

Electronic Supplementary Information (ESI) for
Bifunctional tetrazole-carboxylate ligands based Zn(II) complexes:
Synthesis and their excellent potential anticancer properties

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Table S1 Selected crystallographic data and structure refinement for **1-2**

Complex	1	2
Empirical formula	C ₃₁ H ₃₆ N ₁₅ O ₁₂ Zn	C ₁₆ H ₂₀ N ₁₀ O ₈ Zn
Formula mass	876.12	545.81
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
<i>a</i> (Å)	10.823 (2)	7.1354 (14)
<i>b</i> (Å)	11.011 (2)	9.3422 (19)
<i>c</i> (Å)	16.851 (3)	10.662 (2)
α (°)	78.57 (3)	64.51 (3)
β (°)	73.87 (3)	72.84 (3)
γ (°)	80.02 (3)	79.91 (3)
<i>V</i> (Å ³)	1875.9 (6)	612.0 (2)
<i>Z</i>	2	1

<i>T</i> /K	291(2)	291(2)
<i>D</i> _{calcd} (g.cm ⁻³)	1.549	1.481
<i>u</i> (mm ⁻¹)	0.738	1.06
Reflections collected	17674	6435
Unique Reflections(<i>R</i> _{int})	6572(0.045)	2794(0.033)
No. Observations (<i>I</i> > 2.00)	4647	2347
No. Variables	519	165
<i>R</i> ₁ ^[a] <i>wR</i> ₂ ^[b] (<i>I</i> > 2σ(<i>I</i>))	0.0729, 0.2166	0.0496, 0.1339
GOF ^c	1.395	0.997
Δ/ <i>ρ</i> _{max} (e/Å ³)	1.135	0.400
Δ/ <i>ρ</i> _{min} (e/Å ³)	-0.899	-0.400

$$^{[a]}R = \sum ||F_o| - |F_c|| / \sum |F_o|.$$

$$^{[b]}Rw = \{ \sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2 \}^{1/2}.$$

^[c] GOF = $\{ \sum w((F_o^2 - F_c^2)^2) / (n-p) \}^{1/2}$, where *n* = number of reflections and *p* = total numbers of parameters refined.

Table S2 Selected bond distances and angles for 1-2 (Å/°)

Complex 1			
Zn1–O3A	2.089(4)	Zn1–O1	2.106(4)
Zn1–O7	2.136(3)	Zn1–N14	2.157(4)
Zn1–N15	2.163(4)	Zn1–N13	2.187(4)
O3A–Zn1–O1	175.92(14)	O3A–Zn1–O7	93.41(16)
O1–Zn1–O7	90.10(15)	O3A–Zn1–N14	90.33(15)
O1–Zn1–N14	91.78(15)	O7–Zn1–N14	89.66(15)
O3A–Zn1–N15	90.58(15)	O1–Zn1–N15	87.19(15)
O7–Zn1–N15	92.35(15)	N14–Zn1–N15	177.74(17)
O3A–Zn1–N13	86.54(15)	O1–Zn1–N13	90.00(15)
O7–Zn1–N13	178.60(14)	N14–Zn1–N13	88.94(16)
N15–Zn1–N13	89.05(16)		
Complex 2			
Zn1–O5	2.0793 (17)	Zn1–O1C	2.083 (2)
Zn1–O5A	2.0793 (17)	Zn1–N5A	2.213 (3)
Zn1–O1B	2.083 (2)	Zn1–N5	2.213 (3)
O5–Zn1–N5A	87.49 (9)	O5A–Zn1–O1B	89.50 (8)
O5A–Zn1–N5A	92.51 (9)	O5–Zn1–O1C	89.50 (8)
O1B–Zn1–N5A	90.18 (9)	O5–Zn1–N5	92.51 (9)
O1C–Zn1–N5A	89.82 (9)	O5A–Zn1–N5	87.49 (9)
O5A–Zn1–O1C	90.50 (8)	O1B–Zn1–N5	89.82 (9)

O1B–Zn1–O1C	180.00	O1C–Zn1–N5	90.18*(9)
O5–Zn1–O5A	180.00*(7)	N5A–Zn1–N5	180.00*(14)
O5–Zn1–O1B	90.50*(8)		

Symmetry code:

For 1: A: $-x, -y+1, -z+1$.

For 2 :A: $-x+1, -y, -z$; B: $-x+1, -y+1, -z-1$; C: $x, y-1, z+1$.

