10.1071/CH10302_AC

Australian Journal of Chemistry 2011, 64(3), 345–354

ACCESSORY PUBLICATION

Crystal Structures, Antioxidation and DNA Binding Properties of Sm(III) Complexes

Yongchun Liu,[A,B] *Zhengyin Yang,*[A] *Kejun Zhang,*[B] *Yun Wu,*[B] *Jihua Zhu*[B] and *Tianlin Zhou*[B]

[A]College of Chemistry and Chemical Engineering, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, 730000 Lanzhou, P. R. China. Tel.: +86-931-8913515, Fax: +86-931-8912582. Corresponding author: Zhengyin Yang, Email: yangzy@lzu.edu.cn

[B]College of Chemistry and Chemical Engineering, Key Laboratory of Longdong Biological Resources in Gansu Province, Longdong University, 745000 Qingyang, Gansu, P. R. China.

Table of contents

molar concentration of every investigated compound is 10.0 μM. The molar concentrations of DNA (bps) at approximately saturated titration end points for **1a**, **1b**, **1c**, **2a**, **2b** and **2c** are 20.0, 16.0, 14.0, 16.0, 14.0, 16.0 μM, respectively.

Fig. S1. Spectra of ^{1}H NMR for ligand **1a** (A) and complex **2a** (B).

Fig. S2. Effects of increasing amounts of the investigated compounds on the relative viscosity of CT-DNA in 5 mM Tris–HCl buffer solution (pH 7.20) containing 50 mM NaCl at 25.00±0.01°C. Plots of (A) and (B) represent the ligands–CT-DNA and Sm(III) complexes–CT-DNA systems, respectively. The concentration of CT-DNA was 50 μM (bps).

Fig. S3. UV-vis titration spectra of EB-DNA system (A) and the plot of A/A_o versus C_{DNA}/C_{EB}.

Fig. S4. The fluorescence emission spectra and the corresponding excitation spectra for the fluorescence quenching of EB-DNA systems by the titrations of **2b** and **2c**, respectively.

Fig. S5. McGhee & von Hippel plots for ligands and the Sm(III) complexes titrated by DNA.

Fig. S6. Plots of antioxidation properties for ligands and Sm(III) complexes.

Table S1. Selected bond lengths (Å) and bond angles with the torsion angles (°).

(A) $[SmL^1(NO_3)(DMF)_2]_2$ complex

Bond length (Å)					
Sm(1)–O(2)	2.374(8)	Sm(1)–O(1)#1	2.420(7)	Sm(1)–O(7)	2.431(7)
Sm(1)–O(1)	2.462(7)	Sm(1)–O(6)	2.466(8)	Sm(1)–N(1)	2.545(8)
Sm(1)–O(4)	2.562(7)	Sm(1)–N(2)	2.591(9)	Sm(1)–O(3)	2.606(8)
Sm(1)–Sm(1)#1	4.0713(12)	N(1)–C(2)	1.347(14)	N(1)–C(3)	1.353(14)
N(2)–C(1)	1.283(13)	N(2)–N(3)	1.381(12)	N(3)–C(11)	1.339(14)
N(4)–O(5)	1.224(11)	N(4)–O(3)	1.257(12)	N(4)–O(4)	1.260(12)
N(5)–C(18)	1.314(15)	N(5)–C(20)	1.452(18)	N(5)–C(19)	1.467(15)
N(6)–C(21)	1.314(16)	N(6)–C(22)	1.431(17)	N(6)–C(23)	1.439(16)
O(1)–C(4)	1.345(11)	O(2)–C(11)	1.289(13)	O(6)–C(18)	1.236(13)
O(7)–C(21)	1.201(13)	C(1)–C(2)	1.444(17)	C(2)–C(10)	1.434(15)
C(3)–C(4)	1.427(15)	C(3)–C(8)	1.443(14)	C(4)–C(5)	1.363(15)
C(5)–C(6)	1.420(14)	C(6)–C(7)	1.352(17)	C(7)–C(8)	1.401(17)
C(8)–C(9)	1.399(17)	C(9)–C(10)	1.366(17)	C(11)–C(12)	1.500(17)
C(12)–C(17)	1.379(17)	C(12)–C(13)	1.404(16)	C(13)–C(14)	1.390(16)
C(14)–C(15)	1.367(19)	C(15)–C(16)	1.363(19)	C(16)–C(17)	1.388(18)
Bond angles (°)					
O(2)–Sm(1)–O(1)#1	98.0(2)	O(2)–Sm(1)–O(7)	78.2(3)	O(1)#1–Sm(1)–O(7)	75.4(2)
O(2)–Sm(1)–O(1)	162.6(2)	O(1)#1–Sm(1)–O(1)	67.0(2)	O(7)–Sm(1)–O(1)	89.1(3)
O(2)–Sm(1)–O(6)	77.8(3)	O(1)#1–Sm(1)–O(6)	73.2(2)	O(7)–Sm(1)–O(6)	137.0(3)
O(1)–Sm(1)–O(6)	104.7(3)	O(2)–Sm(1)–N(1)	123.0(3)	O(1)#1–Sm(1)–N(1)	125.5(3)
O(7)–Sm(1)–N(1)	79.6(3)	O(1)–Sm(1)–N(1)	65.0(3)	O(6)–Sm(1)–N(1)	143.2(3)
O(2)–Sm(1)–O(4)	126.1(3)	O(1)#1–Sm(1)–O(4)	112.8(3)	O(7)–Sm(1)–O(4)	150.2(3)
O(1)–Sm(1)–O(4)	70.0(2)	O(6)–Sm(1)–O(4)	70.9(3)	N(1)–Sm(1)–O(4)	72.5(3)
O(2)–Sm(1)–N(2)	61.5(3)	O(1)#1–Sm(1)–N(2)	140.3(3)	O(7)–Sm(1)–N(2)	67.6(3)
O(1)–Sm(1)–N(2)	124.4(3)	O(6)–Sm(1)–N(2)	127.2(3)	N(1)–Sm(1)–N(2)	61.6(3)
O(4)–Sm(1)–N(2)	106.4(3)	O(2)–Sm(1)–O(3)	81.1(3)	O(1)#1–Sm(1)–O(3)	146.5(2)
O(7)–Sm(1)–O(3)	135.8(3)	O(1)–Sm(1)–O(3)	116.2(2)	O(6)–Sm(1)–O(3)	73.9(3)
N(1)–Sm(1)–O(3)	79.7(3)	O(4)–Sm(1)–O(3)	48.8(3)	N(2)–Sm(1)–O(3)	68.2(3)
O(2)–Sm(1)–Sm(1)#1	131.30(18)	O(1)#1–Sm(1)–Sm(1)#1	33.81(17)	O(7)–Sm(1)–Sm(1)#1	80.9(2)
O(1)–Sm(1)–Sm(1)#1	33.16(14)	O(6)–Sm(1)–Sm(1)#1	88.9(2)	N(1)–Sm(1)–Sm(1)#1	95.2(2)
O(4)–Sm(1)–Sm(1)#1	91.33(19)	N(2)–Sm(1)–Sm(1)#1	143.0(2)	O(3)–Sm(1)–Sm(1)#1	139.67(19)
C(2)–N(1)–C(3)	121.8(10)	C(2)–N(1)–Sm(1)	121.1(8)	C(3)–N(1)–Sm(1)	116.6(7)
C(1)–N(2)–N(3)	117.4(10)	C(1)–N(2)–Sm(1)	122.6(9)	N(3)–N(2)–Sm(1)	120.0(7)
C(11)–N(3)–N(2)	108.6(9)	O(5)–N(4)–O(3)	121.8(11)	O(5)–N(4)–O(4)	122.1(11)
O(3)–N(4)–O(4)	116.0(9)	C(18)–N(5)–C(20)	119.9(11)	C(18)–N(5)–C(19)	122.4(13)

