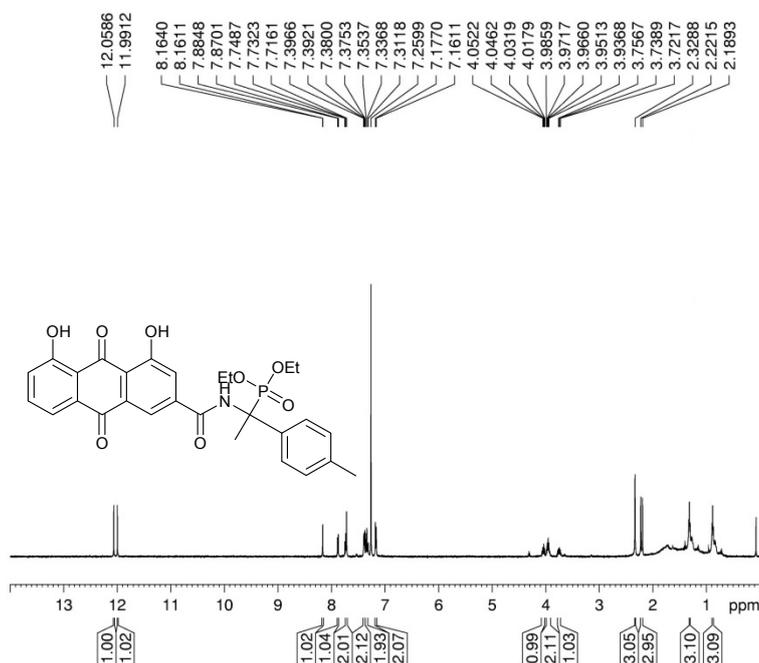


Supplementary Information

NMR spectra of new compounds, **5a–c**

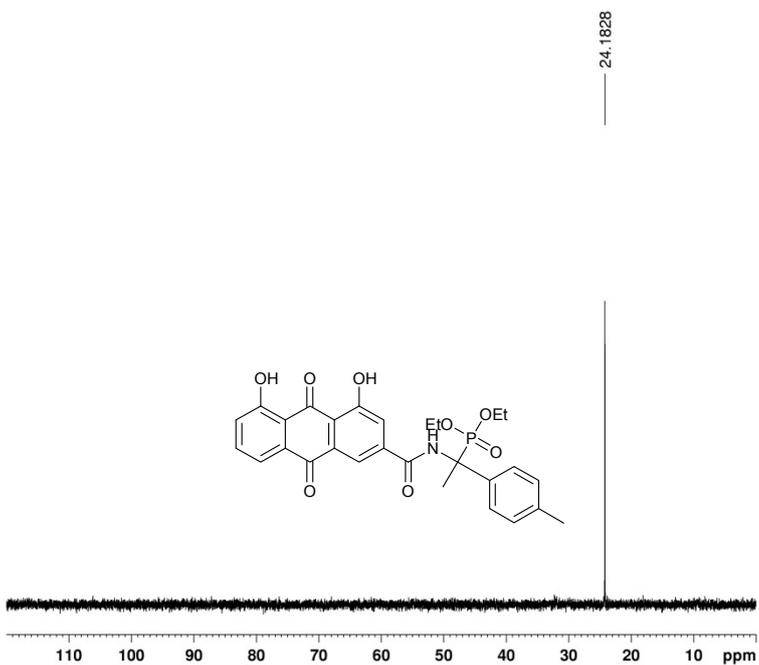
A. Compound **5a**



Current Data Parameters
 NAME whs-ygy-120515jajibe
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20120618
 Time 20.01
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 13
 DS 2
 SWH 8503.401 Hz
 FIDRES 0.129752 Hz
 AQ 3.8536255 sec
 RG 645.1
 DW 58.800 usec
 DE 6.00 usec
 TE 298.5 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
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 P1 7.70 usec
 PL1 1.00 dB
 SFO1 500.1337539 MHz
 F2 - Processing parameters
 SI 16384
 SF 500.1300132 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME whs-ygy-010515jajibenyitong
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date 20120618
 Time 19.59
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpgg
 TD 65536
 SOLVENT CDCl3
 NS 24
 DS 2
 SWH 60606.063 Hz
 FIDRES 0.324775 Hz
 AQ 0.5407302 sec
 RG 23170.5
 DW 8.250 usec
 DE 6.00 usec
 TE 298.4 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 31P
 P0 13.50 usec
 PL1 4.00 dB
 SFO1 202.4765510 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL12 16.10 dB
 PL13 16.10 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

