

# Supplementary Information

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

A. Compound **5a**

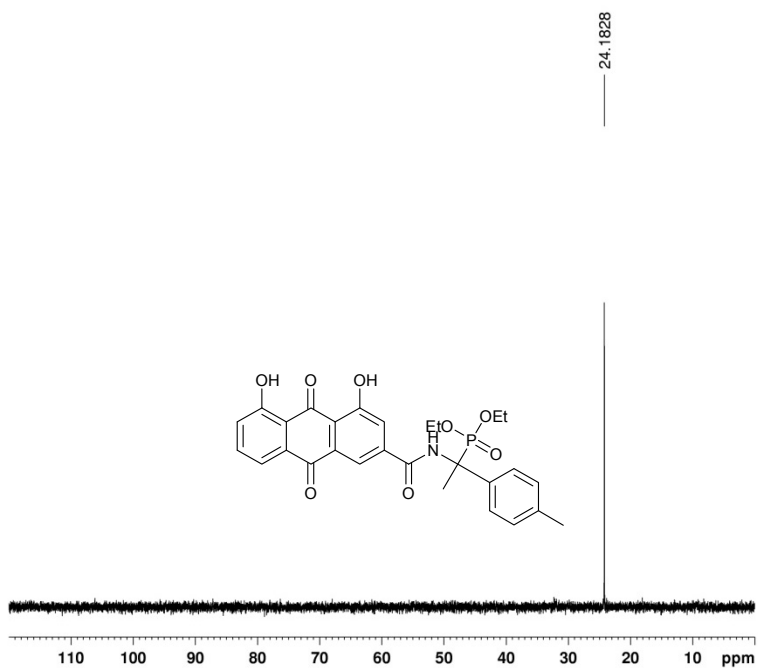


Current Data Parameters  
NAME whs-ygy-120515jiajibe  
EXPNO 1  
PROCNO 1

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 1.00000000 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 500.1300132 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME whs-ygy-010515jiajibenyitong  
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 2.00000000 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

F2 - Processing parameters  
SI 32768  
SF 202.4563100 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## Mass Spectrum List Report

