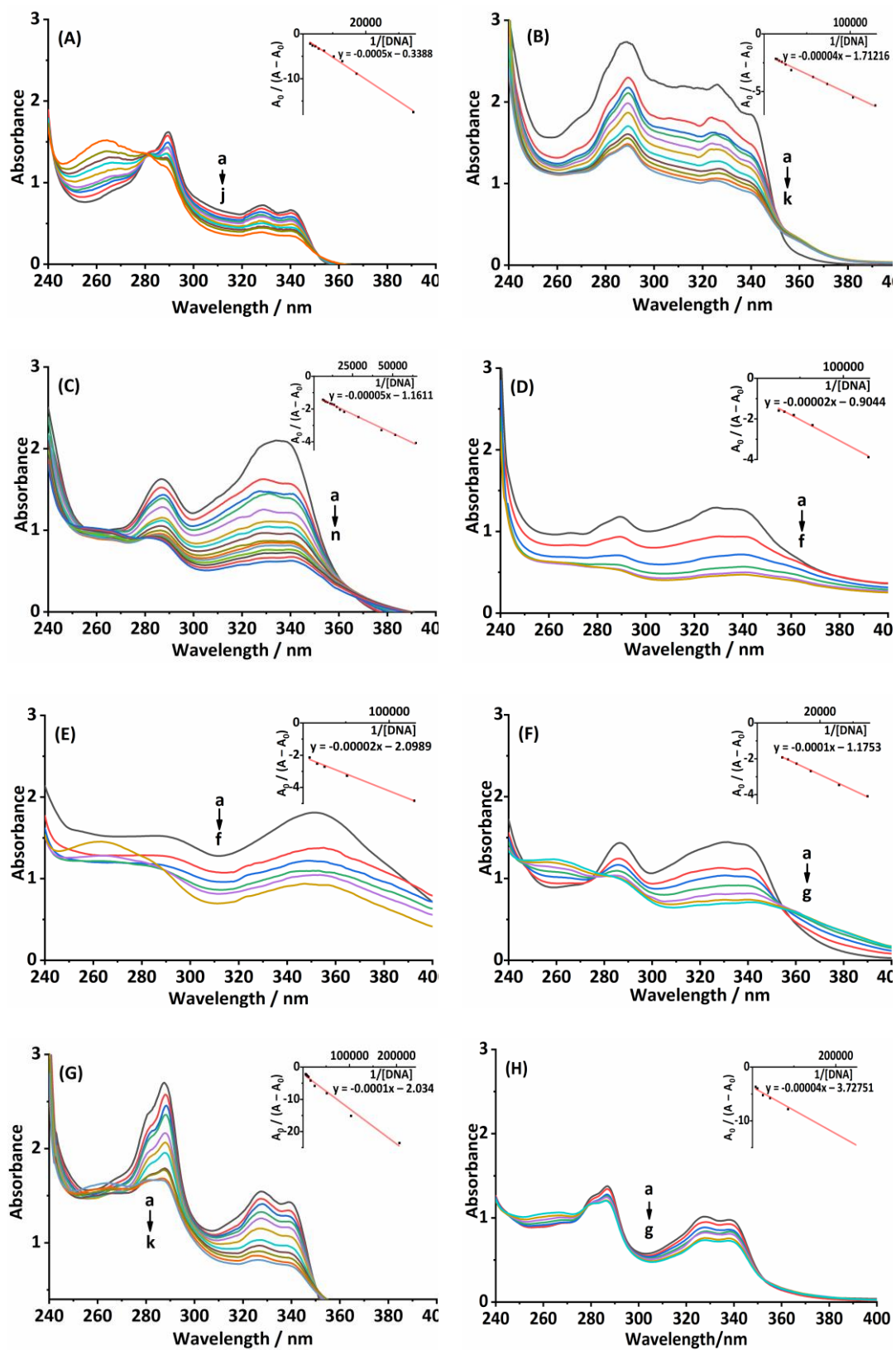


Figure S35 The plots of the cell viability vs. the concentration of compounds **1–10** against RAW 264.7 cell line.



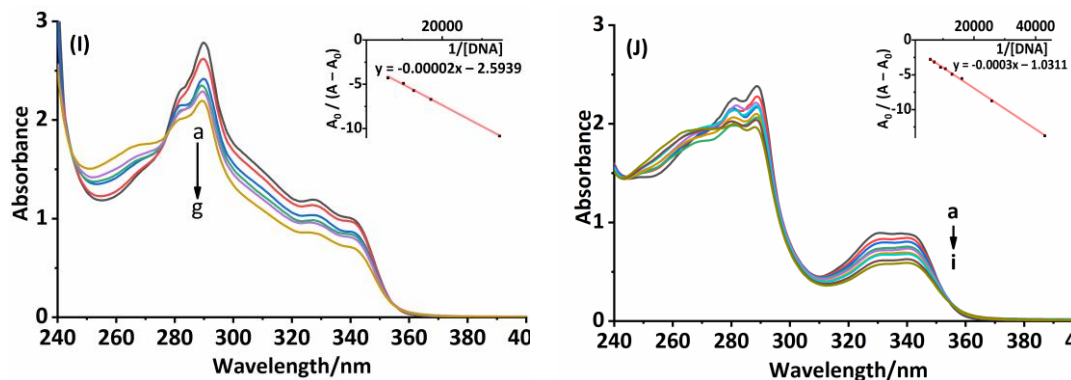


Figure S36 UV-vis spectra for compounds **1–10** in Tris-HCl 1.0×10^{-3} (pH 7.2) with increasing the concentration of CT-DNA, and the inset show plots of $A_0/(A-A_0)$ versus the concentration of CT-DNA. (A) $c(\mathbf{1}) = 67 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 30, 60, 80, 100, 140, 180, 220, 260$ and $320 \mu\text{M}$ corresponding to the curves from a to j, respectively. (B) $c(\mathbf{2}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 8, 10, 14, 18, 32, 40, 48, 56, 64$, and $72 \mu\text{M}$ corresponding to the curves from a to k, respectively. (C) $c(\mathbf{3}) = 67 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 16, 20, 36, 52, 60, 68, 76, 84, 92, 108, 124, 140$, and $156 \mu\text{M}$ corresponding to the curves from a to n, respectively. (D) $c(\mathbf{4}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 8, 16, 24, 32$, and $40 \mu\text{M}$ corresponding to the curves from a to f, respectively. (E) $c(\mathbf{5}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 8, 20, 40, 60$, and $120 \mu\text{M}$ corresponding to the curves from a to f, respectively. (F) $c(\mathbf{6}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 30, 40, 60, 80, 100$ and $120 \mu\text{M}$ corresponding to the curves from a to g, respectively. (G) $c(\mathbf{7}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 5, 10, 20, 40, 60, 80, 100, 120, 140$, and $160 \mu\text{M}$ corresponding to the curves from a to k, respectively. (H) $c(\mathbf{8}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 4, 12, 24, 40, 80$ and $120 \mu\text{M}$ corresponding to the curves from a to g, respectively. (I) $c(\mathbf{9}) = 100 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 30, 60, 80, 100$ and $160 \mu\text{M}$ corresponding to the curves from a to f, respectively. (J) $c(\mathbf{10}) = 80 \mu\text{M}$; $c(\text{CT-DNA}) = 0, 25, 40, 60, 75, 90, 110, 140$ and $170 \mu\text{M}$ corresponding to the curves from a to i, respectively.