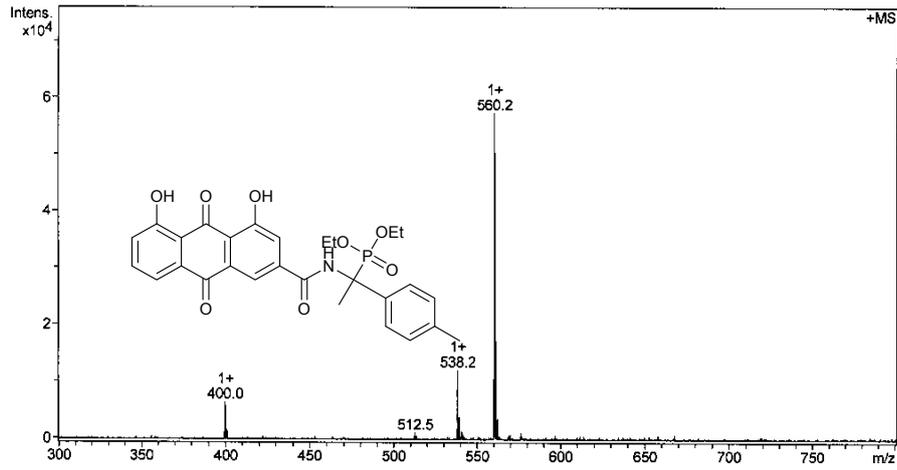
Mass Spectrum List Report

Analysis Info

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 Comment Instrument HCT

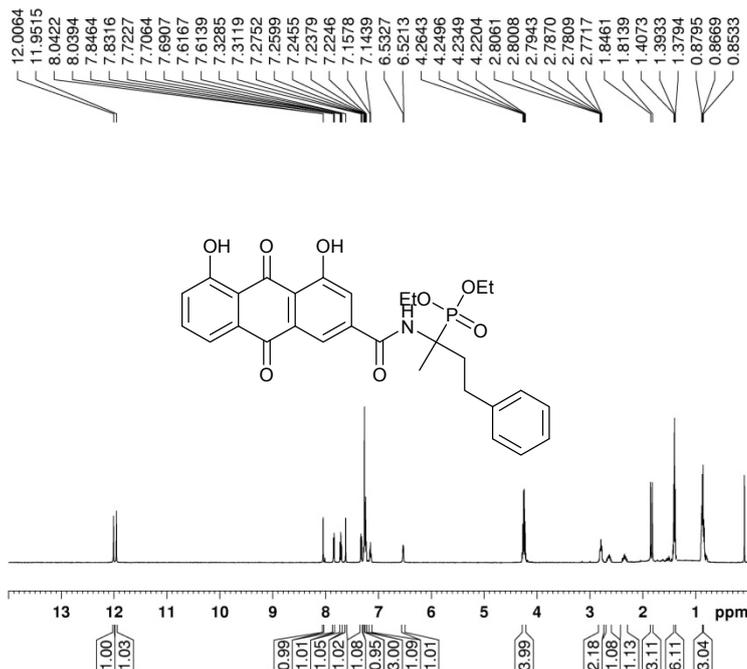
Acquisition Parameter

Ion Source Type ESI Ion Polarity Positive Alternating Ion Polarity off
 Mass Range Mode Std/Enhanced Scan Begin 300 m/z Scan End 800 m/z
 Capillary Exit 126.0 Volt Skimmer 40.0 Volt Trap Drive 120.3
 Accumulation Time 11471 μ s Averages 10 Spectra Auto MS/MS off



#	m/z	I
1	400.0	6319
2	401.1	1637
3	512.5	1101
4	538.2	12048
5	539.2	3868
6	540.6	1334
7	560.2	57236
8	561.2	17212
9	562.2	3504
10	576.1	3980