## Analysis Info

Analysis Name D:\Data\wanghengshan\yaoguiyang\ESI-whs-ygy-120515.d

Method aHCT\_ESI\_Profile.MS.m

Comment

Operator

hct

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

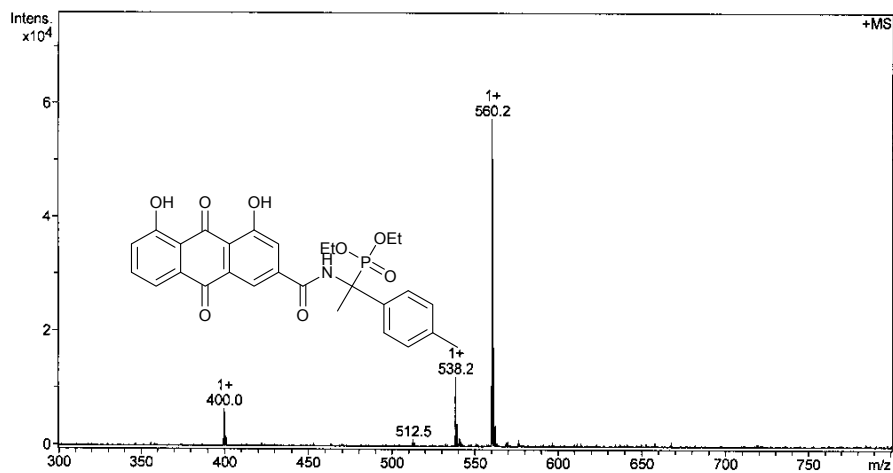
Accumulation Time 11471  $\mu$ s

Averages

10 Spectra

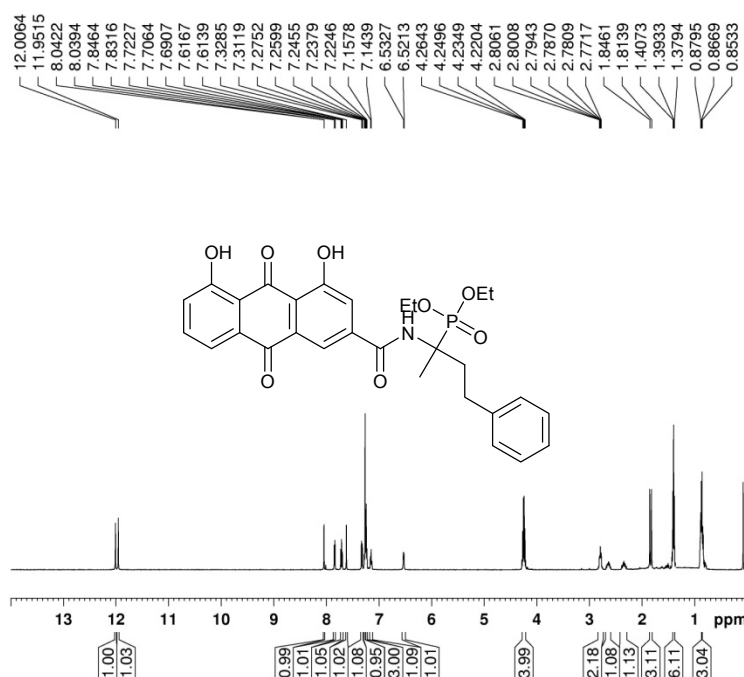
Auto MS/MS

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

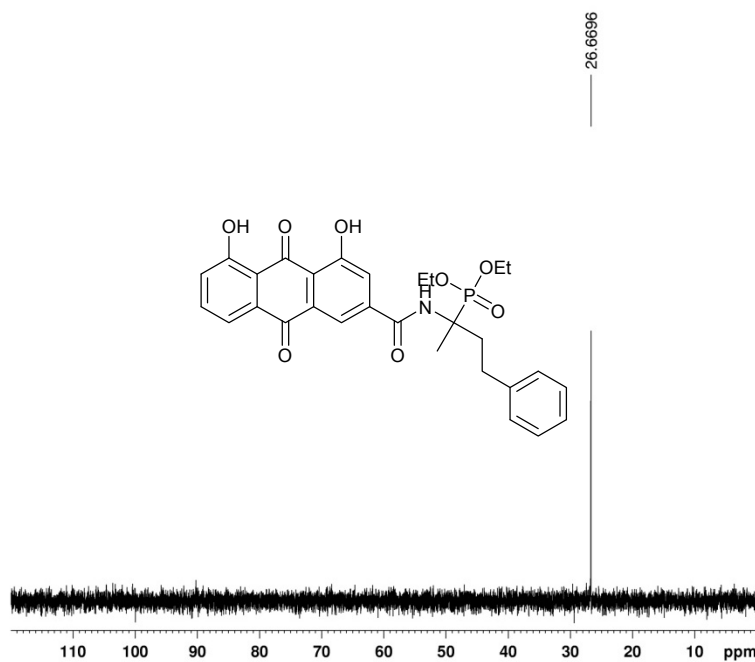


Current Data Parameters  
NAME whs-ygy-120512  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120518  
Time 19.47  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 8503.401 Hz  
FIDRES 0.129752 Hz  
AQ 3.8536255 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 zgpg  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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

