Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Trifluoromethyl-pyridine carboxylic acid Zn(II) complexes: isomeric effects on coordination and biological activity

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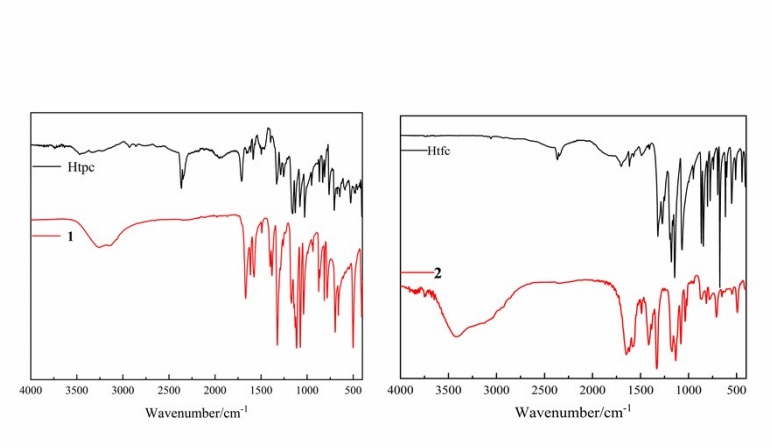

Fig S1. IR spectra of ligands and complexes

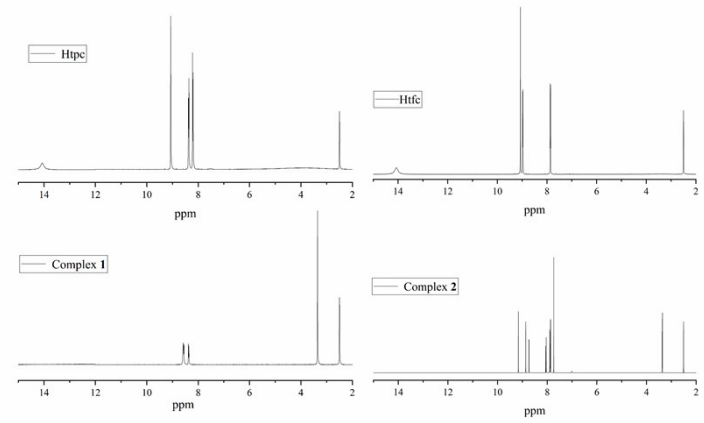

Fig S2. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of ligands and complexes