Table S3 Hydrogen-bonding Geometry (Å and °) for 1-2

<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>[D...A]</i>	$\angle D-H...A$
Complex 1				
O(7)–H(7A)···O(11) ^{#1}	0.85	1.79	2.633(17)	172
O(7)–H(7A)···O(12) ^{#2}	0.85	2.45	2.845(9)	109
O(7)–H(7B)···O(12) ^{#2}	0.85	2.51	2.845(9)	105
O(8)–H(8D)···O(2) ^{#3}	0.85	1.99	2.580(10)	126
O(8)–H(8E)···O(12)	0.85	2.08	2.706(10)	130
O(9)–H(9A)···O(4) ^{#4}	0.85	2.01	2.746(12)	145
O(9)–H(9B)···O(8)	0.85	2.54	3.036(15)	118
O(10)–H(10A)···O(9) ^{#5}	0.85	1.95	2.589(17)	131
O(10)–H(10A)···O(7) ^{#6}	0.85	2.01	2.720(10)	140
O(11)–H(11C)···O(10)	0.85	1.77	2.22(2)	111
O(11)–H(11E)···N(7) ^{#7}	0.85	2.59	3.014(18)	112
O(12)–H(12A)···O(7) ^{#2}	0.85	2.57	2.845(9)	100
O(12)–H(12A)···O(11) ^{#8}	0.85	1.98	2.30(2)	101
C(11)–H(11A)···N(9) ^{#7}	0.97	2.52	3.353(9)	144
C(11)–H(11B)···O(9) ^{#9}	0.97	2.5	3.236(12)	132
C(14)–H(14B)···O(12) ^{#8}	0.97	2.47	3.427(12)	169
C(19)–H(19A)···N(3) ^{#10}	0.93	2.5	3.292(7)	143
C(24)–H(24A)···O(4) ^{#4}	0.93	2.45	3.272(8)	147
C(31)–H(31A)···O(4) ^{#4}	0.96	2.5	3.302(10)	141
Complex 2				
O(5)–H(5C)···O(7) ^{#3}	0.84	1.81	2.649(3)	170
O(7)–H(7A)···N(4) ^{#1}	0.85	2.36	2.793(16)	112
O(7)–H(7B)···O(1) ^{#2}	0.84	1.93	2.741(3)	164
C(13)–H(13B)···O(7) ^{#1}	0.97	2.58	3.262(4)	127

Symmetry codes

For 1: # 1: $-1+x, 1+y, z$; # 2: $-1-x, 1-y, 2-z$; # 3: $x, -1+y, z$; # 4: $-1+x, y, 1+z$; # 5: $1+x, y, z$; # 6: $-x, 1-y, 2-z$; # 7: $1-x, 1-y, 1-z$; # 8: $-x, -y, 2-z$; # 9: $-x, 1-y, 1-z$; # 10: $-x, 2-y, 1-z$.

For 2: # 1: $1-x, -y, -z$; # 2: $1-x, 1-y, -z$; # 3: $1+x, y, -1+z$.