C(20)–N(5)–C(19)	117.4(12)	C(21)–N(6)–C(22)	120.4(12)	C(21)–N(6)–C(23)	122.0(14)
C(22)–N(6)–C(23)	117.6(13)	C(4)–O(1)–Sm(1)#1	127.4(7)	C(4)–O(1)–Sm(1)	118.8(7)
Sm(1)#1–O(1)–Sm(1)	113.0(2)	C(11)–O(2)–Sm(1)	122.6(8)	N(4)–O(3)–Sm(1)	96.5(6)
N(4)–O(4)–Sm(1)	98.6(6)	C(18)–O(6)–Sm(1)	130.9(8)	C(21)–O(7)–Sm(1)	144.5(9)
N(2)–C(1)–C(2)	116.2(12)	N(1)–C(2)–C(10)	118.7(12)	N(1)–C(2)–C(1)	117.3(10)
N(1)–C(3)–C(4)	117.4(10)	N(1)–C(3)–C(8)	121.9(11)	O(1)–C(4)–C(5)	124.5(11)
O(1)–C(4)–C(3)	118.4(11)	O(2)–C(11)–N(3)	125.5(11)	O(2)–C(11)–C(12)	118.6(11)
N(3)–C(11)–C(12)	115.9(11)	O(6)–C(18)–N(5)	125.1(12)	O(7)–C(21)–N(6)	127.1(14)

(B) $[SmL^2(NO_3)(DMF)_2]_2$ complex

Bond length (Å)					
Sm(1)–O(2)	2.382(3)	Sm(1)–O(5)	2.415(3)	Sm(1)–O(1)#1	2.426(3)
Sm(1)–O(4)	2.434(3)	Sm(1)–O(1)	2.445(3)	Sm(1)–N(1)	2.522(3)
Sm(1)–O(7)	2.569(3)	Sm(1)–N(2)	2.582(3)	Sm(1)–Sm(1)#1	4.0599(5)
Sm(1)–O(6)	2.594(3)	C(1)–N(1)	1.361(5)	C(1)–C(6)	1.421(6)
C(1)–C(2)	1.428(6)	C(1)–O(1)	1.331(4)	C(2)–C(3)	1.368(6)
C(3)–C(4)	1.409(6)	C(4)–C(5)	1.359(7)	C(5)–C(6)	1.393(7)
C(6)–C(7)	1.395(7)	C(7)–C(8)	1.354(7)	C(8)–C(9)	1.420(6)
C(9)–N(1)	1.329(5)	C(9)–C(10)	1.464(7)	C(10)–N(2)	1.284(5)
C(11)–O(2)	1.280(5)	C(11)–N(3)	1.332(6)	C(11)–C(12)	1.485(6)
C(12)–C(13)	1.384(6)	C(12)–C(17)	1.406(6)	C(13)–C(14)	1.384(7)
C(14)–C(15)	1.384(7)	C(15)–C(16)	1.339(7)	C(16)–C(17)	1.402(7)
C(17)–O(3)	1.336(6)	C(18)–O(4)	1.240(6)	C(18)–N(4)	1.304(6)
C(19)–N(4)	1.437(7)	C(20)–N(4)	1.445(8)	C(21)–O(5)	1.207(6)
C(21)–N(5)	1.302(6)	C(22)–N(5)	1.429(8)	C(23)–N(5)	1.437(9)
N(2)–N(3)	1.368(5)	N(6)–O(8)	1.220(5)	N(6)–O(6)	1.255(5)
N(6)–O(7)	1.255(5)				
Bond angles (°)					
O(2)–Sm(1)–O(5)	78.75(12)	O(2)–Sm(1)–O(1)#1	97.89(9)	O(5)–Sm(1)–O(1)#1	75.31(10)
O(2)–Sm(1)–O(4)	77.74(11)	O(5)–Sm(1)–O(4)	137.65(11)	O(1)#1–Sm(1)–O(4)	73.66(10)
O(2)–Sm(1)–O(1)	162.48(10)	O(5)–Sm(1)–O(1)	88.34(11)	O(1)#1–Sm(1)–O(1)	67.09(10)
O(4)–Sm(1)–O(1)	105.06(11)	O(2)–Sm(1)–N(1)	122.67(11)	O(5)–Sm(1)–N(1)	78.59(11)
O(1)#1–Sm(1)–N(1)	125.46(10)	O(4)–Sm(1)–N(1)	143.58(11)	O(1)–Sm(1)–N(1)	65.11(10)
O(2)–Sm(1)–O(7)	125.67(10)	O(5)–Sm(1)–O(7)	149.26(11)	O(1)#1–Sm(1)–O(7)	114.12(10)
O(4)–Sm(1)–O(7)	71.40(10)	O(1)–Sm(1)–O(7)	70.71(9)	N(1)–Sm(1)–O(7)	72.32(11)
O(2)–Sm(1)–N(2)	61.34(11)	O(5)–Sm(1)–N(2)	67.40(11)	O(1)#1–Sm(1)–N(2)	139.86(10)
O(4)–Sm(1)–N(2)	127.04(12)	O(1)–Sm(1)–N(2)	124.26(11)	N(1)–Sm(1)–N(2)	61.35(12)
O(7)–Sm(1)–N(2)	105.58(11)	O(2)–Sm(1)–O(6)	80.41(11)	O(5)–Sm(1)–O(6)	135.16(11)
O(1)#1–Sm(1)–O(6)	147.06(10)	O(4)–Sm(1)–O(6)	73.85(11)	O(1)–Sm(1)–O(6)	117.08(10)
N(1)–Sm(1)–O(6)	80.11(11)	O(7)–Sm(1)–O(6)	48.79(10)	N(2)–Sm(1)–O(6)	67.76(11)
O(2)–Sm(1)–Sm(1)#1	131.02(7)	O(5)–Sm(1)–Sm(1)#1	80.27(9)	O(1)#1–Sm(1)–Sm(1)#1	33.69(7)
O(4)–Sm(1)–Sm(1)#1	89.33(8)	O(1)–Sm(1)–Sm(1)#1	33.40(6)	N(1)–Sm(1)–Sm(1)#1	95.35(8)