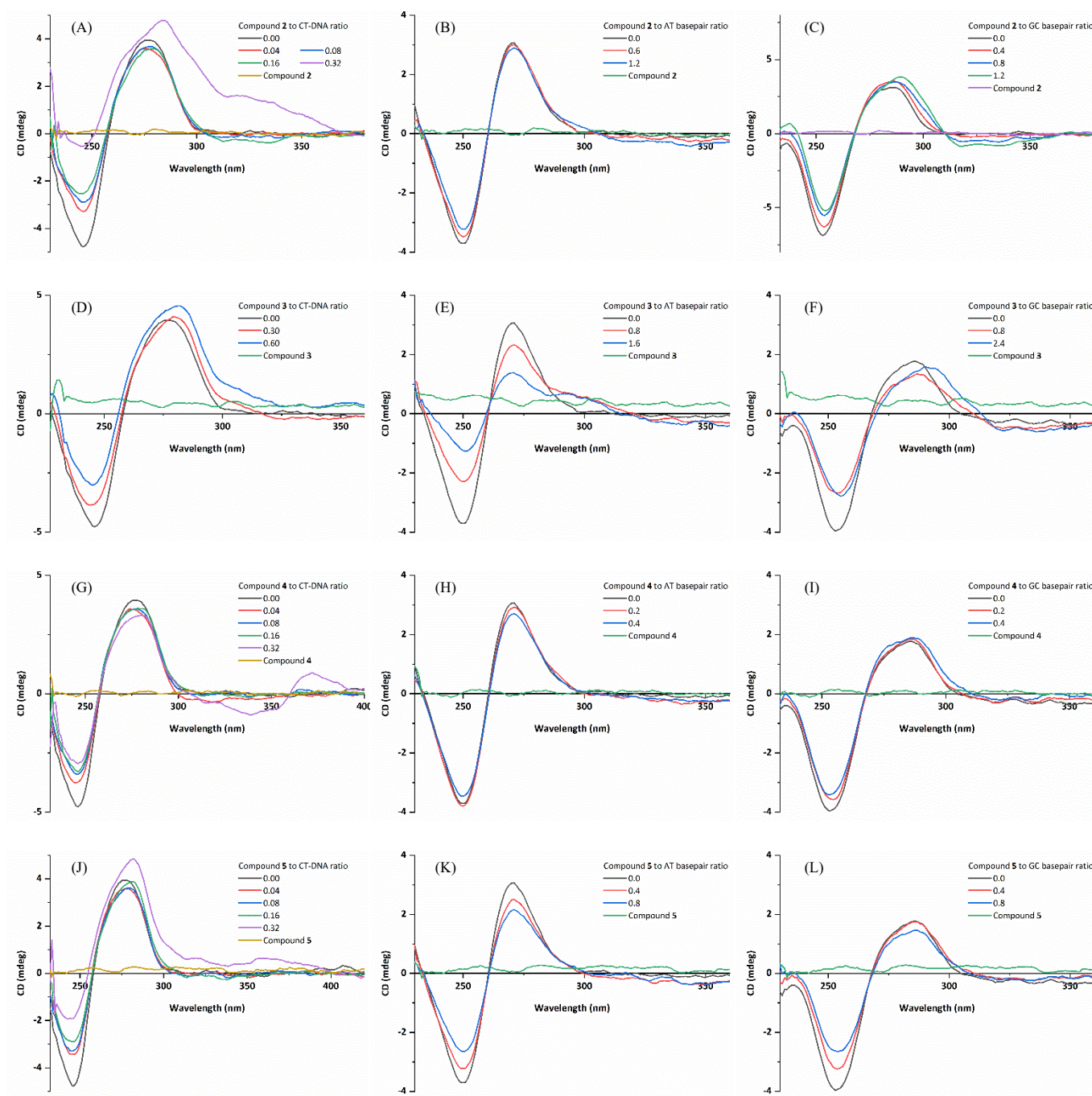


Figure S37 Circular dichroism spectra of three kinds of DNA in the presence or absence of compounds **2–5** in Tris-HCl buffer (pH 7.2), at 20 °C. (A) CT-DNA (4.0×10^{-4} M) treated with compound **2**, (B) ds(AT)₆ (1.44×10^{-5} M) treated with compound **2**, (C) ds(GC)₆ (1.58×10^{-5} M) treated with compound **2**, (D) CT-DNA (4.0×10^{-4} M) treated with compound **3**, (E) ds(AT)₆ (1.44×10^{-5} M) treated with compound **3**, (F) ds(GC)₆ (8.7×10^{-6} M) treated with compound **3**, (G) CT-DNA (4.0×10^{-4} M) treated with compound **4**, (H) ds(AT)₆ (1.44×10^{-5} M) treated with compound **4**, (I) ds(GC)₆ (8.7×10^{-6} M) treated with compound **4**, (J) CT-DNA (4.0×10^{-4} M) treated with compound **5**, (K) ds(AT)₆ (1.44×10^{-5} M) treated with compound **5**, (L) ds(GC)₆ (8.7×10^{-6} M) treated with compound **5**.

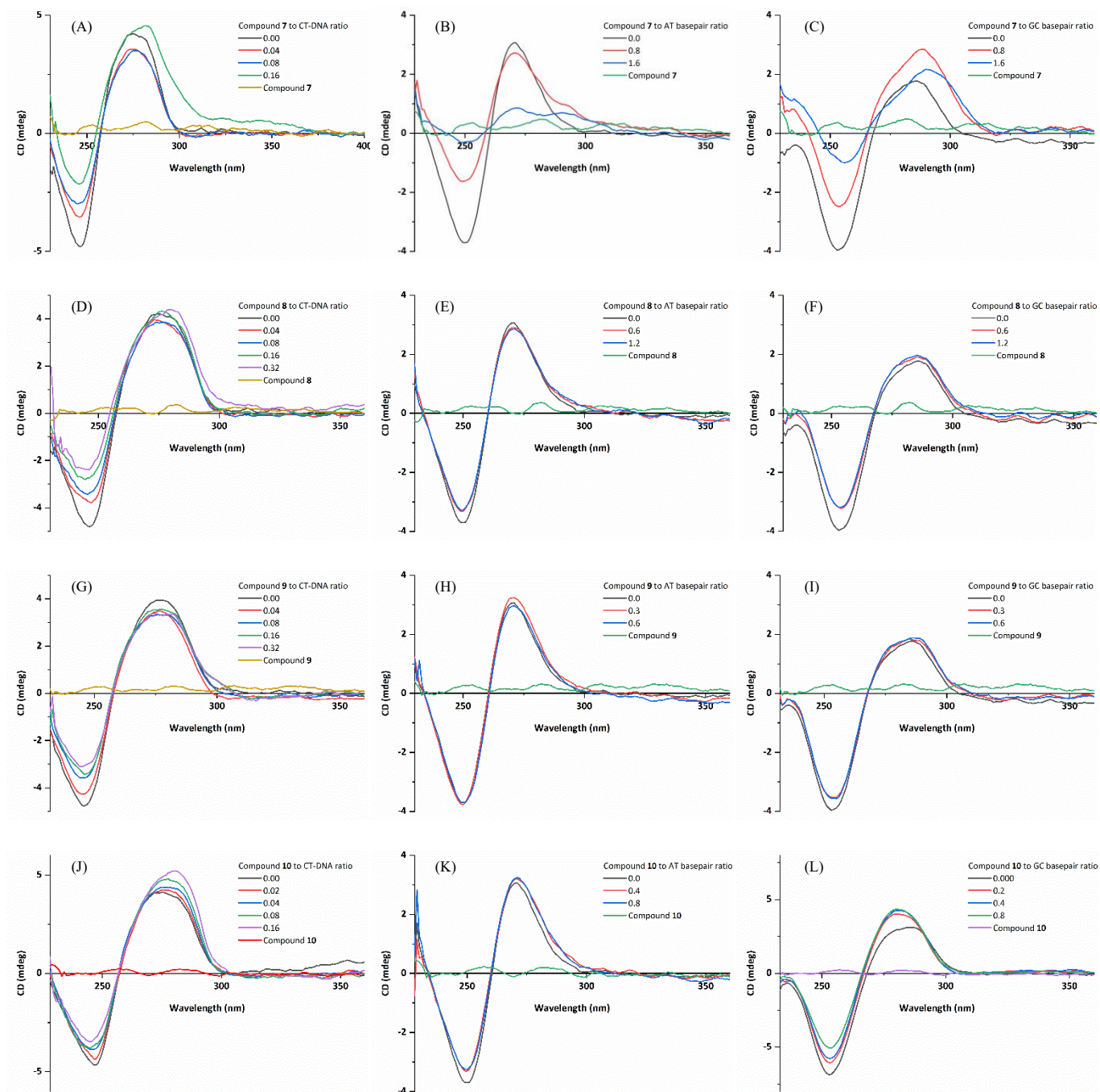


Figure S38 Circular dichroism spectra of three kinds of DNA in the presence or absence of compounds 7–10 in Tris-HCl buffer (pH 7.2), at 20 °C. (A) CT-DNA (4.0×10^{-4} M) treated with compound 7, (B) ds(AT)₆ (1.44×10^{-5} M) treated with compound 7, (C) ds(GC)₆ (1.58×10^{-5} M) treated with compound 7, (D) CT-DNA (4.0×10^{-4} M) treated with compound 8, (E) ds(AT)₆ (1.44×10^{-5} M) treated with compound 8, (F) ds(GC)₆ (8.7×10^{-6} M) treated with compound 8, (G) CT-DNA (4.0×10^{-4} M) treated with compound 9, (H) ds(AT)₆ (1.44×10^{-5} M) treated with compound 9, (I) ds(GC)₆ (8.7×10^{-6} M) treated with compound 9, (J) CT-DNA (4.0×10^{-4} M) treated with compound 10, (K) ds(AT)₆ (1.44×10^{-5} M) treated with compound 10, (L) ds(GC)₆ (1.58×10^{-5} M) treated with compound 10.