B. Compound 5b

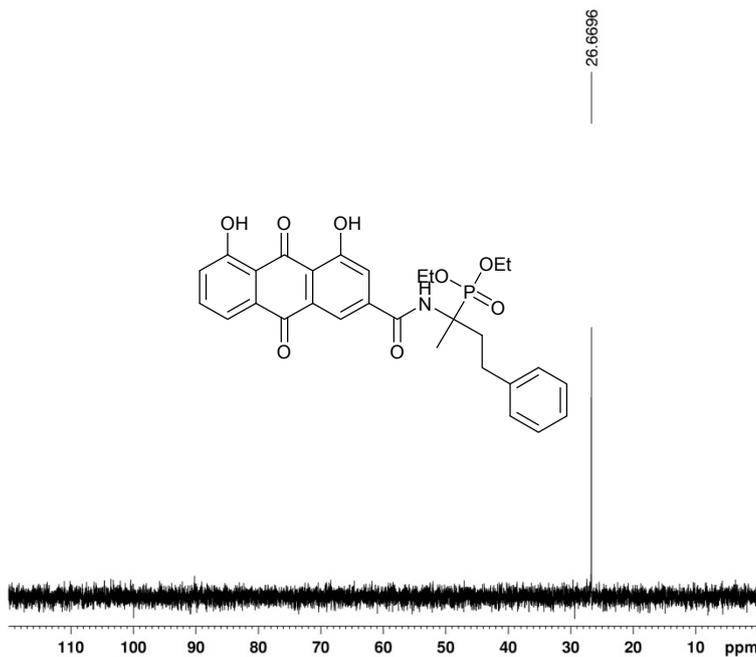


Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 Time 19.47
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8503.401 Hz
 FIDRES 0.129752 Hz
 AQ 3.8538255 sec
 RG 181
 DW 58.800 usec
 DE 6.00 usec
 TE 300.5 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 1.00 dB
 SFO1 500.1337539 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300137 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME whs-ygy-120512
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 20.56
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpgg
 TD 65536
 SOLVENT CDCl3
 NS 27
 DS 2
 SWH 60606.063 Hz
 FIDRES 0.924775 Hz
 AQ 0.5407302 sec
 RG 23170.5
 DW 8.250 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 31P
 P0 13.50 usec
 PL1 4.00 dB
 SFO1 202.4765510 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL12 16.10 dB
 PL13 16.10 dB
 SFO2 500.1320005 MHz

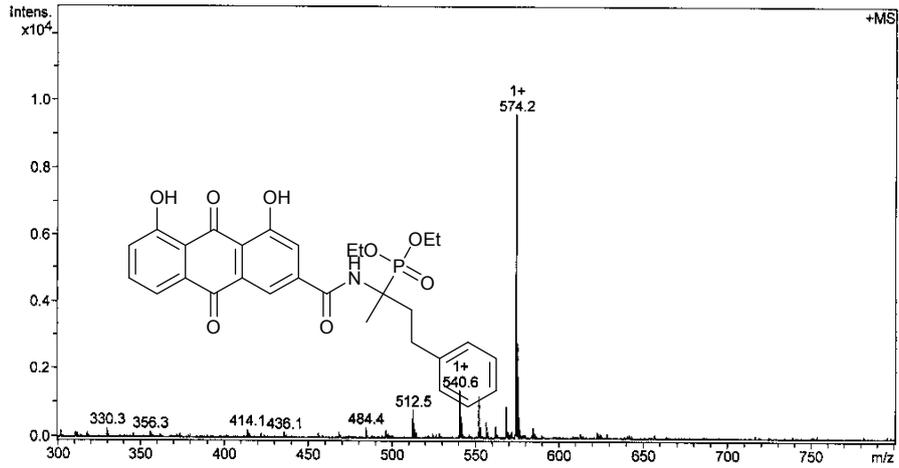
Mass Spectrum List Report

Analysis Info

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 Method aHCT_ESI_Profile.MS.m Operator hct
 Comment Instrument HCT