O(7)–Sm(1)–Sm(1)#1	92.60(7)	N(2)–Sm(1)–Sm(1)#1	142.73(8)	O(6)–Sm(1)–Sm(1)#1	140.87(7)
N(1)–C(1)–C(6)	122.3(4)	N(1)–C(1)–C(2)	116.8(4)	N(1)–C(9)–C(8)	121.4(5)
O(1)–C(2)–C(3)	124.3(4)	O(1)–C(2)–C(1)	118.2(4)	N(1)–C(9)–C(10)	115.3(4)
N(2)–C(10)–C(9)	116.4(4)	O(2)–C(11)–N(3)	124.6(4)	O(2)–C(11)–C(12)	119.1(4)
N(3)–C(11)–C(12)	116.3(4)	O(3)–C(17)–C(16)	118.6(5)	O(3)–C(17)–C(12)	123.4(5)
O(4)–C(18)–N(4)	125.4(5)	O(5)–C(21)–N(5)	125.7(5)	C(1)–N(1)–Sm(1)	116.6(2)
C(9)–N(1)–C(1)	119.5(4)	C(9)–N(1)–Sm(1)	123.2(3)	N(3)–N(2)–Sm(1)	119.8(3)
C(10)–N(2)–N(3)	117.9(4)	C(10)–N(2)–Sm(1)	122.3(3)	C(18)–N(4)–C(20)	120.3(5)
C(11)–N(3)–N(2)	110.0(4)	C(18)–N(4)–C(19)	122.7(5)	C(21)–N(5)–C(23)	119.7(5)
C(19)–N(4)–C(20)	116.6(5)	C(21)–N(5)–C(22)	123.5(5)	O(8)–N(6)–O(7)	122.5(4)
C(22)–N(5)–C(23)	116.8(6)	O(8)–N(6)–O(6)	121.1(4)	C(2)–O(1)–Sm(1)	119.3(2)
O(6)–N(6)–O(7)	116.3(4)	C(2)–O(1)–Sm(1)#1	126.9(2)	C(18)–O(4)–Sm(1)	131.5(3)
Sm(1)–O(1)–Sm(1)#1	112.91(10)	C(11)–O(2)–Sm(1)	123.0(3)	N(6)–O(7)–Sm(1)	98.0(2)
C(21)–O(5)–Sm(1)	142.4(3)	N(6)–O(6)–Sm(1)	96.8(3)		

(C) $2[SmL^3(NO_3)(DMF)_2]_2\cdot 5DMF$ complex

Bond length (Å)					
Sm(1)–O(1)	2.377(4)	Sm(1)–O(2)#1	2.423(4)	Sm(1)–O(2)	2.441(4)
Sm(1)–O(7)	2.447(4)	Sm(1)–O(6)	2.448(4)	Sm(1)–O(3)	2.539(4)
Sm(1)–N(4)	2.544(4)	Sm(1)–N(2)	2.562(5)	Sm(1)–O(4)	2.621(4)
Sm(1)–Sm(1)#1	4.0291(5)	Sm(2)–O(8)	2.385(4)	Sm(2)–O(14)	2.414(5)
Sm(2)–O(9)#2	2.436(3)	Sm(2)–O(9)	2.440(3)	Sm(2)–O(13)	2.455(4)
Sm(2)–N(11)	2.531(4)	Sm(2)–O(10)	2.553(4)	Sm(2)–N(9)	2.568(4)
Sm(2)–O(11)	2.625(4)	Sm(2)–Sm(2)#2	4.0171(5)	N(1)–C(1)	1.320(8)
N(1)–N(2)	1.383(7)	N(2)–C(7)	1.284(7)	N(3)–C(2)	1.296(11)
N(3)–C(6)	1.355(11)	N(4)–C(8)	1.324(8)	N(4)–C(12)	1.347(8)
N(5)–O(5)	1.226(6)	N(5)–O(4)	1.254(6)	N(5)–O(3)	1.259(6)
N(6)–C(17)	1.316(8)	N(6)–C(19)	1.424(11)	N(6)–C(18)	1.462(9)
N(7)–C(20)	1.272(9)	N(7)–C(21)	1.440(11)	N(7)–C(22)	1.478(13)
N(8)–C(23)	1.309(7)	N(8)–N(9)	1.388(6)	N(9)–C(29)	1.270(7)
N(10)–C(24)	1.298(9)	N(10)–C(28)	1.324(10)	N(11)–C(30)	1.333(7)
N(11)–C(34)	1.347(7)	N(12)–O(12)	1.222(7)	N(12)–O(11)	1.248(6)
N(12)–O(10)	1.260(6)	N(13)–C(39)	1.305(7)	N(13)–C(40)	1.428(9)
N(13)–C(41)	1.446(8)	N(14)–C(42)	1.296(9)	N(14)–C(44)	1.423(12)
N(14)–C(43)	1.481(11)	N(15)–C(45)	1.318(9)	N(15)–C(47)	1.411(10)
N(15)–C(46)	1.434(9)	N(16)–C(48)	1.34(12)	N(16)–C(49)	1.5(4)
N(16)–C(50)	1.49(8)	O(1)–C(1)	1.277(7)	O(2)–C(13)	1.342(6)
O(2)–Sm(1)#1	2.423(4)	O(6)–C(17)	1.242(7)	O(7)–C(20)	1.196(8)
O(8)–C(23)	1.286(6)	O(9)–C(35)	1.335(6)	O(9)–Sm(2)#2	2.436(3)
O(13)–C(39)	1.244(6)	O(14)–C(42)	1.187(8)	O(15)–C(45)	1.234(9)
O(16)–C(48)	1.22(8)	C(1)–C(4)	1.502(9)	C(2)–C(3)	1.378(10)
C(3)–C(4)	1.378(10)	C(4)–C(5)	1.367(10)	C(5)–C(6)	1.384(10)