Table S1 CD spectra bands of CT-DNA, ds(AT)₆, ds(GC)₆ and with compounds **1–10**: wavelength λ
(degree of ellipticity, Φ)

	λ/nm ($\Phi/^\circ$)	
	(-) band	(+) band
400 μM CT-DNA	246(-4.77)	277(3.94)
400 μM CT-DNA + 128 μM compound 1	245(-3.79)	279(4.69)
400 μM CT-DNA + 256 μM compound 1	245(-3.04)	279(4.73)
400 μM CT-DNA + 512 μM compound 1	244(-2.53)	282(6.45)
400 μM CT-DNA + 16 μM compound 2	246(-3.30)	276(3.57)
400 μM CT-DNA + 32 μM compound 2	246(-2.89)	277(3.67)
400 μM CT-DNA + 64 μM compound 2	245(-2.54)	278(3.59)
400 μM CT-DNA + 128 μM compound 2	245(-0.55)	285(4.76)
400 μM CT-DNA + 160 μM compound 3	245(-3.85)	280(4.07)
400 μM CT-DNA + 320 μM compound 3	245(-3.02)	282(4.55)
400 μM CT-DNA + 16 μM compound 4	245(-3.76)	274(3.60)
400 μM CT-DNA + 32 μM compound 4	246(-3.40)	277(3.56)
400 μM CT-DNA + 64 μM compound 4	246(-3.29)	281(3.59)
400 μM CT-DNA + 128 μM compound 4	246(-2.94)	281(3.30)
400 μM CT-DNA + 16 μM compound 5	246(-3.42)	278(3.59)
400 μM CT-DNA + 32 μM compound 5	245(-3.29)	280(3.61)
400 μM CT-DNA + 64 μM compound 5	245(-2.90)	282(3.88)
400 μM CT-DNA + 128 μM compound 5	243(-1.93)	282(4.85)
400 μM CT-DNA + 8 μM compound 6	246(-3.54)	277(3.60)
400 μM CT-DNA + 16 μM compound 6	246(-3.62)	277(3.39)
400 μM CT-DNA + 32 μM compound 6	246(-3.19)	277(3.42)
400 μM CT-DNA + 64 μM compound 6	246(-2.34)	279(3.64)
400 μM CT-DNA + 128 μM compound 6	246(-1.28)	283(4.47)
400 μM CT-DNA + 256 μM compound 6	246(0.66)	288(5.71)
400 μM CT-DNA + 8 μM compound 7	246(-3.57)	275(3.54)
400 μM CT-DNA + 32 μM compound 7	246(-2.96)	278(3.48)
400 μM CT-DNA + 64 μM compound 7	246(-2.15)	281(4.55)
400 μM CT-DNA + 16 μM compound 8	247(-3.79)	274(3.95)
400 μM CT-DNA + 32 μM compound 8	246(-3.44)	276(3.85)
400 μM CT-DNA + 64 μM compound 8	245(-2.79)	277(4.31)
400 μM CT-DNA + 128 μM compound 8	245(-2.37)	279(4.40)
400 μM CT-DNA + 16 μM compound 9	246(-4.27)	276(3.48)
400 μM CT-DNA + 32 μM compound 9	246(-3.59)	277(3.32)
400 μM CT-DNA + 64 μM compound 9	246(-3.43)	277(3.56)
400 μM CT-DNA + 128 μM compound 9	245(-3.11)	280(3.35)
400 μM CT-DNA + 8 μM compound 10	246(-4.35)	277(4.21)
400 μM CT-DNA + 16 μM compound 10	246(-3.87)	278(4.35)
400 μM CT-DNA + 32 μM compound 10	245(-3.80)	278(4.82)
400 μM CT-DNA + 64 μM compound 10	245(-3.48)	280(5.20)
15.7 μM ds(AT) ₆	250(-4.43)	271(3.59)
15.7 μM ds(AT) ₆ + 160 μM compound 1	249(-2.97)	271(3.00)
15.7 μM ds(AT) ₆ + 320 μM compound 1	251(-0.82)	275(1.40)
15.7 μM ds(AT) ₆ + 480 μM compound 1	251(-0.37)	275(1.09)
14.4 μM ds(AT) ₆	250(-3.70)	271(3.07)
14.4 μM ds(AT) ₆ + 108 μM compound 2	250(-3.48)	271(3.00)
14.4 μM ds(AT) ₆ + 180 μM compound 2	250(-3.23)	271(2.90)
14.4 μM ds(AT) ₆ + 144 μM compound 3	250(-2.30)	271(2.33)
14.4 μM ds(AT) ₆ + 288 μM compound 3	251(-1.27)	271(1.38)
14.4 μM ds(AT) ₆ + 36 μM compound 4	250(-3.79)	271(2.92)
14.4 μM ds(AT) ₆ + 72 μM compound 4	250(-3.46)	271(2.70)
14.4 μM ds(AT) ₆ + 72 μM compound 5	250(-3.22)	271(2.51)
14.4 μM ds(AT) ₆ + 144 μM compound 5	250(-2.65)	271(2.16)
14.4 μM ds(AT) ₆ + 108 μM compound 6	251(-2.11)	271(2.33)
14.4 μM ds(AT) ₆ + 216 μM compound 6	253(-0.33)	271(0.84)
14.4 μM ds(AT) ₆ + 144 μM compound 7	249(-1.63)	271(2.72)
14.4 μM ds(AT) ₆ + 288 μM compound 7	249(-0.31)	271(0.86)
14.4 μM ds(AT) ₆ + 108 μM compound 8	250(-3.28)	271(2.86)
14.4 μM ds(AT) ₆ + 216 μM compound 8	250(-3.32)	271(2.90)
14.4 μM ds(AT) ₆ + 72 μM compound 9	251(-3.70)	271(2.97)
14.4 μM ds(AT) ₆ + 144 μM compound 9	250(-3.78)	271(3.24)

14.4 μM ds(AT) ₆ + 72 μM compound 10	250(-3.31)	271(3.21)
14.4 μM ds(AT) ₆ + 144 μM compound 10	250(-3.26)	271(3.25)
15.8 μM ds(GC) ₆	253(-7.10)	284(3.27)
15.8 μM ds(GC) ₆ + 160 μM compound 1	254(-4.56)	286(3.69)
15.8 μM ds(GC) ₆ + 320 μM compound 1	257(-2.23)	296(4.65)
15.8 μM ds(GC) ₆ + 400 μM compound 1	259(-1.49)	296(5.01)
15.8 μM ds(GC) ₆ + 80 μM compound 2	253(-6.26)	285(3.52)
15.8 μM ds(GC) ₆ + 160 μM compound 2	253(-5.50)	287(3.49)
15.8 μM ds(GC) ₆ + 320 μM compound 2	254(-5.20)	290(3.82)
15.8 μM ds(GC) ₆ + 80 μM compound 6	254(-5.11)	291(4.16)
15.8 μM ds(GC) ₆ + 160 μM compound 6	255(-1.83)	295(6.11)
15.8 μM ds(GC) ₆ + 320 μM compound 6	256(0.21)	296(6.69)
15.8 μM ds(GC) ₆ + 40 μM compound 10	253(-6.06)	280(4.01)
15.8 μM ds(GC) ₆ + 80 μM compound 10	253(-5.77)	281(4.27)
15.8 μM ds(GC) ₆ + 160 μM compound 10	253(-5.07)	280(4.34)
8.7 μM ds(GC) ₆	253(-3.97)	286(1.77)
8.7 μM ds(GC) ₆ + 90 μM compound 3	254(-2.68)	287(1.34)
8.7 μM ds(GC) ₆ + 180 μM compound 3	255(-2.78)	290(1.58)
8.7 μM ds(GC) ₆ + 20 μM compound 4	255(-3.57)	286(1.84)
8.7 μM ds(GC) ₆ + 40 μM compound 4	255(-3.35)	287(1.89)
8.7 μM ds(GC) ₆ + 40 μM compound 5	255(-3.24)	287(1.75)
8.7 μM ds(GC) ₆ + 80 μM compound 5	255(-2.66)	287(1.45)
8.7 μM ds(GC) ₆ + 90 μM compound 7	253(-2.47)	289(2.85)
8.7 μM ds(GC) ₆ + 180 μM compound 7	256(-0.99)	290(2.16)
8.7 μM ds(GC) ₆ + 60 μM compound 8	254(-3.23)	286(1.90)
8.7 μM ds(GC) ₆ + 120 μM compound 8	254(-3.18)	286(1.95)
8.7 μM ds(GC) ₆ + 30 μM compound 9	254(-3.54)	287(1.80)
8.7 μM ds(GC) ₆ + 60 μM compound 9	254(-3.54)	289(1.86)