Analysis Name D:\Data\wanghengshan\yaoguiyang\ESI-whs-ygy-120512.d

Method aHCT\_ESI\_Profile.MS.m

Comment

Operator

hct

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

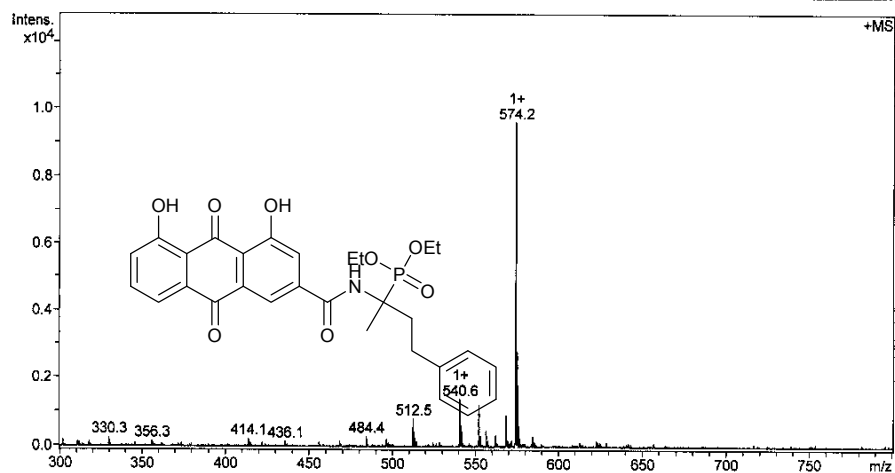
Accumulation Time 72696  $\mu$ s

Averages

10 Spectra

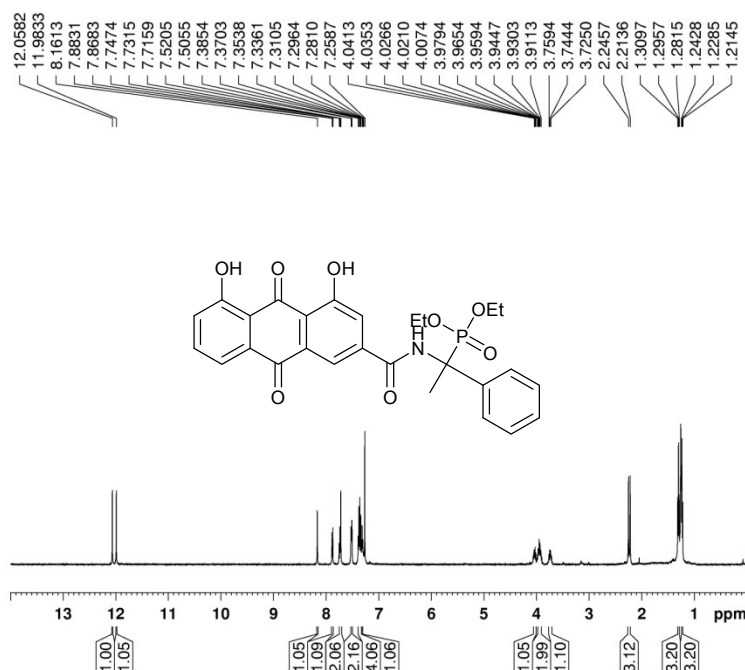
Auto MS/MS

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

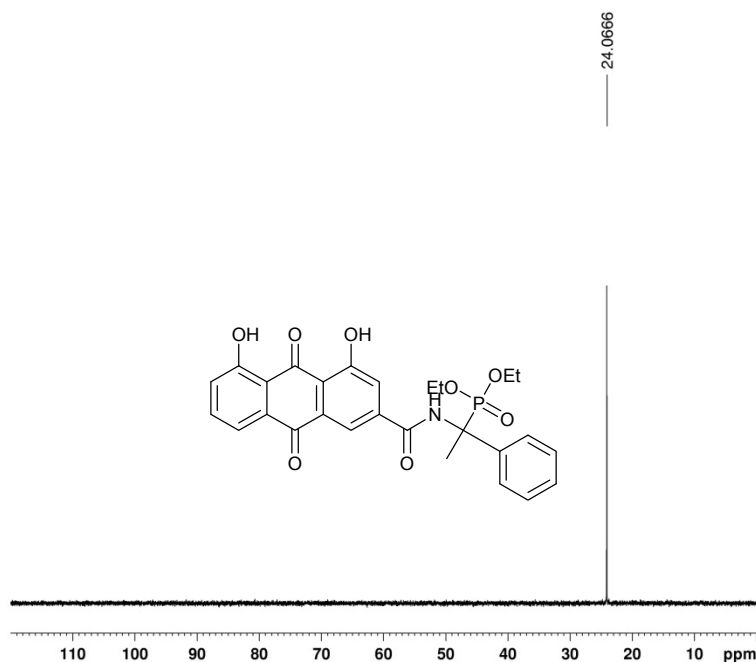


Current Data Parameters  
 NAME whs-ygy-120422benyit  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120618  
 Time 20.29  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 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  
 MCOREST 0.00000000 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 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-ygy-120422benyit  
 EXPNO 31  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120618  
 Time 20.27  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 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  