C(7)–C(8)	1.447(9)	C(8)–C(9)	1.428(8)	C(9)–C(10)	1.348(9)
C(10)–C(11)	1.393(9)	C(11)–C(16)	1.397(9)	C(11)–C(12)	1.421(8)
C(12)–C(13)	1.421(8)	C(13)–C(14)	1.364(8)	C(14)–C(15)	1.423(8)
C(15)–C(16)	1.344(10)	C(23)–C(26)	1.491(8)	C(24)–C(25)	1.375(9)
C(25)–C(26)	1.367(9)	C(26)–C(27)	1.360(9)	C(27)–C(28)	1.381(10)
C(29)–C(30)	1.463(8)	C(30)–C(31)	1.408(7)	C(31)–C(32)	1.353(8)
C(32)–C(33)	1.421(8)	C(33)–C(38)	1.398(8)	C(33)–C(34)	1.419(7)
C(34)–C(35)	1.432(7)	C(35)–C(36)	1.374(7)	C(36)–C(37)	1.410(7)
C(37)–C(38)	1.358(8)	N(17)–C(51)	1.30(7)	N(17)–C(52)	1.45(6)
N(17)–C(53)	1.48(6)	O(17)–C(51)	1.22(6)		
Bond angles (°)					
O(1)–Sm(1)–O(2)#1	98.56(13)	O(1)–Sm(1)–O(2)	166.17(13)	O(2)#1–Sm(1)–O(2)	68.14(14)
O(1)–Sm(1)–O(7)	81.25(15)	O(2)#1–Sm(1)–O(7)	74.70(14)	O(2)–Sm(1)–O(7)	91.17(14)
O(1)–Sm(1)–O(6)	79.15(14)	O(2)#1–Sm(1)–O(6)	71.67(13)	O(2)–Sm(1)–O(6)	99.32(13)
O(7)–Sm(1)–O(6)	137.68(15)	O(1)–Sm(1)–O(3)	121.38(13)	O(2)#1–Sm(1)–O(3)	117.39(14)
O(2)–Sm(1)–O(3)	70.23(13)	O(7)–Sm(1)–O(3)	149.18(14)	O(6)–Sm(1)–O(3)	71.42(13)
O(1)–Sm(1)–N(4)	123.68(16)	O(2)#1–Sm(1)–N(4)	O(2)–Sm(1)–N(4)	123.09(14)	64.76(14)
O(7)–Sm(1)–N(4)	76.17(15)	O(6)–Sm(1)–N(4)	144.91(15)	O(3)–Sm(1)–N(4)	73.70(14)
O(1)–Sm(1)–N(2)	62.00(15)	O(2)#1–Sm(1)–N(2)	141.69(15)	O(2)–Sm(1)–N(2)	126.15(14)
O(7)–Sm(1)–N(2)	70.06(15)	O(6)–Sm(1)–N(2)	128.89(14)	O(3)–Sm(1)–N(2)	100.68(15)
N(4)–Sm(1)–N(2)	61.87(16)	O(1)–Sm(1)–O(4)	73.90(14)	O(2)#1–Sm(1)–O(4)	142.13(13)
O(2)–Sm(1)–O(4)	118.79(13)	O(7)–Sm(1)–O(4)	137.44(15)	O(6)–Sm(1)–O(4)	70.46(13)
O(3)–Sm(1)–O(4)	48.95(13)	N(4)–Sm(1)–O(4)	89.49(14)	N(2)–Sm(1)–O(4)	67.86(15)
O(1)–Sm(1)–Sm(1)#1	132.67(10)	O(2)#1–Sm(1)–Sm(1)#1	34.22(8)	O(2)–Sm(1)–Sm(1)#1	33.92(8)
O(7)–Sm(1)–Sm(1)#1	81.59(11)	O(6)–Sm(1)–Sm(1)#1	84.78(10)	O(3)–Sm(1)–Sm(1)#1	94.11(10)
N(4)–Sm(1)–Sm(1)#1	94.01(11)	N(2)–Sm(1)–Sm(1)#1	146.02(11)	O(4)–Sm(1)–Sm(1)#1	140.04(10)
O(8)–Sm(2)–O(14)	82.84(15)	O(8)–Sm(2)–O(9)#2	96.92(12)	O(14)–Sm(2)–O(9)#2	74.45(13)
O(8)–Sm(2)–O(9)	165.17(13)	O(14)–Sm(2)–O(9)	88.57(14)	O(9)#2–Sm(2)–O(9)	69.04(12)
O(8)–Sm(2)–O(13)	77.78(13)	O(14)–Sm(2)–O(13)	138.33(14)	O(9)#2–Sm(2)–O(13)	71.78(12)
O(9)–Sm(2)–O(13)	101.26(12)	O(8)–Sm(2)–N(11)	123.63(13)	O(14)–Sm(2)–N(11)	76.20(15)
O(9)#2–Sm(2)–N(11)	125.42(13)	O(9)–Sm(2)–N(11)	65.24(12)	O(13)–Sm(2)–N(11)	144.54(14)
O(8)–Sm(2)–O(10)	123.08(14)	O(14)–Sm(2)–O(10)	147.62(14)	O(9)#2–Sm(2)–O(10)	116.24(13)
O(9)–Sm(2)–O(10)	69.50(13)	O(13)–Sm(2)–O(10)	71.46(13)	N(11)–Sm(2)–O(10)	73.08(14)
O(8)–Sm(2)–N(9)	61.89(13)	O(14)–Sm(2)–N(9)	71.47(15)	O(9)#2–Sm(2)–N(9)	141.57(14)
O(9)–Sm(2)–N(9)	126.44(13)	O(13)–Sm(2)–N(9)	126.91(14)	N(11)–Sm(2)–N(9)	61.90(14)
O(10)–Sm(2)–N(9)	102.08(15)	O(8)–Sm(2)–O(11)	76.31(14)	O(14)–Sm(2)–O(11)	139.36(15)
O(9)#2–Sm(2)–O(11)	141.90(13)	O(9)–Sm(2)–O(11)	117.55(13)	O(13)–Sm(2)–O(11)	70.14(13)
N(11)–Sm(2)–O(11)	86.87(14)	O(10)–Sm(2)–O(11)	48.70(14)	N(9)–Sm(2)–O(11)	67.96(15)
O(8)–Sm(2)–Sm(2)#2	131.31(9)	O(14)–Sm(2)–Sm(2)#2	79.77(11)	O(9)#2–Sm(2)–Sm(2)#2	34.55(8)
O(9)–Sm(2)–Sm(2)#2	34.49(8)	O(13)–Sm(2)–Sm(2)#2	85.93(9)	N(11)–Sm(2)–Sm(2)#2	95.57(10)
O(10)–Sm(2)–Sm(2)#2	93.18(10)	N(9)–Sm(2)–Sm(2)#2	146.69(11)	O(11)–Sm(2)–Sm(2)#2	139.30(10)
C(1)–N(1)–N(2)	108.1(5)	C(7)–N(2)–N(1)	117.6(5)	C(7)–N(2)–Sm(1)	122.0(5)
N(1)–N(2)–Sm(1)	120.4(3)	C(2)–N(3)–C(6)	119.5(8)	C(8)–N(4)–C(12)	119.8(5)
C(8)–N(4)–Sm(1)	122.4(4)	C(12)–N(4)–Sm(1)	117.6(4)	O(5)–N(5)–O(4)	121.5(5)