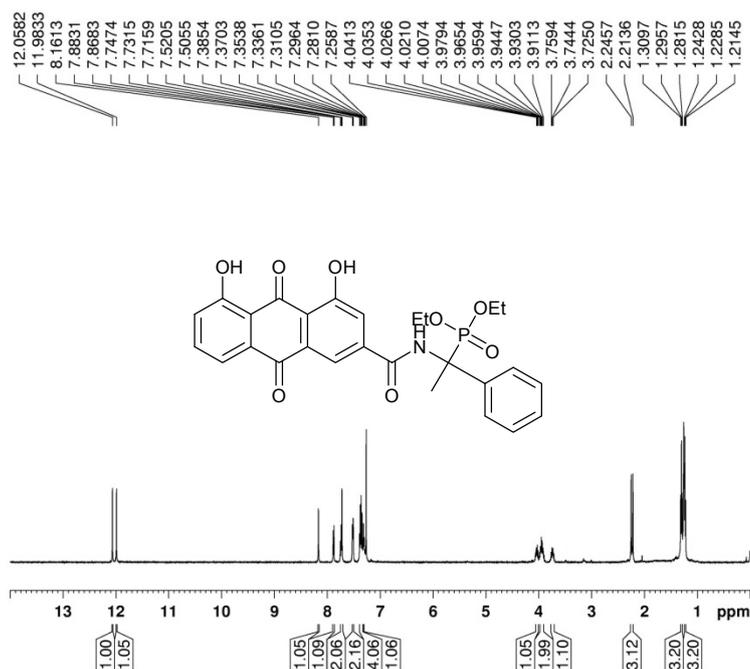
Acquisition Parameter

Ion Source Type ESI Ion Polarity Positive Alternating Ion Polarity off
 Mass Range Mode Std/Enhanced Scan Begin 300 m/z Scan End 800 m/z
 Capillary Exit 126.0 Volt Skimmer 40.0 Volt Trap Drive 120.3
 Accumulation Time 72696 μ s Averages 10 Spectra Auto MS/MS off



#	m/z	I
1	512.5	809
2	540.6	1382
3	541.5	620
4	552.2	1212
5	556.5	456
6	568.6	910
7	574.2	9595
8	575.2	2767
9	576.2	594
10	590.2	1064

C. Compound 5c

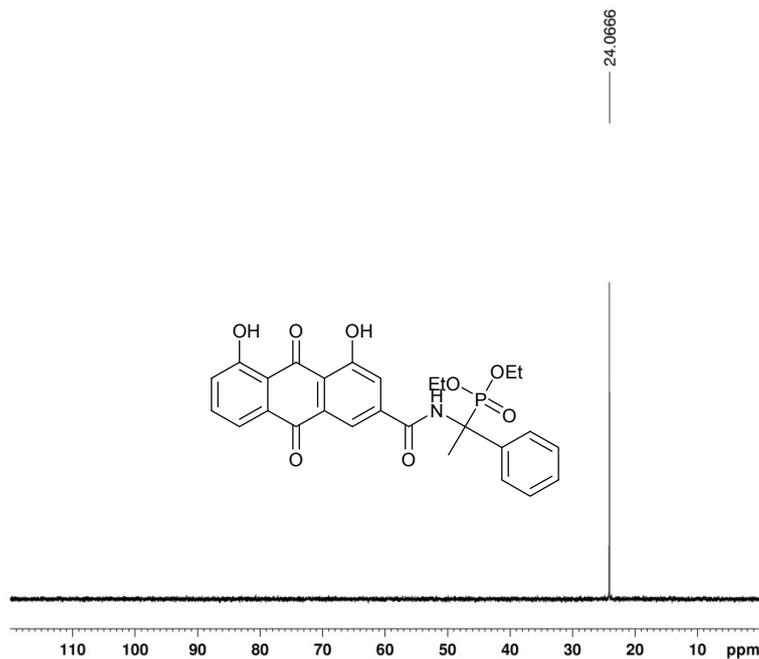


Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 20:23
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 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 2
 SWH 8503.401 Hz
 FIDRES 0.129752 Hz
 AQ 3.8536255 sec
 RG 724.1
 DW 58.800 usec
 DE 6.00 usec
 TE 298.4 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 1.00 dB
 SFO1 500.1337539 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300135 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME whs-yyg-120422benyit
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120618
 Time 20:27
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg0pg
 TD 65536
 SOLVENT CDCl3
 NS 21
 DS 2
 SWH 60606.063 Hz
 FIDRES 0.924775 Hz
 AQ 0.5407302 sec
 RG 16384
 DW 8.250 usec
 DE 6.00 usec
 TE 298.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 31P
 P1 13.50 usec
 PL1 4.00 dB
 SFO1 202.4765510 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL12 16.10 dB
 PL13 16.10 dB
 SFO2 500.1320005 MHz

