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SUPPLEMENTARY MATERIAL TO

Structure and DNA/BSA binding study of zinc(II) complex with 4-ethynyl-2,2'-bipyridine

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ANALYTICAL DATA FOR EBPY LIGAND AND THE COMPLEX

Anal. Calcd. for $C_{12}H_8N_2$ (MW 180.21): C, 79.98; H, 4.47; N, 15.55 %. Found: C, 79.82; H, 4.52; N, 15.68 %. ^{1}H NMR (200 MHz, DMSO-d_6): δ = 4.69 (*s*, 1H, CCH), 7.52 (*m*, 2H, C5H and C5'H), 7.98 (*dd*, J = 8.6, 6.9 Hz, 1H, C4'H), 8.39 (*d*, J = 6.9 Hz, 2H, C3H and C3'H), 8.72 (*d*, J = 5.0 Hz, C6H and C6'H) ppm. IR (KBr, ν, cm^{-1}): 3224m (ν(C_{alkyne}–H)), 3059w, 3029w, 3011w (ν(C_{ar}–H)), 2108m (ν(C≡C)), 1584vs, 1564m, 1540s, 1457vs (ν(C_{ar}=C_{ar}) and ν(C_{ar}=N)), 794s (γ(C_{ar}–H)), 626m (γ(C_{alkyne}–H)). UV-Vis (DMSO, λ_{max}, nm): 283 (ε = 1.0 × 10^4 M^{-1} cm^{-1}), 308 (*sh*, ε = 5.3 × 10^3 M^{-1} cm^{-1}). Λ_M (DMSO): 1.50 Ω^{-1}cm^{2}mol^{-1}.

Anal. Calcd. for $C_{12}H_8Cl_2N_2Zn$ (MW 316.47): C, 45.54; H, 2.55; N, 8.85 %. Found: C, 45.41; H, 2.52; N, 8.92 %. ^{1}H NMR (200 MHz, DMSO-d_6): δ = 4.84 (*s*, 1H, CCH), 7.67 (*m*, 2H, C5H and C5'H), 8.12 (*t*, J = 7.4 Hz, 1H, C4'H), 8.57 (*s*, 2H, C3H and C3'H), 8.72 (*d*, J = 4.8 Hz, C6H and C6'H) ppm. IR (KBr, ν, cm^{-1}): 3215s (ν(C_{alkyne}–H)), 3114w, 3080w, 3057w (ν(C_{ar}–H)), 2109m (ν(C≡C)), 1604vs, 1571w, 1542m, 1480m, 1440s, 1406s (ν(C_{ar}=C_{ar}) and ν(C_{ar}=N)), 792s (γ(C_{ar}–H)), 623m (γ(C_{alkyne}–H)). UV-Vis (DMSO, λ_{max}, nm): 283 (ε = 9.3 × 10^3 M^{-1} cm^{-1}), 308 (*sh*, ε = 4.8 × 10^3 M^{-1} cm^{-1}). Λ_M (DMSO): 4.82 Ω^{-1}cm^{2}mol^{-1}.

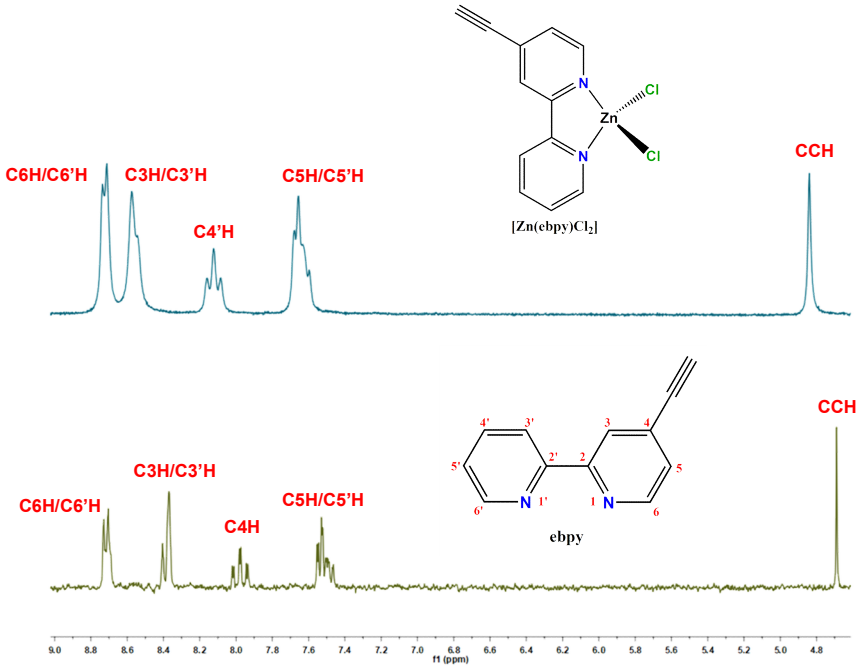

Fig. S-1. The parts of ^{1}H NMR spectrum of [Zn(ebpy)Cl_2] measured in DMSO-d_6 in comparison to that of ebpy.