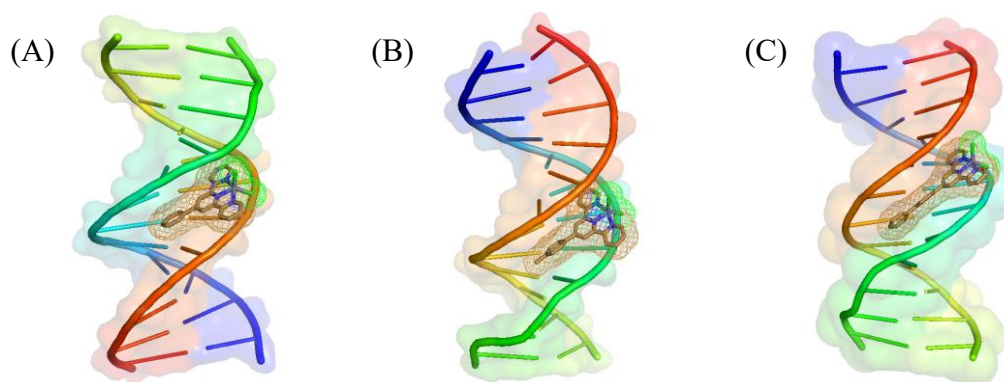


Figure S39 The most favorable orientation of (A): compound **1**, (B): compound **2** and (C): compound **4** bound with the minor groove of the CT-DNA (PDB ID: 1BNA).

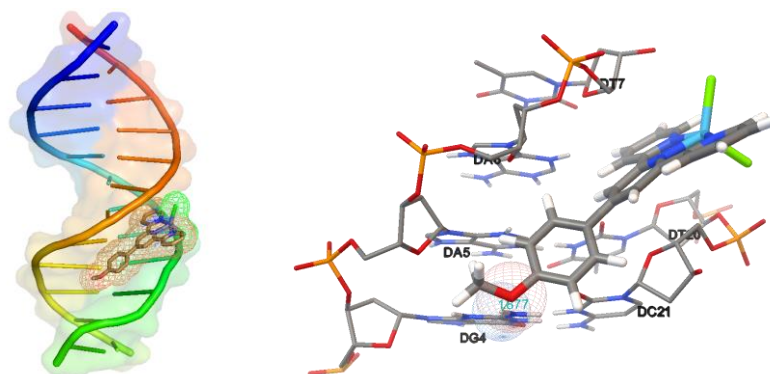


Figure S40 The most favorable orientation of compound **3** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

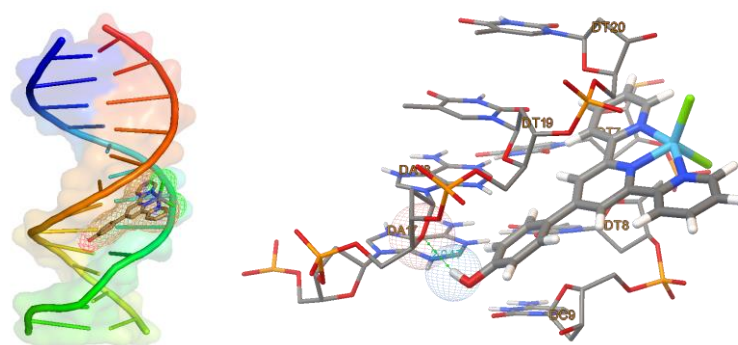


Figure S41 The most favorable orientation of compound **6** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

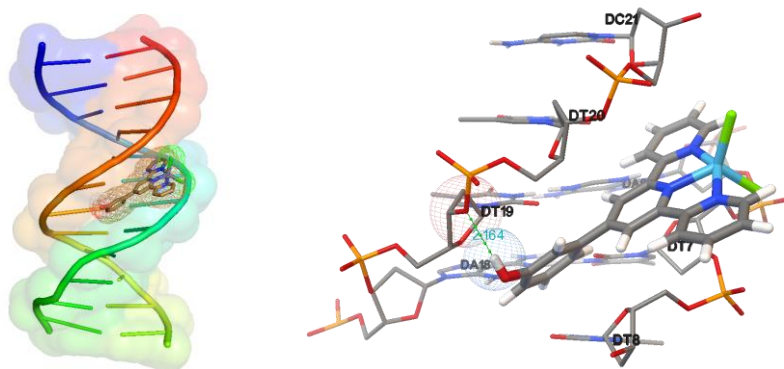


Figure S42 The most favorable orientation of compound **7** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

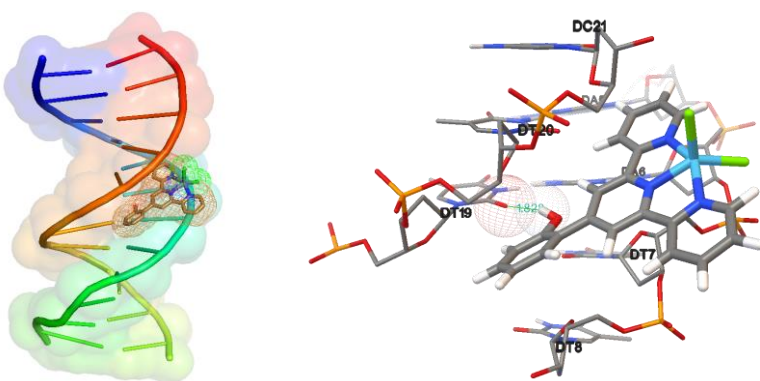


Figure S43 The most favorable orientation of compound **8** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

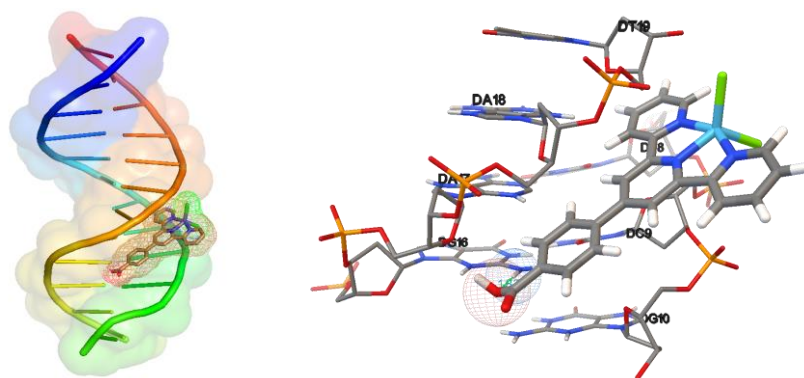


Figure S44 The most favorable orientation of compound **9** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

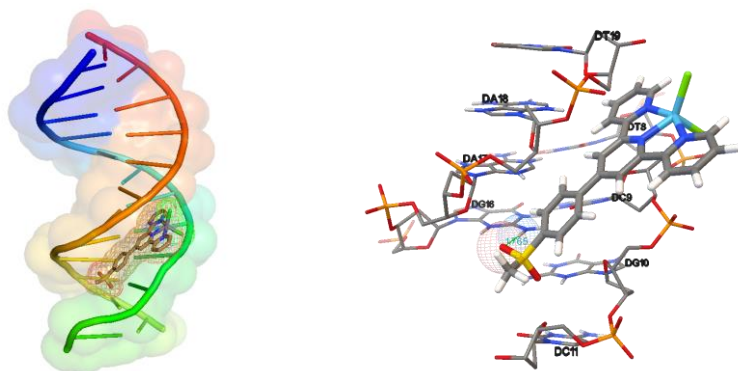


Figure S45 The most favorable orientation of compound **10** bound with the minor groove of the B-DNA (PDB ID: 1BNA). The formed hydrogen bond and distance have been marked.