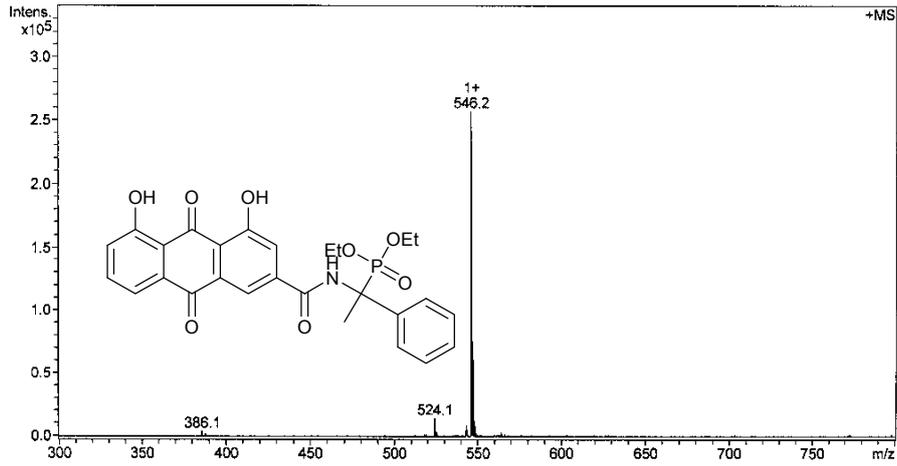
Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\wanghengshan\yaoguiyang\ESI-whs-ygy-120422-01.d
 Method aHCT_ESI_Pfile.MS.m Operator hct
 Comment Instrument HCT

Acquisition Parameter

Ion Source Type ESI Ion Polarity Positive Alternating Ion Polarity off
 Mass Range Mode Std/Enhanced Scan Begin 300 m/z Scan End 800 m/z
 Capillary Exit 126.0 Volt Skimmer 40.0 Volt Trap Drive 120.3
 Accumulation Time 2685 μ s Averages 10 Spectra Auto MS/MS off



#	m/z	I
1	386.1	3727
2	524.1	14403
3	525.2	3780
4	543.1	8473
5	543.6	5184
6	546.2	256566
7	547.2	75351
8	548.2	12066
9	562.1	28998
10	563.1	8790

Figure S1. UV-Vis absorption spectra of complex **5a** in the absence (---) and presence (—) of ct-DNA with increasing [DNA]/[**5a**] ratios in the range from 1:1 to 7:1.

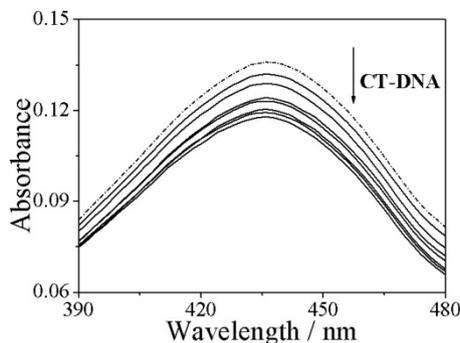


Figure S2. UV-Vis absorption spectra of complex **5c** in the absence (---) and presence (—) of ct-DNA with increasing [DNA]/[**5c**] ratios in the range from 1:1 to 7:1.

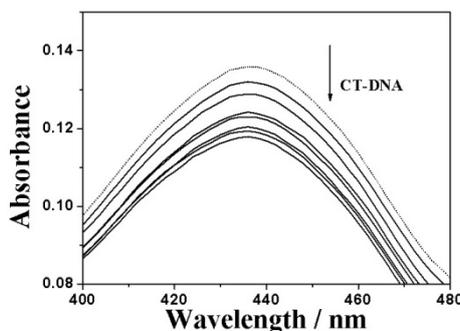


Figure S3. Fluorescence emission spectra of GelRed bound with ct-DNA ($[DNA] = 2.0 \times 10^{-3}$ M, $[GelRed] = 2.0 \times 10^{-3}$ M) in the absence (dash line) and presence (solid lines) of **5a** with [**5a**]/[GelRed] ratios range from 1:1 to 8:1. Inset: linear fitting for quenching constant K_q based on Stern-Volmer equation.