 MCOREST 0.00000000 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 <sup>31</sup>P  
 P0 13.50 usec  
 PL1 4.00 dB  
 SFO1 202.4765510 MHz

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

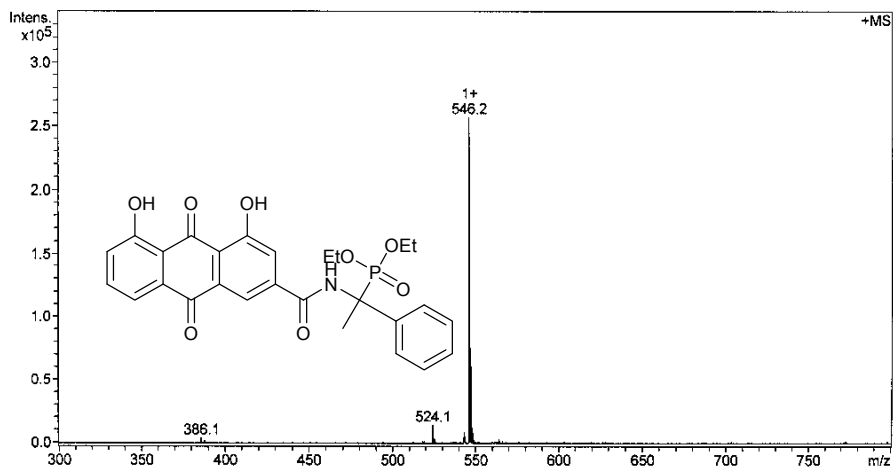
## Mass Spectrum List Report

## Analysis Info

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

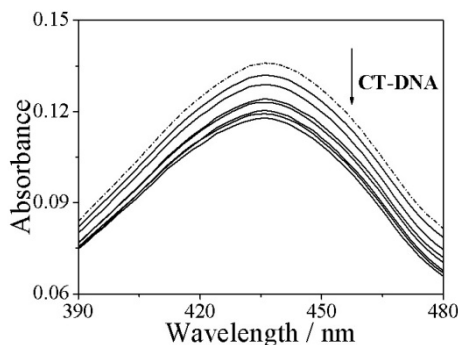
## Acquisition Parameter

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	2685 $\mu$ s	Averages	10 Spectra	Auto MS/MS	off

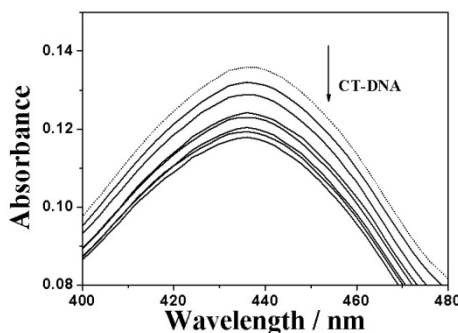


#	m/z	I
1	386.1	3727
2	524.1	14403
3	525.2	3780
4	543.1	8473
5	543.6	5184
6	546.2	256566
7	547.2	75351
8	548.2	12086
9	562.1	28998
10	563.1	8790

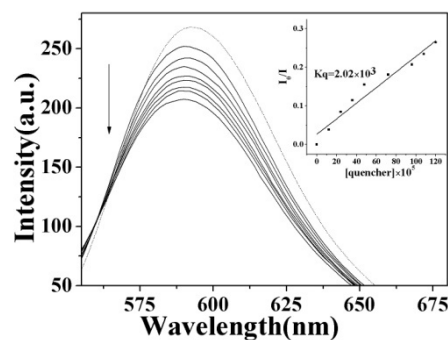
**Figure S1.** UV-Vis absorption spectra of complex **5a** in the absence (---) and presence (—) of ct-DNA with increasing [DNA]/[**5a**] ratios in the range from 1:1 to 7:1.