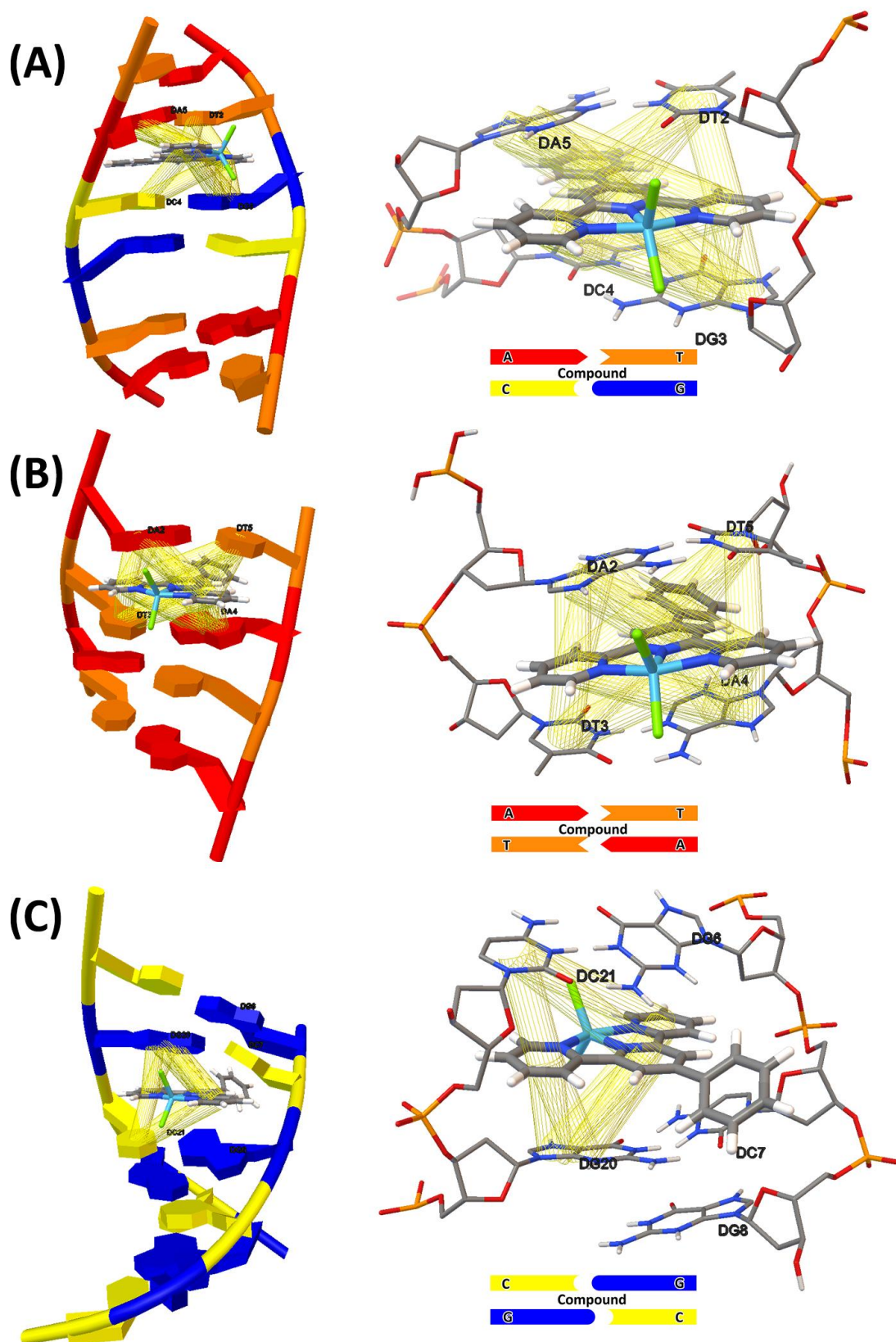


Figure S46 View of the energy minimized docked poses of compound **1** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

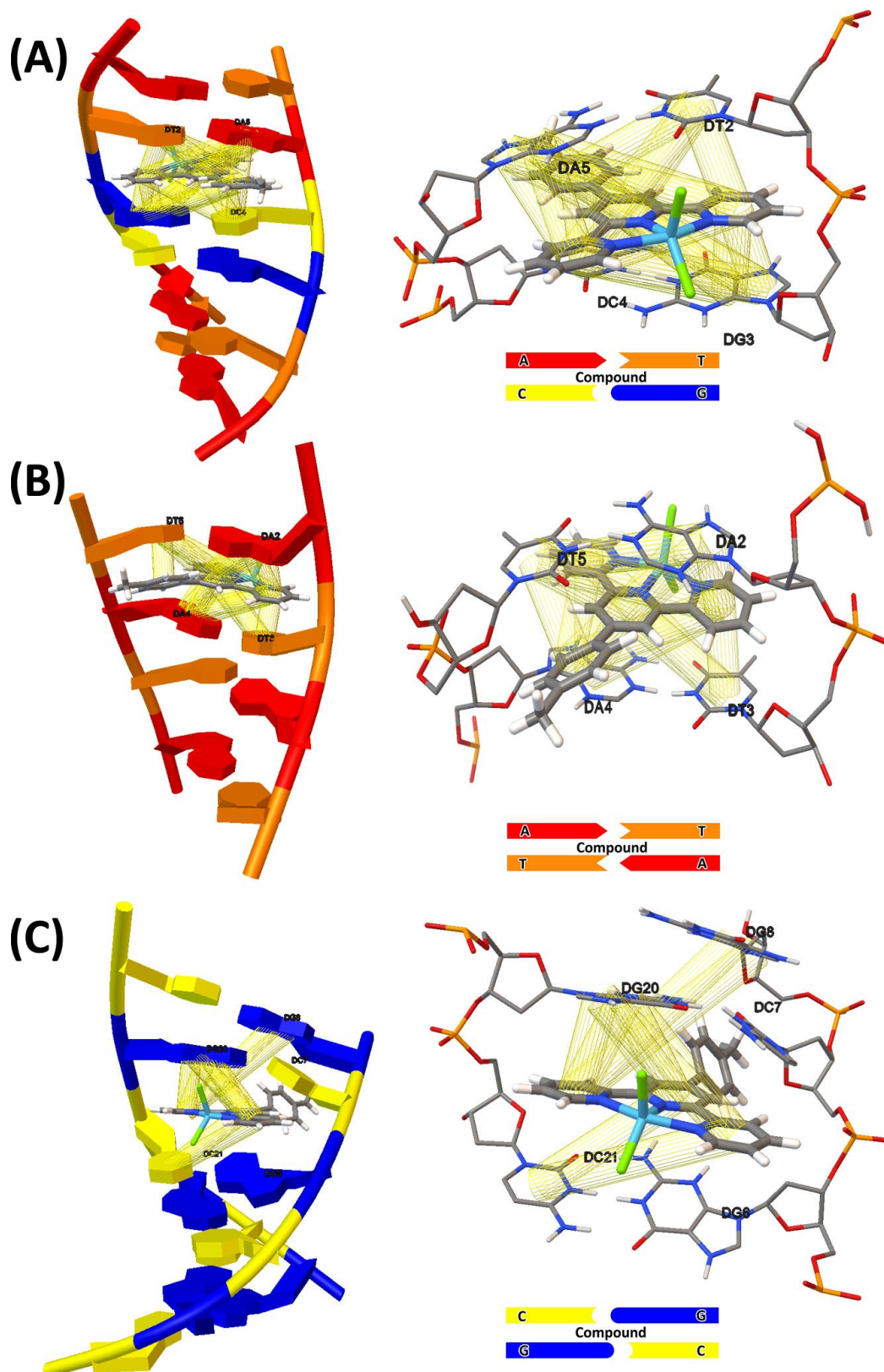


Figure S47 View of the energy minimized docked poses of compound **2** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