O(5)–N(5)–O(3)	121.7(5)	O(4)–N(5)–O(3)	116.7(5)	C(17)–N(6)–C(19)	121.0(6)
C(17)–N(6)–C(18)	119.9(7)	C(19)–N(6)–C(18)	119.1(7)	C(20)–N(7)–C(21)	125.9(8)
C(20)–N(7)–C(22)	117.5(8)	C(21)–N(7)–C(22)	115.1(8)	C(23)–N(8)–N(9)	108.9(4)
C(29)–N(9)–N(8)	117.5(5)	C(29)–N(9)–Sm(2)	122.4(4)	N(8)–N(9)–Sm(2)	120.1(3)
C(24)–N(10)–C(28)	115.6(7)	C(30)–N(11)–C(34)	119.8(4)	C(30)–N(11)–Sm(2)	122.6(4)
C(34)–N(11)–Sm(2)	117.3(3)	O(12)–N(12)–O(11)	122.4(6)	O(12)–N(12)–O(10)	120.8(6)
O(11)–N(12)–O(10)	116.8(5)	C(39)–N(13)–C(40)	120.4(5)	C(39)–N(13)–C(41)	121.3(6)
C(40)–N(13)–C(41)	118.2(6)	C(42)–N(14)–C(44)	127.1(9)	C(42)–N(14)–C(43)	118.5(8)
C(44)–N(14)–C(43)	113.2(8)	C(45)–N(15)–C(47)	121.4(7)	C(45)–N(15)–C(46)	120.2(7)
C(47)–N(15)–C(46)	118.1(7)	C(48)–N(16)–C(50)	116(5)	C(49)–N(16)–C(50)	127(10)
C(48)–N(16)–C(49)	117(10)	C(13)–O(2)–Sm(1)#1	125.5(3)	C(13)–O(2)–Sm(1)	119.8(3)
C(1)–O(1)–Sm(1)	121.6(4)	N(5)–O(3)–Sm(1)	98.8(3)	N(5)–O(4)–Sm(1)	94.9(3)
Sm(1)#1–O(2)–Sm(1)	111.86(14)	C(20)–O(7)–Sm(1)	135.7(5)	C(23)–O(8)–Sm(2)	121.8(3)
C(17)–O(6)–Sm(1)	130.3(4)	C(35)–O(9)–Sm(2)	119.5(3)	Sm(2)#2–O(9)–Sm(2)	110.96(12)
C(35)–O(9)–Sm(2)#2	127.1(3)	N(12)–O(11)–Sm(2)	95.4(3)	C(39)–O(13)–Sm(2)	127.0(4)
N(12)–O(10)–Sm(2)	98.5(3)	O(1)–C(1)–N(1)	127.6(6)	O(1)–C(1)–C(4)	117.1(6)
C(42)–O(14)–Sm(2)	136.6(5)	N(1)–C(1)–C(4)	115.3(6)	N(3)–C(2)–C(3)	122.0(8)
N(3)–C(6)–C(5)	120.7(9)	N(2)–C(7)–C(8)	118.0(6)	N(4)–C(8)–C(9)	121.1(6)
N(4)–C(8)–C(7)	115.6(5)	N(4)–C(12)–C(11)	122.2(6)	N(4)–C(12)–C(13)	116.7(5)
O(6)–C(17)–N(6)	124.8(7)	O(7)–C(20)–N(7)	129.1(8)	O(8)–C(23)–N(8)	127.2(5)
O(8)–C(23)–C(26)	117.4(5)	N(8)–C(23)–C(26)	115.5(5)	N(10)–C(24)–C(25)	123.7(7)
N(10)–C(28)–C(27)	124.5(8)	N(9)–C(29)–C(30)	117.7(5)	N(11)–C(30)–C(31)	121.5(5)
N(11)–C(30)–C(29)	115.2(5)	N(11)–C(34)–C(33)	122.1(5)	N(11)–C(34)–C(35)	116.9(4)
O(9)–C(35)–C(36)	124.3(5)	O(9)–C(35)–C(34)	118.4(4)	O(13)–C(39)–N(13)	124.4(6)
O(14)–C(42)–N(14)	125.1(8)	O(15)–C(45)–N(15)	124.1(8)	O(16)–C(48)–N(16)	118(8)
C(51)–N(17)–C(52)	128(8)	C(51)–N(17)–C(53)	120(8)	C(52)–N(17)–C(53)	113(5)
O(17)–C(51)–N(17)	120(10)				

Table S2. The characteristic IR band data (ν_{max}/cm^{-1}) of the metal complexes