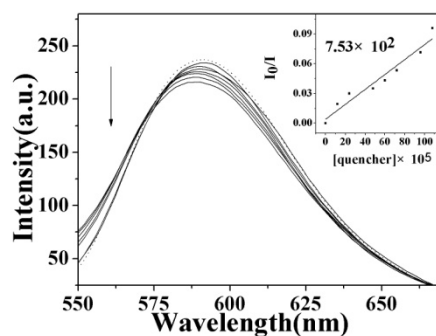
**Figure S2.** UV-Vis absorption spectra of complex **5c** in the absence (---) and presence (—) of ct-DNA with increasing [DNA]/[**5c**] ratios in the range from 1:1 to 7:1.



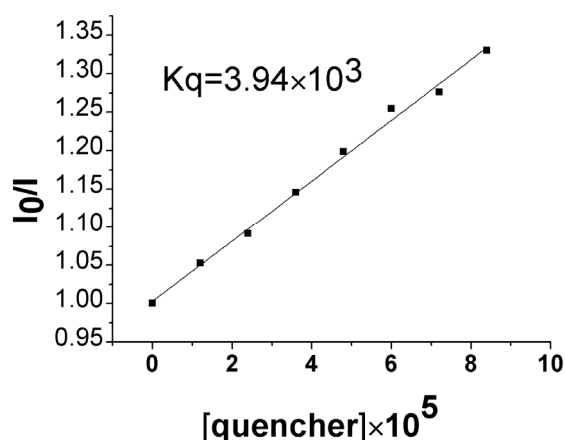
**Figure S3.** Fluorescence emission spectra of GelRed bound with ct-DNA ( $[\text{DNA}] = 2.0 \times 10^{-3} \text{ M}$ ,  $[\text{GelRed}] = 2.0 \times 10^{-3} \text{ M}$ ) in the absence (dash line) and presence (solid lines) of **5a** with [**5a**]/[GelRed] ratios range from 1:1 to 8:1. Inset: linear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



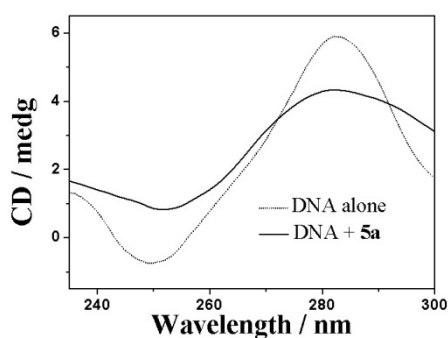
**Figure S4.** Fluorescence emission spectra of GelRed bound with ct-DNA ( $[\text{DNA}] = 2.0 \times 10^{-3} \text{ M}$ ,  $[\text{GelRed}] = 2.0 \times 10^{-3} \text{ M}$ ) in the absence (dash line) and presence (solid lines) of **5c** with  $[\text{5c}]/[\text{GelRed}]$  ratios range from 1:1 to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



**Figure S5.** The quenching constant  $K_q$  of rhein.

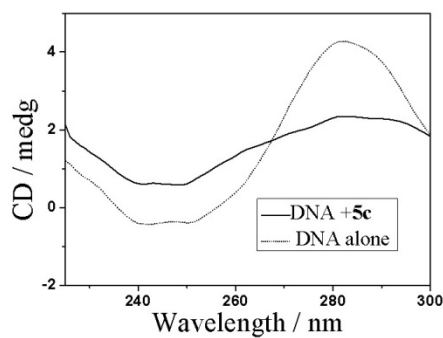


**Figure S6.** CD spectra of ct-DNA (2 mL solution,  $1.5 \times 10^{-4} \text{ M}$ ) in the absence and presence of **5a** ( $1.5 \times 10^{-5} \text{ M}$ ).





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



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