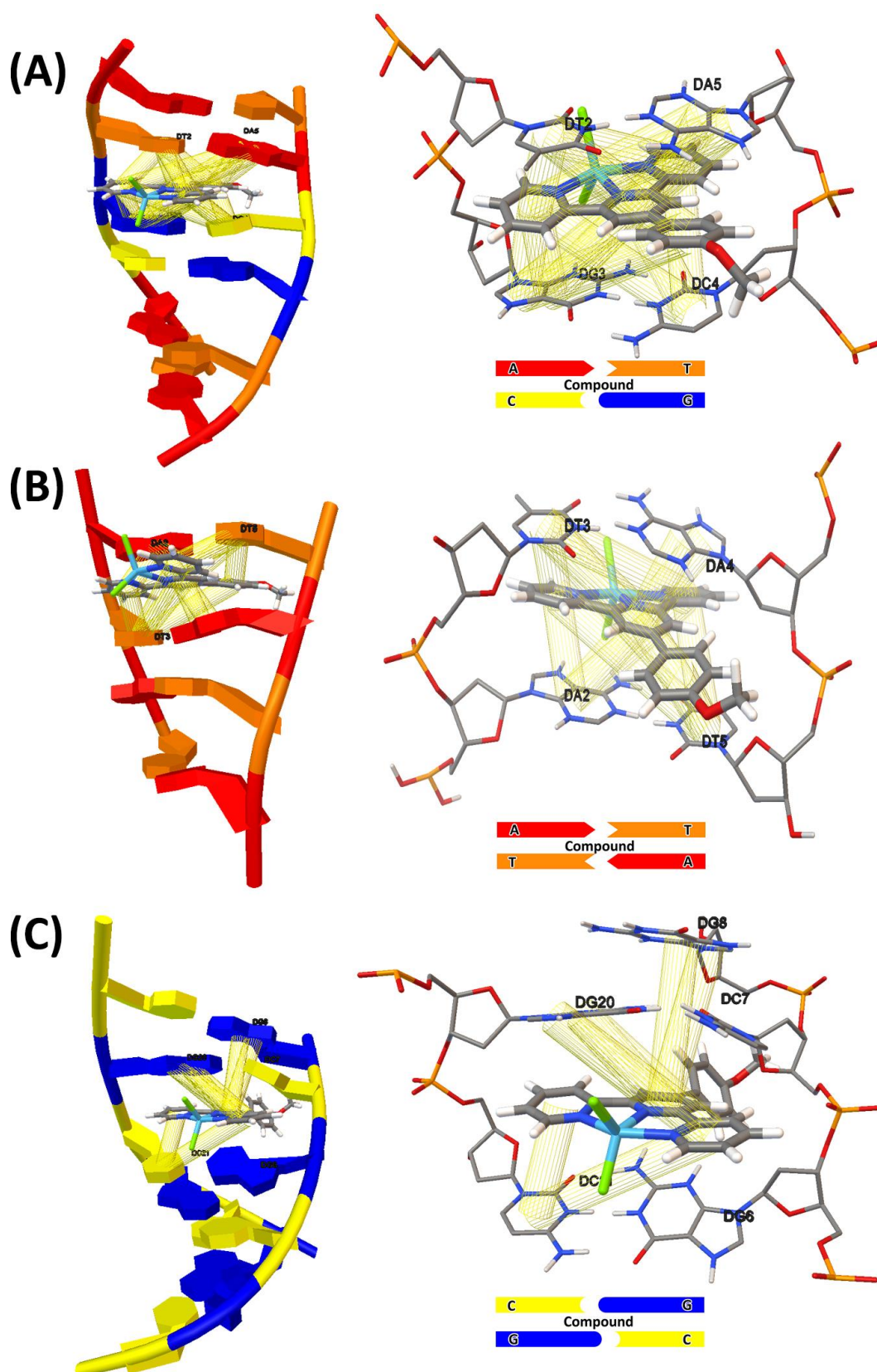


Figure S48 View of the energy minimized docked poses of compound **3** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

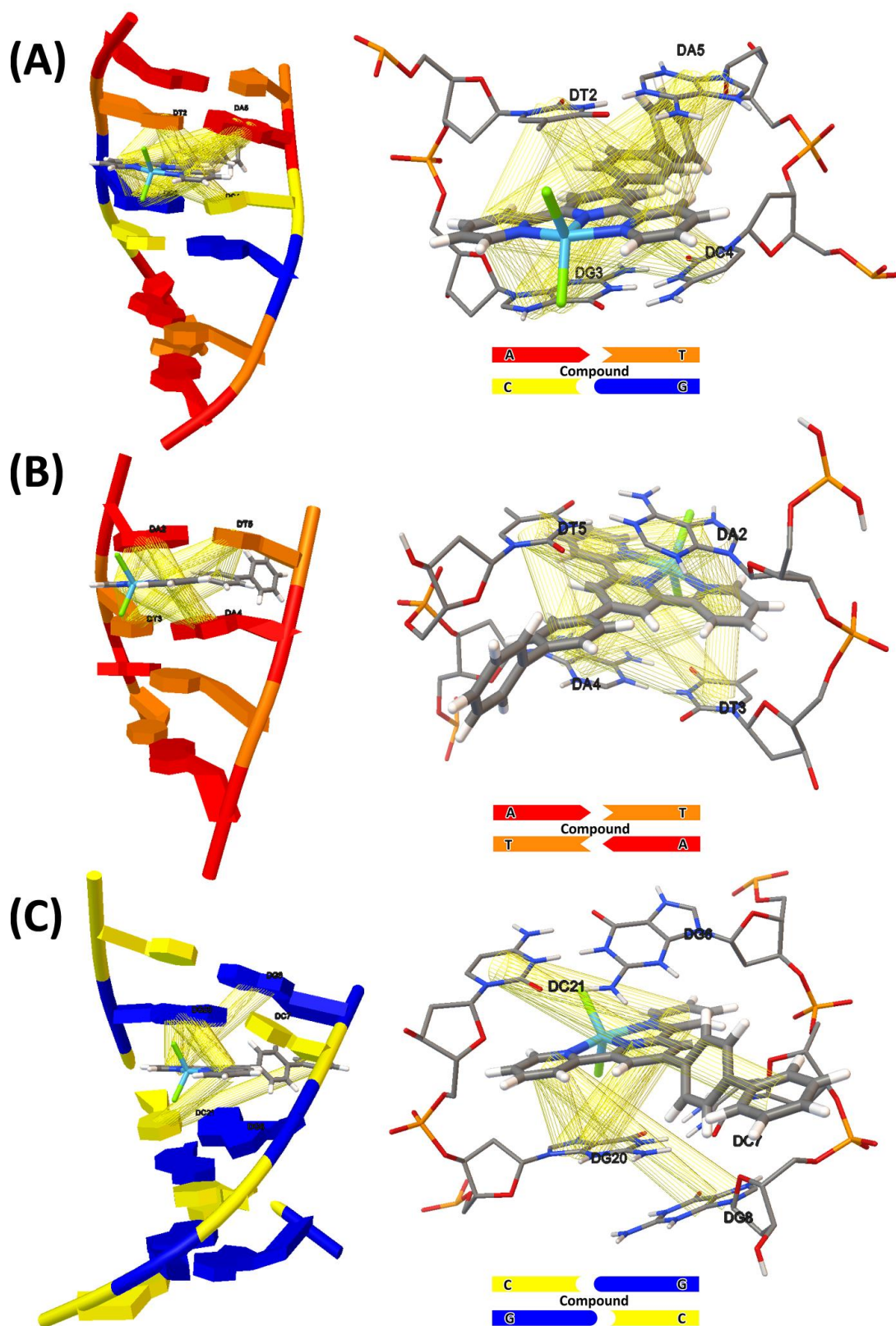


Figure S49 View of the energy minimized docked poses of compound 4 with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