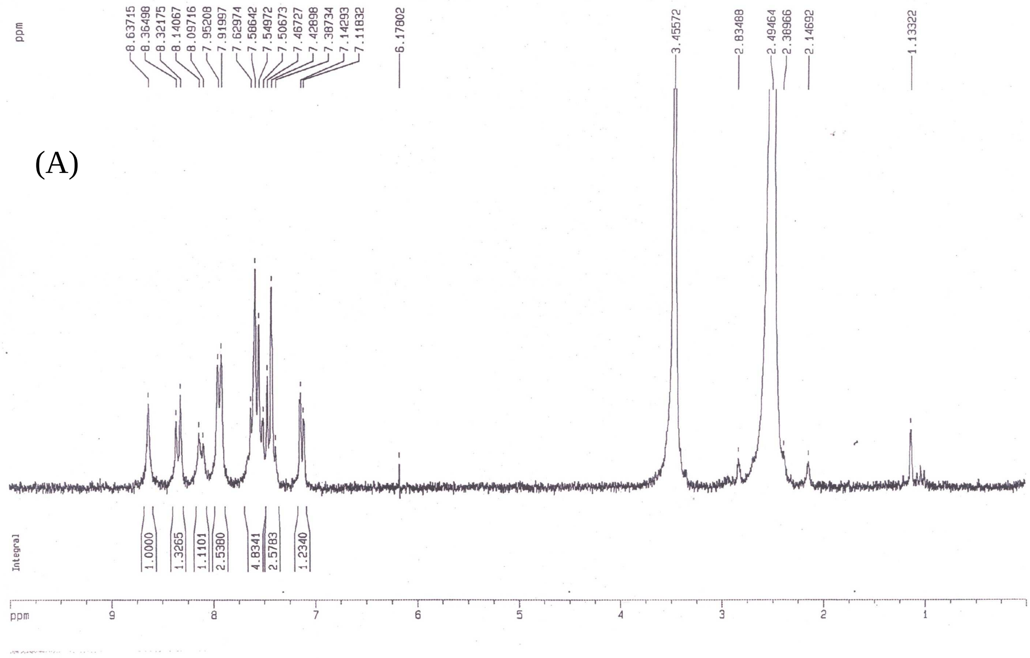
Complexes	ν (OH) H_2O	ν (OH) phenolic	ν (CN) azomethine	ν (CN) pyridine	ν (C–OH) free	ν (C–O) bound	NO_3^- ν_1	NO_3^- ν_4	NO_3^- ν_2	NO_3^- ν_3	NO_3^- ν_5	ρ_r H_2O	ρ_w H_2O	ν (MO)	ν (MN)
$[L^1Sm(NO_3)(OH_2)_2]_2$	3415	–	1618	1556	–	1104	1495	1311	1034	812	765	947	656	521	488
$[L^2Sm(NO_3)(OH_2)_2]_2$	3429	3184	1601	1548	1277	1102	1492	1314	1037	839	756	942	652	535	487
$[L^3Sm(NO_3)(OH_2)_2]_2$	3399	–	1635	1591,1565	–	1100	1498	1316	1061	811	759	935	639	522	486

Table S3. The UV-vis spectra values of λ_{max} (nm), ε_{max} (M^{-1} cm^{-1}), hypochromicity and shifts of λ_{max} after additions of DNA for ligands and the Sm(III) complexes. The molar concentration of every investigated compound is 10.0 μM. The molar concentrations of DNA (bps) at approximately saturated titration end points for **1a**, **1b**, **1c**, **2a**, **2b** and **2c** are 20.0, 16.0, 14.0, 16.0, 14.0, 16.0 μM, respectively.

Ligands	π–π* aromatic ring		π–π* C=N and C=O		Complexes	π–π* conjugated aromatic ring		π–π* C=N–N=C	
	λ_{max} (ε)	Hypochromicity (λ_{max} shifts)	λ_{max} (ε)	Hypochromicity (λ_{max} shifts)		λ_{max} (ε)	Hypochromicity (λ_{max} shifts)	λ_{max} (ε)	Hypochromicity (λ_{max} shifts)
1a	295 (3.55)	34.3% (1 nm, red)	323 (2.11)	11.1% (1 nm, blue)	**2a**	324 (4.14)	24.9% (1 nm, red)	371 (2.75)	22.3% (0 nm)
1b	294 (3.16)	30.1% (3 nm, red)	329 (2.36)	18.1% (3 nm, blue)	**2b**	323 (3.66)	20.6% (2 nm, red)	378 (3.55)	21.5% (0 nm)
1c	290 (2.86)	8.4% (0 nm)	325 (1.78)	1.0% (0 nm)	**2c**	327 (4.39)	0.54% (0 nm)	374 (3.60)	0.94% (0 nm)

Fig. S1. Spectra of ^{1}H NMR for ligand **1a** (A) and complex **2a** (B).

(A)



(B)

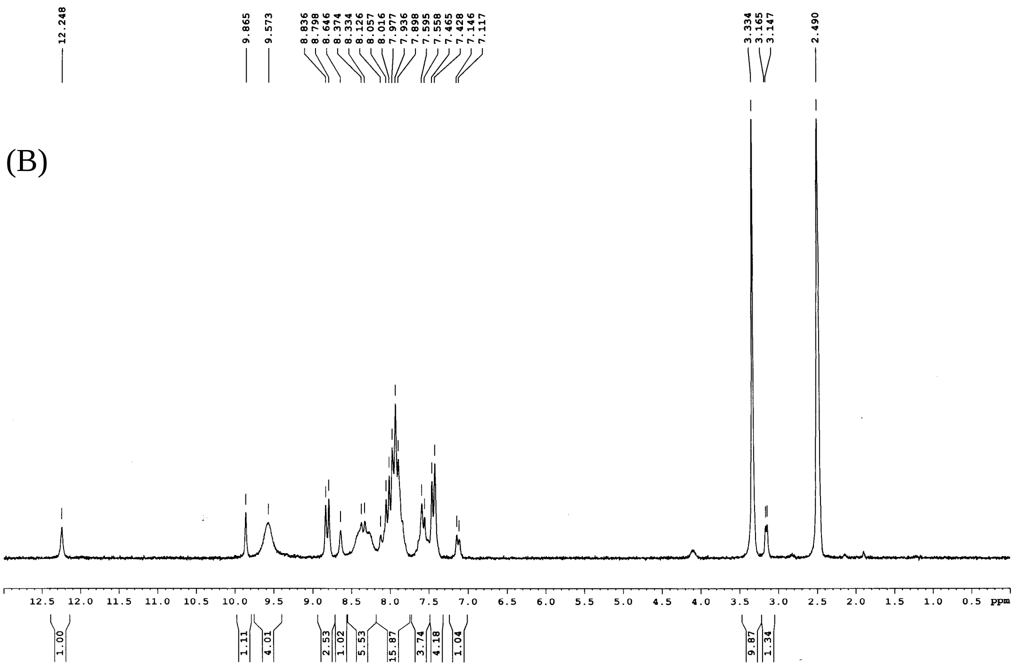
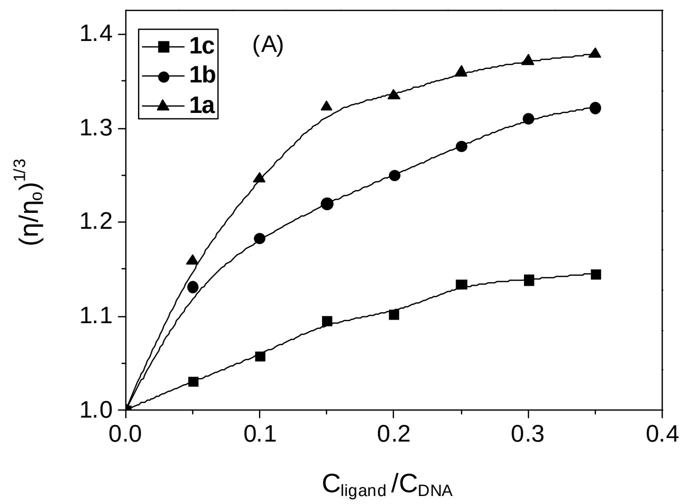