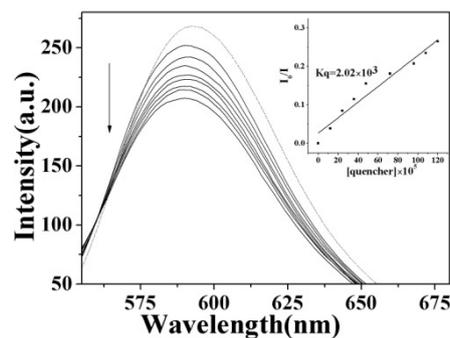


Figure S4. Fluorescence emission spectra of GelRed bound with ct-DNA ($[DNA] = 2.0 \times 10^{-3} \text{ M}$, $[GelRed] = 2.0 \times 10^{-3} \text{ M}$) in the absence (dash line) and presence (solid lines) of **5c** with $[5c]/[GelRed]$ ratios range from 1:1 to 7:1. Inset: linear fitting for quenching constant K_q based on Stern-Volmer equation.

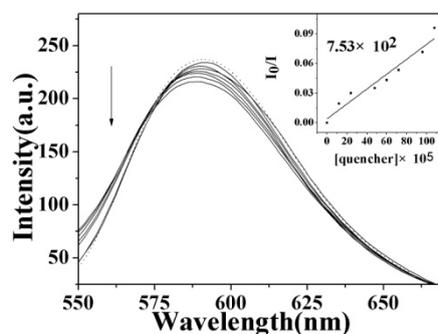


Figure S5. The quenching constant K_q of rhein.

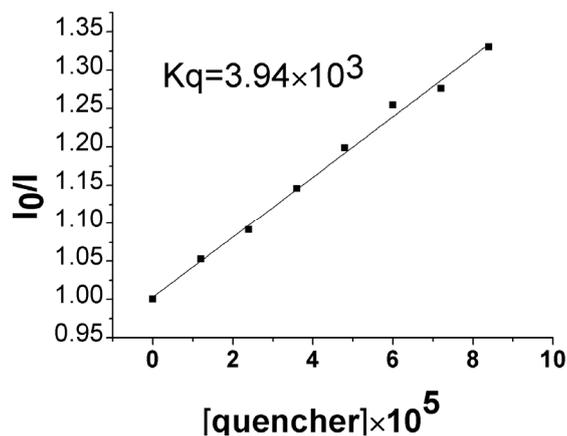


Figure S6. CD spectra of ct-DNA (2 mL solution, $1.5 \times 10^{-4} \text{ M}$) in the absence and presence of **5a** ($1.5 \times 10^{-5} \text{ M}$).

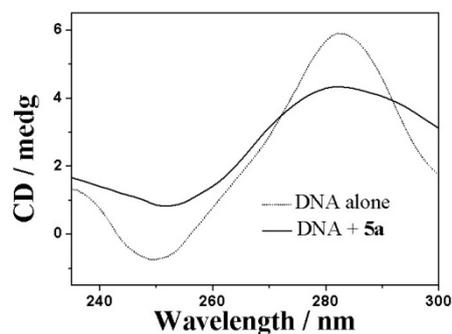
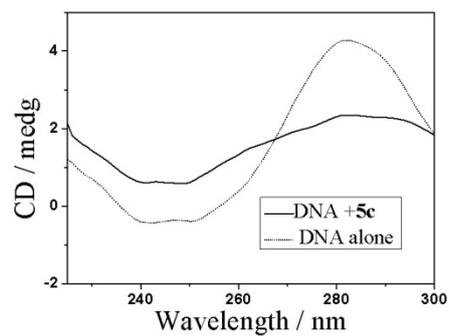


Figure S7. CD spectra of ct-DNA (2 mL solution, 1.5×10^{-4} M) in the absence and presence of **5c** (1.5×10^{-5} M).



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