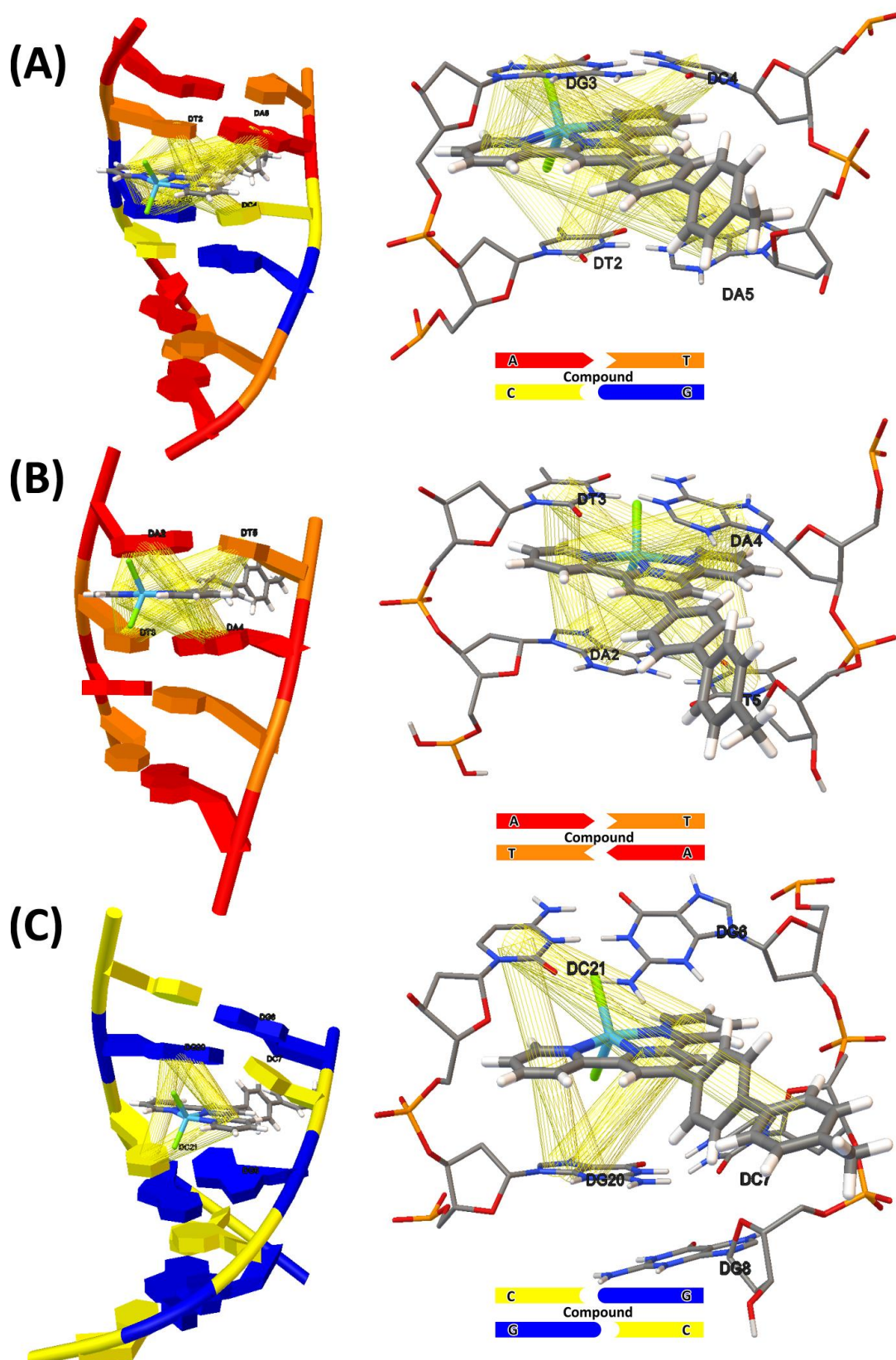


Figure S50 View of the energy minimized docked poses of compound **5** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

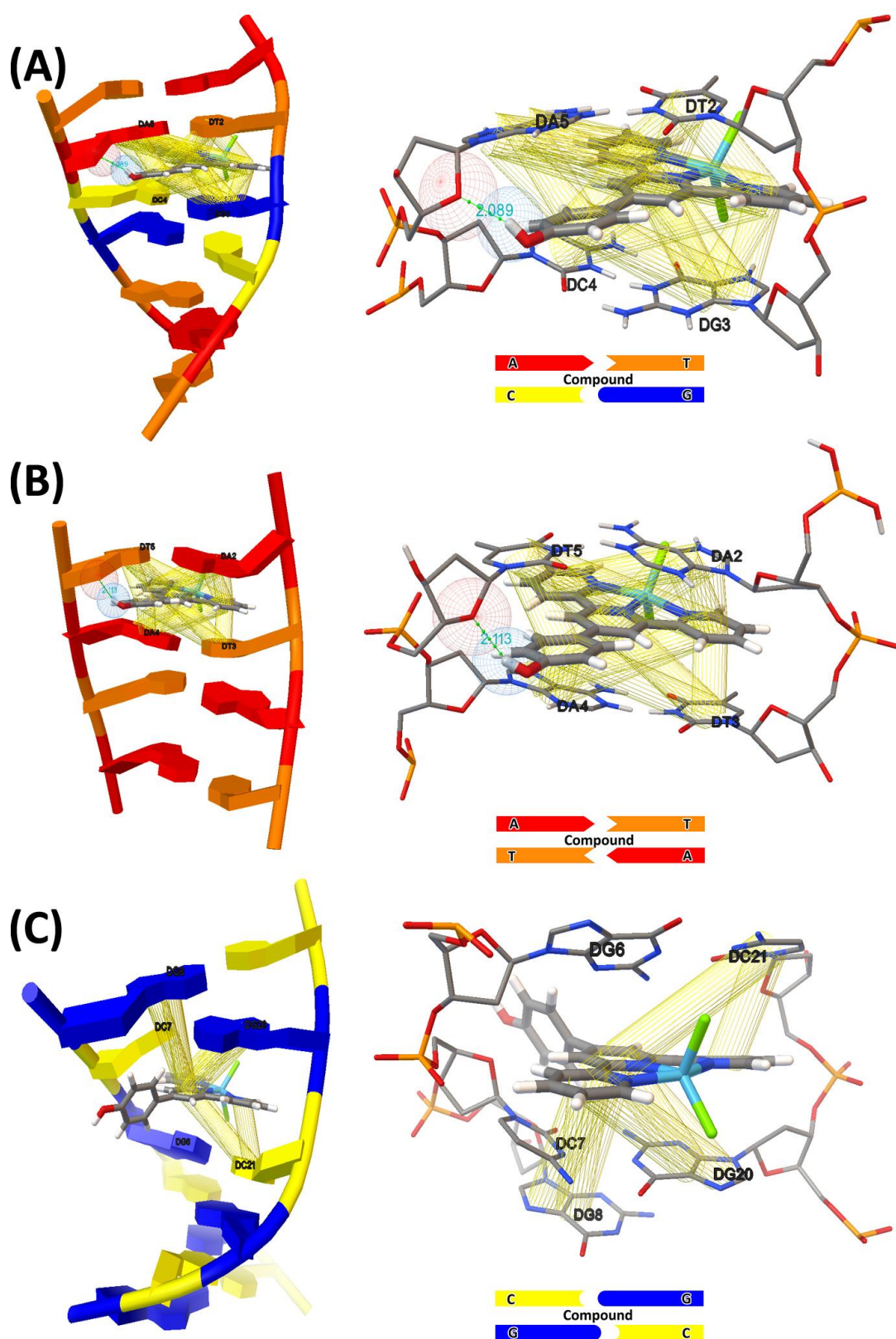


Figure S51 View of the energy minimized docked poses of compound **6** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

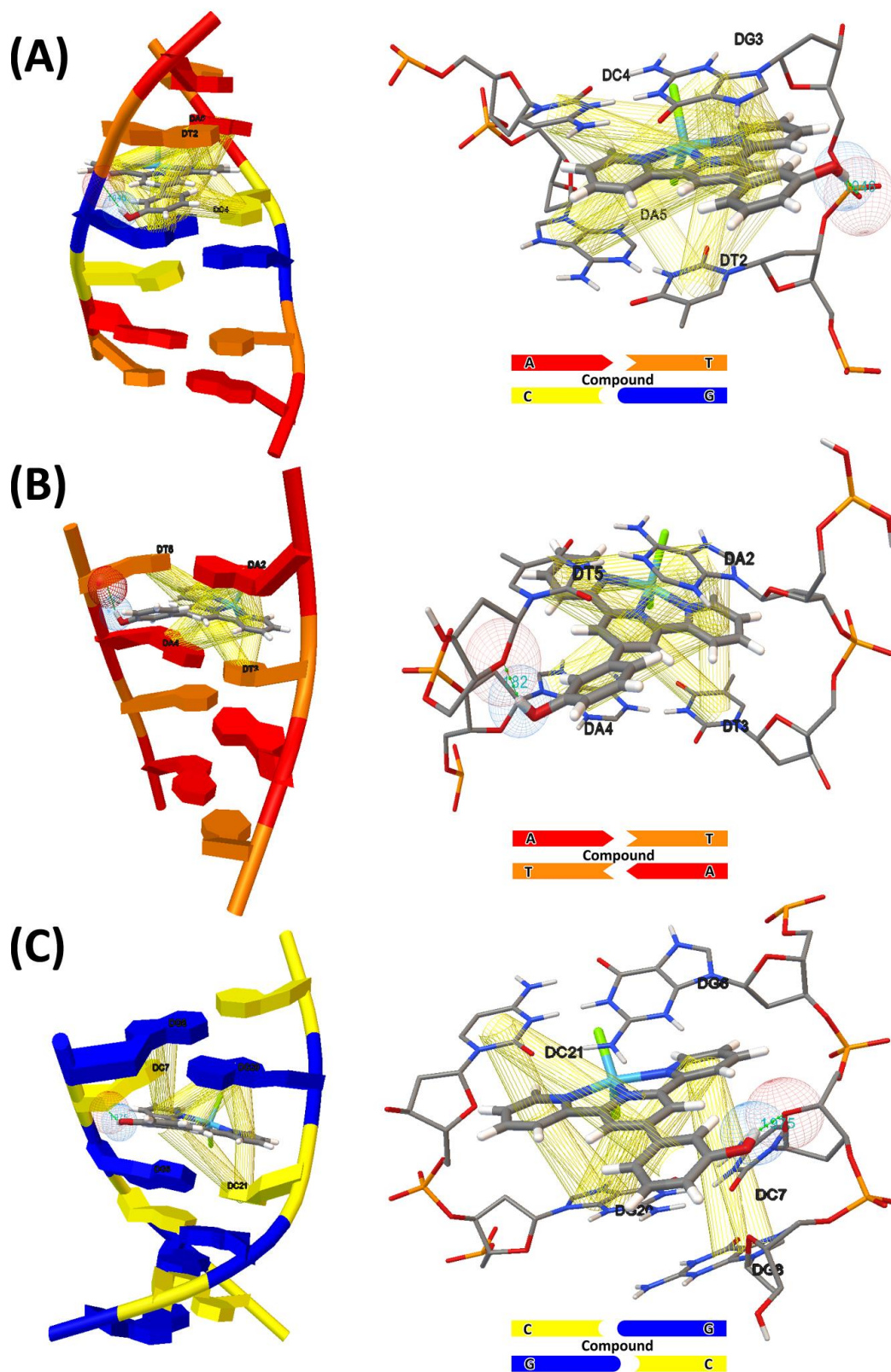


Figure S52 View of the energy minimized docked poses of compound **7** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