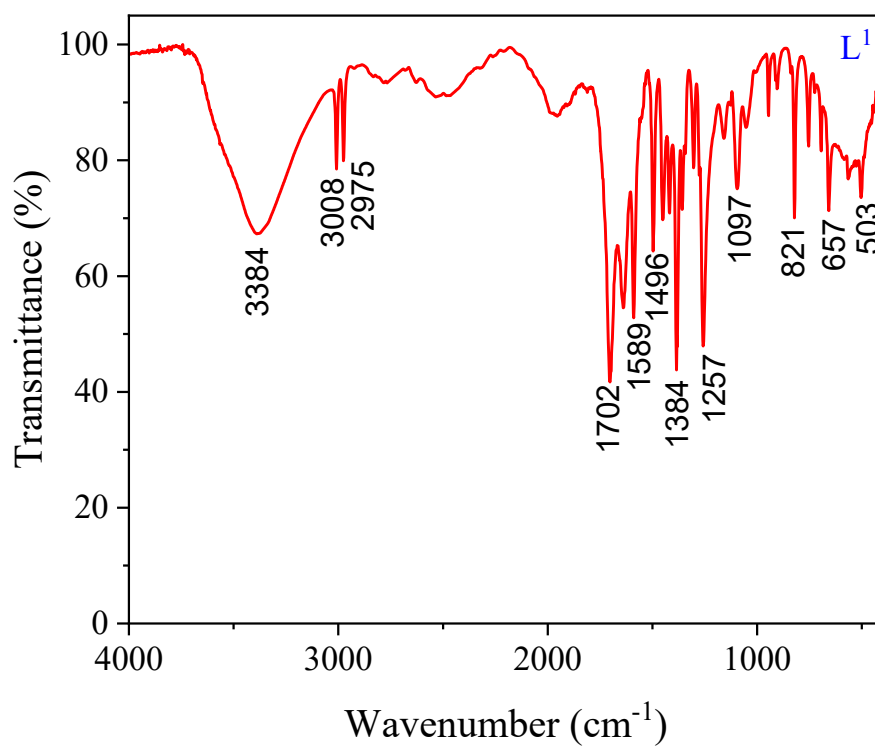


Fig. S1 The IR spectrum of L¹

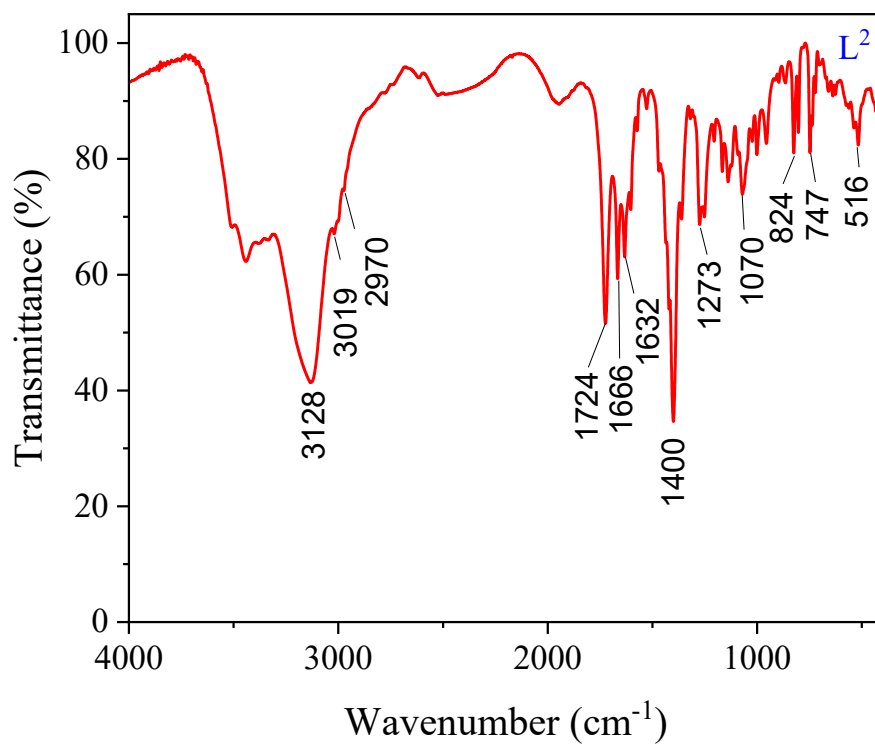


Fig. S2 The IR spectrum of L^2

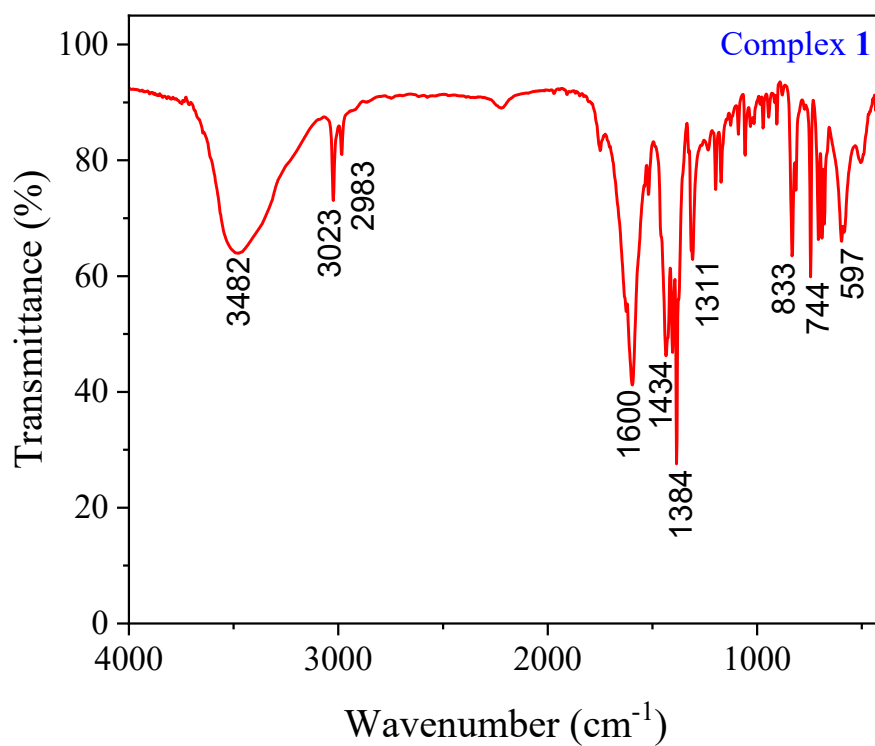