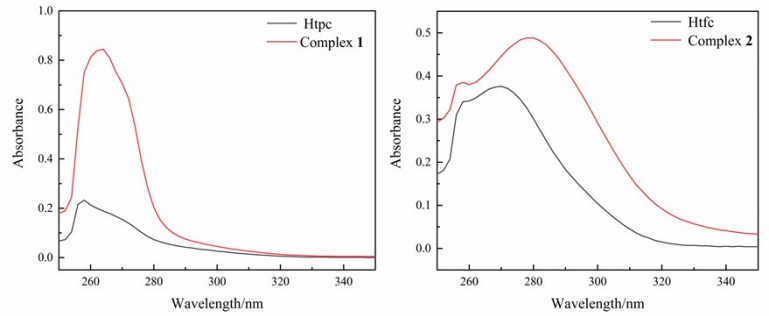

Fig S3. UV-Vis spectra of ligands and the corresponding complexes in DMSO

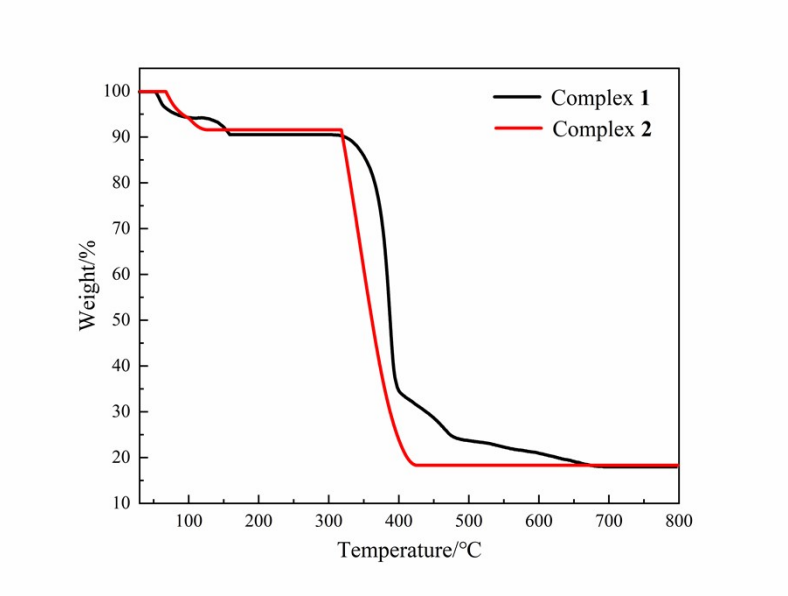

Fig S4. TG curves of complexes **1** and **2**

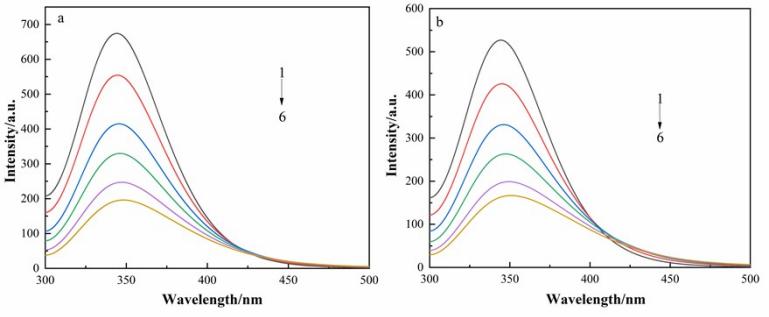

Fig S5. Fluorescence quenching of BSA by complexes **1** (a) and **2** (b) at 35 °C

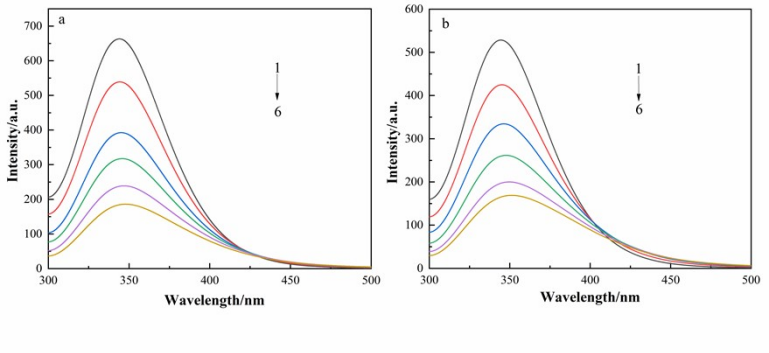

Fig S6. Fluorescence quenching of BSA by complexes **1** (a) and **2** (b) at 45 °C

Table S1. Partial Bond Lengths for complex **1**

Bond	Dist.	Bond	Dist.
Zn(1)–O(2)	2.070(4)	Zn(1)–O(3)	2.122(4)
Zn(1)–O(2)^{i}	2.070(4)	Zn(1)–O(3)^{i}	2.122(4)
Zn(1)–N(1)	2.138(3)	Zn(1)–N(2)^{i}	2.138(4)

Table S2. Partial Bond Angles for complex **1**

Angle	(°)	Angle	(°)
O(2)–Zn(1)–O(3)	179.31(9)	O(2)–Zn(1)–N(2)	100.55(9)
O(2)–Zn(1)–O(5)	89.45(10)	O(3)–Zn(1)–O(5)	91.16(10)
O(2)–Zn(1)–O(6)	89.34(11)	O(3)–Zn(1)–O(6)	90.05(10)
O(2)–Zn(1)–N(1)	79.55(9)	N(1)–Zn(1)–N(2)	179.73(11)

Table S3. Partial Bond Lengths for complex **2**

Bond	Dist.	Bond	Dist.
Zn(1)–O(1)	2.123(14)	Zn(1)–N(1)	2.175(17)
Zn(1)–O(1)^{i}	2.123(14)	Zn(1)–N(1)^{i}	2.175(17)
Zn(1)–O(3)	2.075(15)	Zn(1)–O(3)^{i}	2.075(15)

Symmetry code: ^{i} -x+1, -y, -z+1

Table S4. Partial Bond Angles for complex **2**

Angle	(°)	Angle	(°)
O(1)–Zn(1)–O(1)^{i}	180.00(7)	O(3)–Zn(1)–N(1)	94.47(6)
O(3)–Zn(1)–O(3)^{i}	180.00(7)	O(3)–Zn(1)–N(1)^{i}	94.47(6)
O(1)–Zn(1)–N(1)	88.74(6)	O(1)–Zn(1)–O(3)	88.15(6)
O(1)–Zn(1)–N(1)^{i}	91.26(6)	N(1)–Zn(1)–N(1)^{i}	180.00(6)

Symmetry code: ^{i} -x+1, -y, -z+1

Table S5. Hydrogen-bonded parameters for complex **1**

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠DHA
O3-H3A···O5	0.93	1.87	2.767(6)	160.51
O6-H6B···O4	0.93	1.85	2.711(6)	152.12