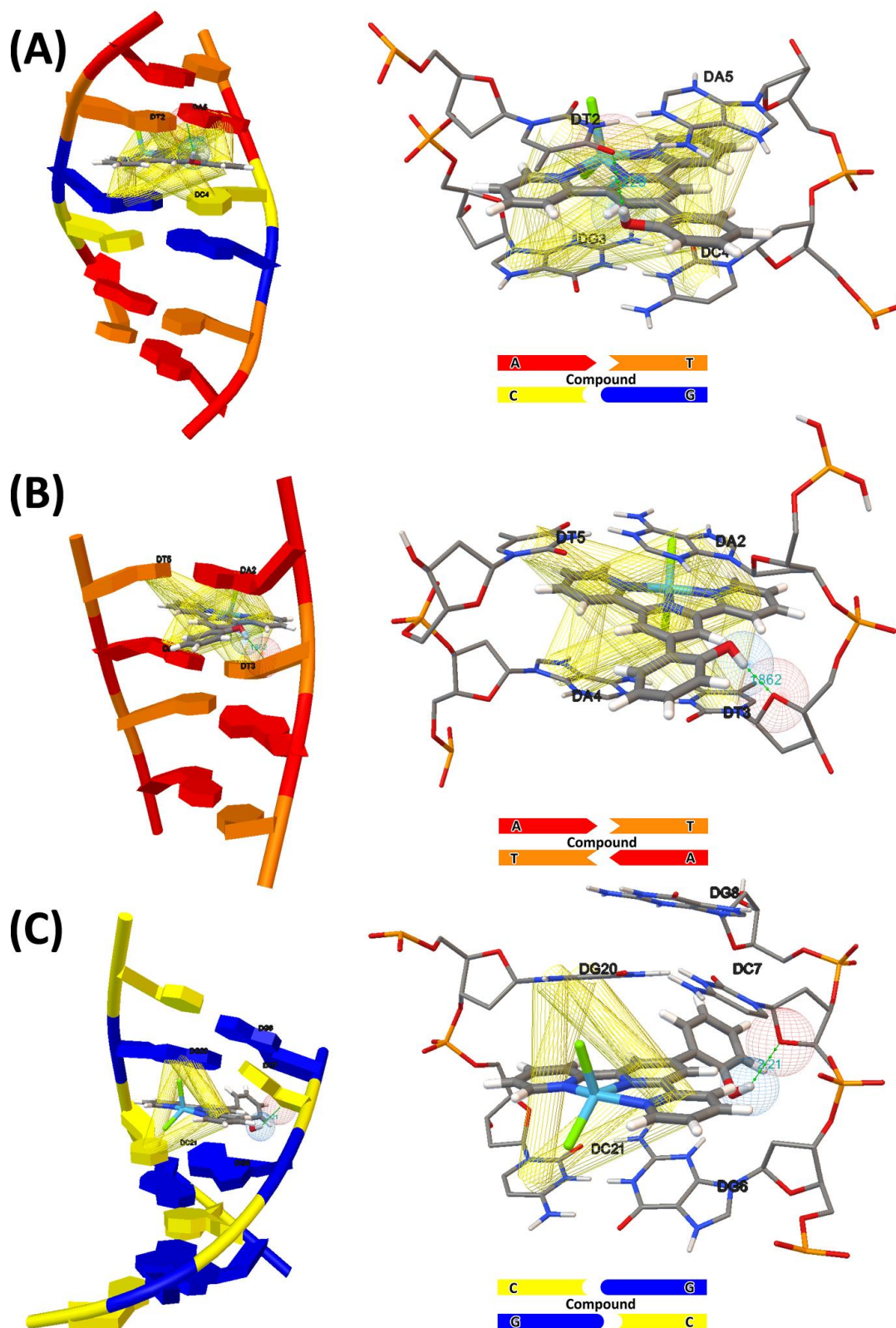


Figure S53 View of the energy minimized docked poses of compound **8** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).

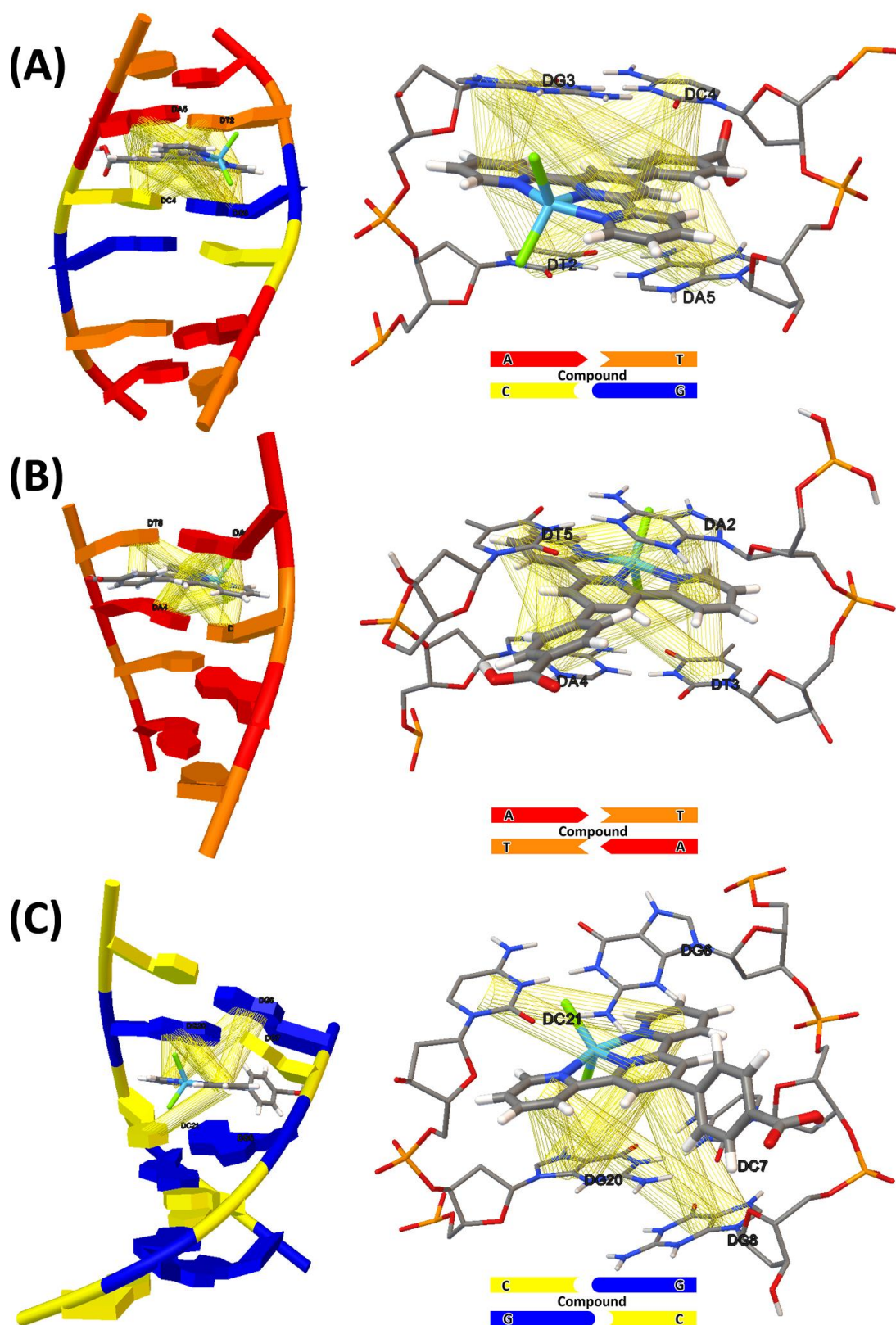


Figure S54 View of the energy minimized docked poses of compound **9** with (A) ds(ATGCAT)₂ (PDB ID: 4JD8), (B) ds(ATAT)₂ (PDB ID: 2DA8M), and (C) ds(CGCGCG)₂ (PDB ID: 2ROUM).