Fig. S2. Effects of increasing amounts of the investigated compounds on the relative viscosity of CT-DNA in 5 mM Tris–HCl buffer solution (pH 7.20) containing 50 mM NaCl at 25.00±0.01°C. Plots of (A) and (B) represent the ligands–CT-DNA and Sm(III) complexes–CT-DNA systems, respectively. The concentration of CT-DNA was 50 μM (bps).



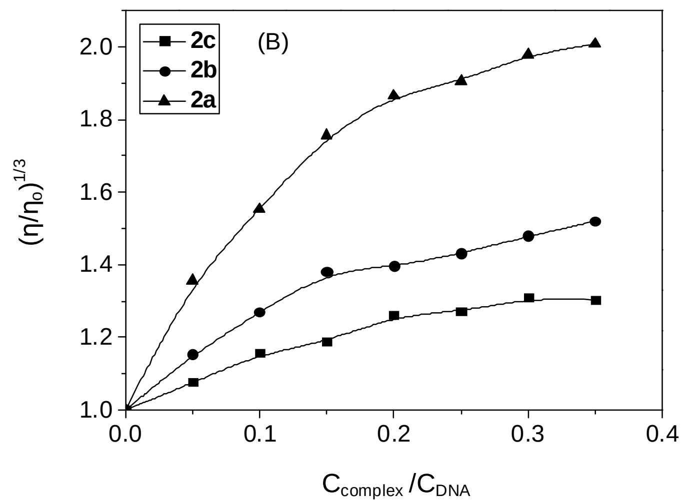
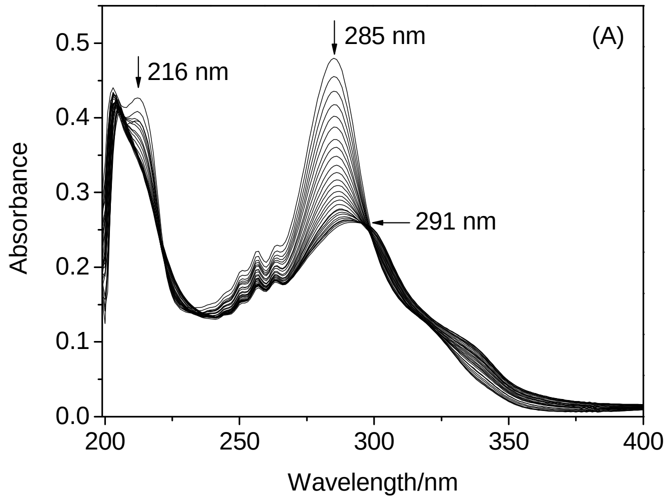


Fig. S3. UV-vis titration spectra of EB-DNA system (A) and the plot of A/A_o versus C_{DNA}/C_{EB} at 285 nm (B) in 5 mM Tris–HCl buffer solution (pH 7.20) containing 50 mM NaCl. The molar concentration of EB is 10.0 μM and the molar concentration of CT-DNA added by every titration at 5 μL of 2.0 mM increases from 0 to 104.0 μM (nucleotides). A_o and A are the absorbances of EB containing solution at 285 nm in the absence and in the presence of CT-DNA, respectively.



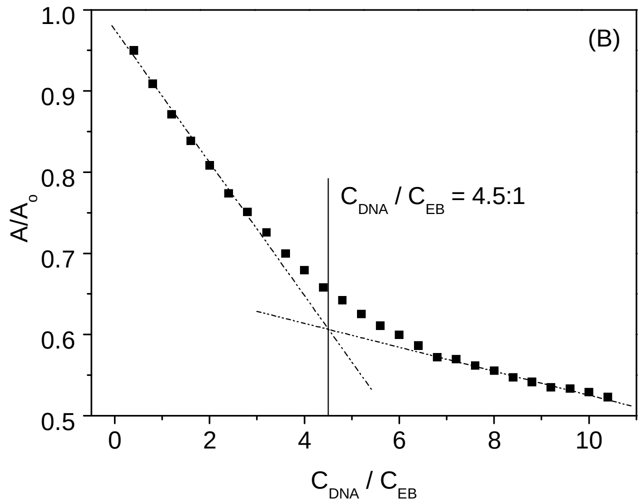
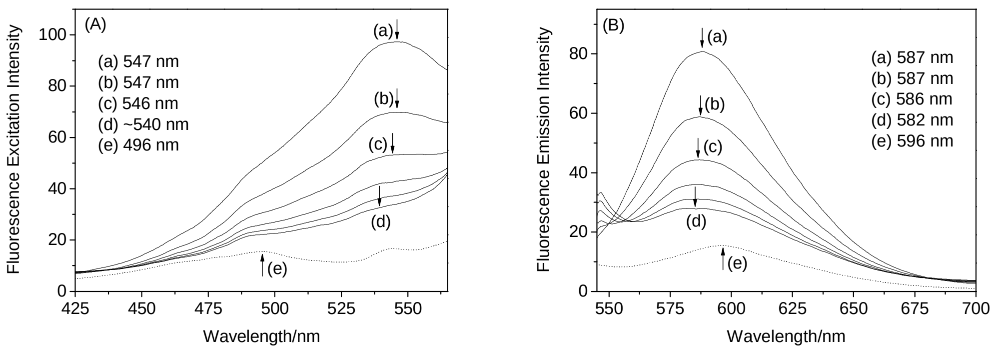


Fig. S4. The fluorescence emission spectra and the corresponding excitation spectra for the fluorescence quenching of EB-DNA systems by the titrations of **2b** and **2c** complexes, respectively. Plots of (A) and (B) represent the fluorescence excitation spectra at λ_{em} = 587 nm and the fluorescence emission spectra at λ_{ex} = 525 nm for **2b**, respectively. The molar concentration of **2b** added in EB-DNA system by titration increase from 0 (a) to 20.0 μM (d). Plots of (C) and (D) represent the fluorescence excitation spectra at λ_{em} = 587 nm and the fluorescence emission spectra at λ_{ex} = 525 nm for **2c**, respectively. The molar concentration of **2c** added in EB-DNA system by titration increase from 0 (a) to 56.0 μM (d). Both curves of (e) depicted by dots (······) in plots (A) and (C) represent the fluorescence excitation spectra of free EB at λ_{em} = 596 nm, and both curves of (e) depicted by dots (······) in plots (B) and (D) represent the fluorescence emission spectra of free EB at λ_{ex} = 496 nm. All the tests were performed under the conditions of 5 mM Tris–HCl buffer solution (pH = 7.20) containing 50 mM NaCl at 298 K. C_{DNA} = 2 μM (bps), C_{EB} = 0.32 μM.