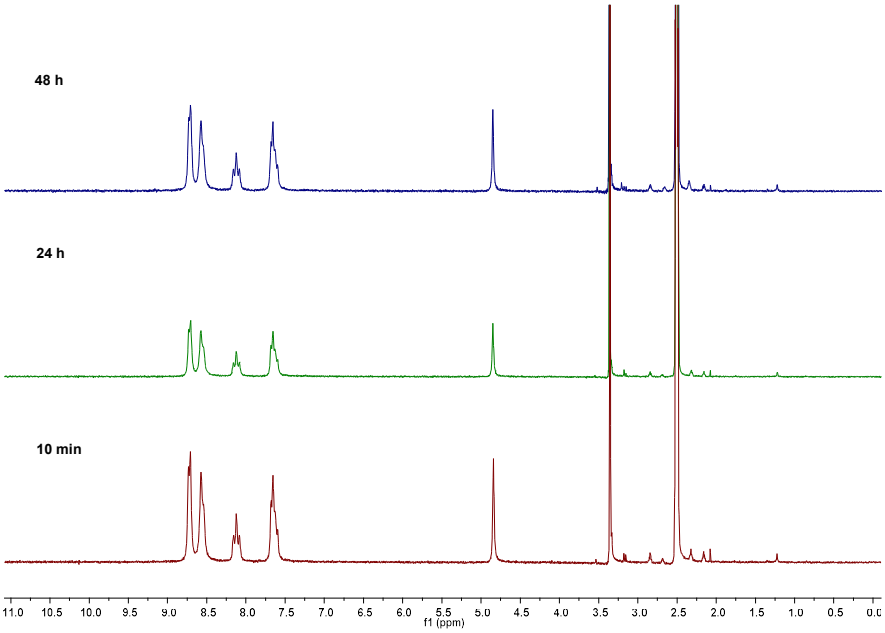

Fig. S-2. Time-dependent ^{1}H NMR spectra of [Zn(ebpy)Cl$_2$] measured in DMSO-d_6 at ambient temperature over 48 h.

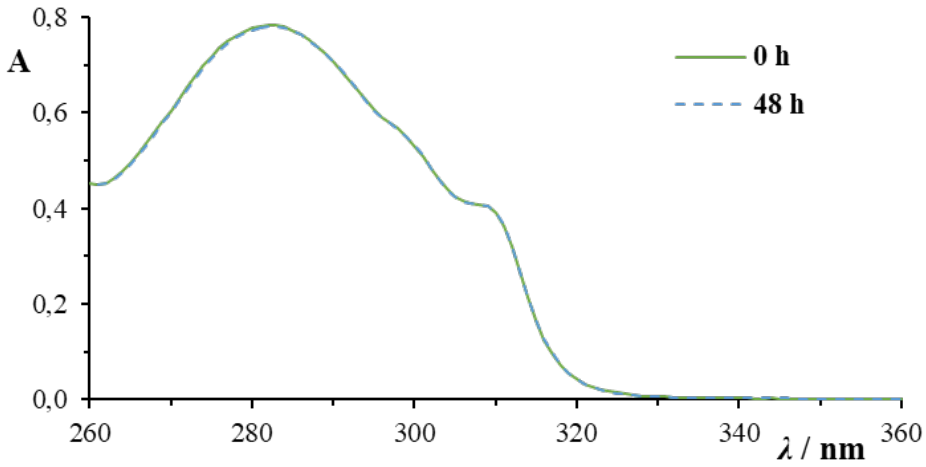

Fig. S-3. UV-Vis spectra of [Zn(ebpy)Cl$_2$] measured in DMSO right after its dissolution and after 48 h standing at ambient temperature.

TABLE S-I. Details of the crystal structure determination of $[Zn(ebpy)Cl_2]$

	$[Zn(ebpy)Cl_2]$
Empirical formula	$C_{12}H_8Cl_2N_2Zn$
Molecular weight	316.47
Crystal system, space group	monoclinic, $P2_1/m$
a (Å)	7.9738(7)
b (Å)	7.2991(8)
c (Å)	11.0462(10)
β (°)	98.749(7)
V (Å^3)	635.43(11)
F_{000}	316
Z	2
X-radiation, λ /Å	Mo-K_α 0.71073
data collect. temperat. / K	250(2)
Calculated density (g cm^{-3})	1.654
Absorption coefficient (mm^{-1})	2.329
Crystal size (mm^3)	0.19 × 0.143 × 0.08
2θ range (°)	3.73 to 52.644
index ranges h, k, l	-9 ... 9, -9 ... 9, -13 ... 13
No. of collected and independent reflections	5319, 1363
R_{int}	0.0361
Data / restraints / parameters	1363 / 0 / 100
Goodness-on-fit on F^2	1.079
Final R indices [$I \geq 2\sigma(I)$]	0.0280, 0.0660
Final R indices (all data)	0.0332, 0.0702
Difference density: max, min (e Å^{-3})	0.27, -0.33
CCDC number	2266337

TABLE S-II. Selected bond distances (Å) and valence angles (°) in $[Zn(ebpy)Cl_2]$

$[Zn(ebpy)Cl_2]$	
Zn1—N1	2.045(3)
Zn1—N2	2.048(3)
Zn1—Cl1	2.1981(7)
Cl1^i—Zn1—Cl1	116.77(4)
N1—Zn1—Cl1^i	113.93(3)
N1—Zn1—Cl1	113.93(3)
N1—Zn1—N2	80.46(10)
N2—Zn1—Cl1^i	113.25(3)
N2—Zn1—Cl1	113.25(3)
C1—N1—Zn1	126.5(2)
C5—N1— Zn1	114.5(2)
C6—N2— Zn1	114.2(2)
C10—N2— Zn1	126.8(2)

Symmetry code: (i) x, 1/2-y, z