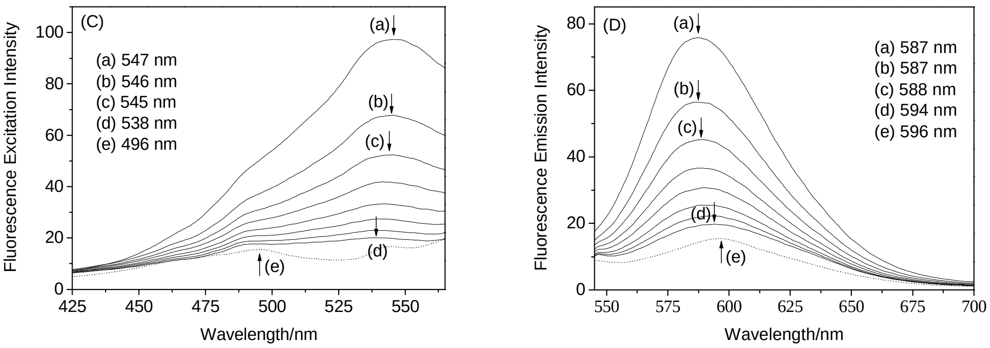
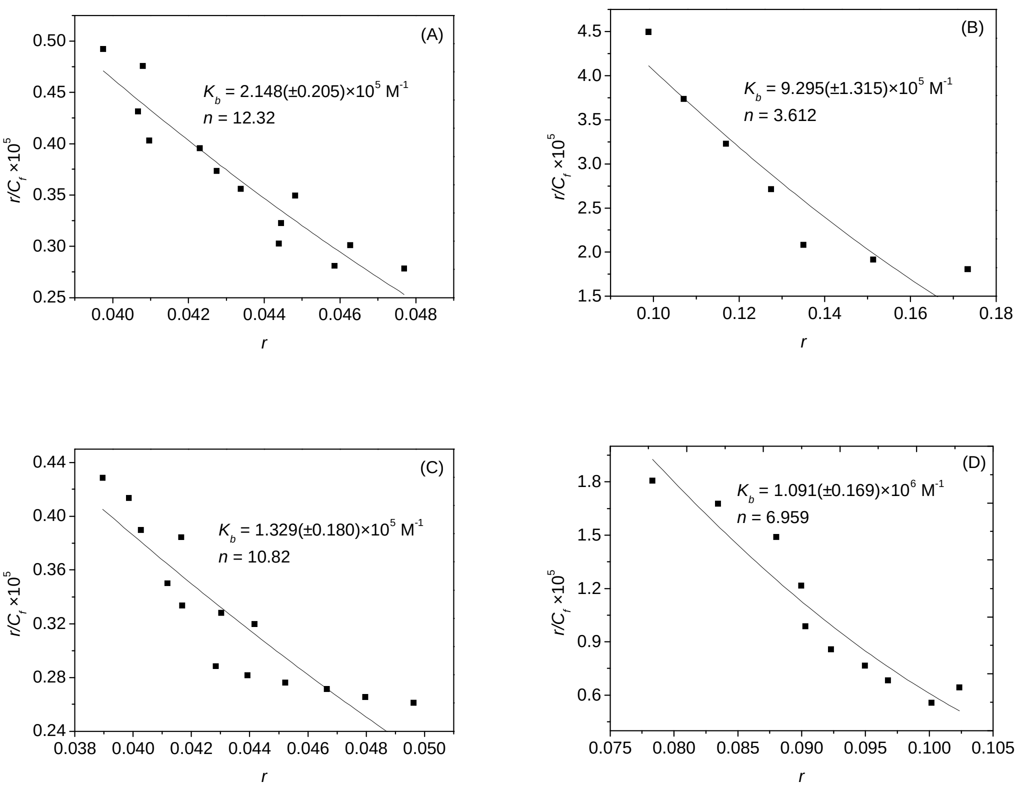


Fig. S5. McGhee & von Hippel plots for ligands and the Sm(III) complexes titrated by DNA (bps) (P < 0.05). Plots of (A), (B) and (C) for **1a-**, **1b-** and **1c**-DNA systems at λ_{ex} = 321–325 nm and λ_{em} = 442–443 nm, respectively; Plots of (D), (E) and (F) for **2a-**, **2b-** and **2c**-DNA systems at λ_{ex} = 321–323 nm and λ_{em} = 440–445 nm, respectively. n is the exclusion parameter in DNA base pairs.



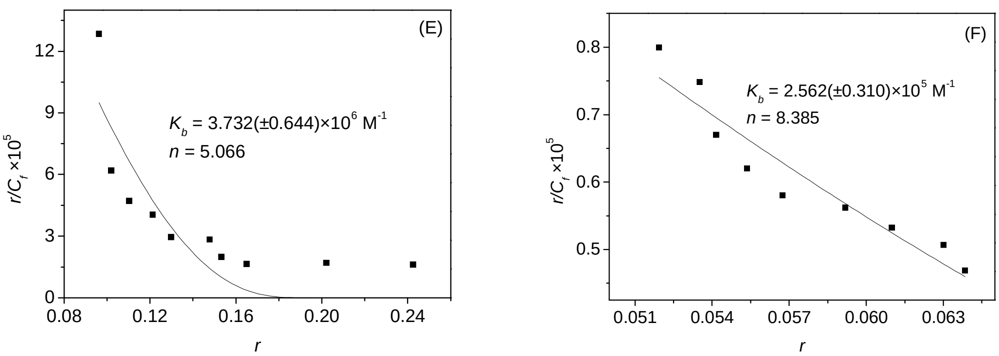


Fig. S6. Plots of antioxidation properties for ligands and Sm(III) complexes. (A) and (B) represent the hydroxyl radical scavenging effect (%) for ligands and Sm(III) complexes, respectively. (C) and (D) represent the superoxide radical scavenging effect (%) for ligands and Sm(III) complexes, respectively.