Fig. S3 The IR spectrum of complex 1

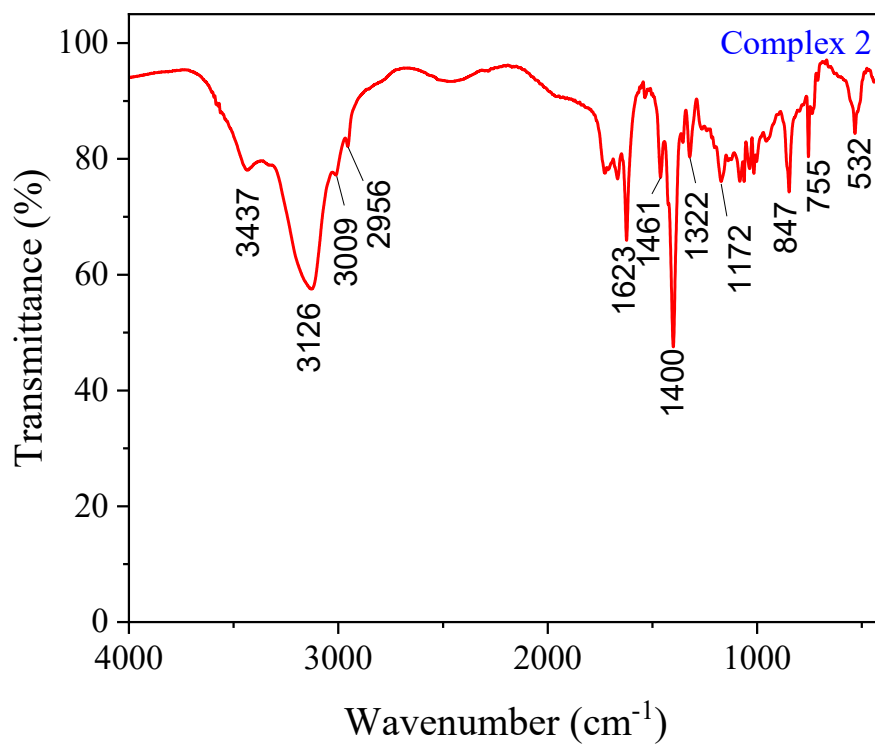


Fig. S4 The IR spectrum of complex 2

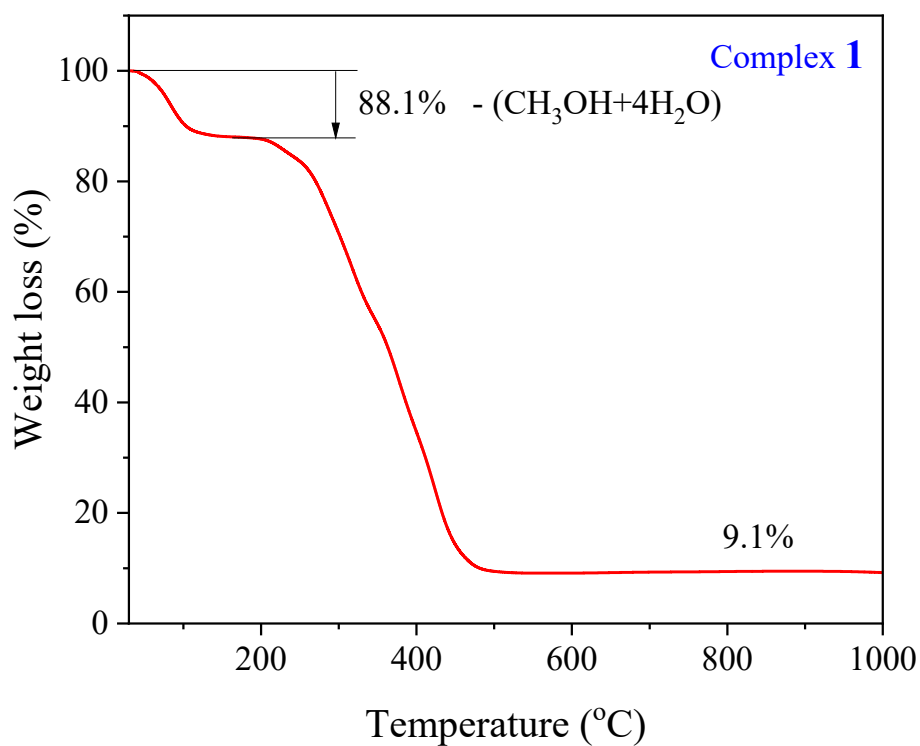


Fig. S5 Thermogravimetric analysis curve of complex 1

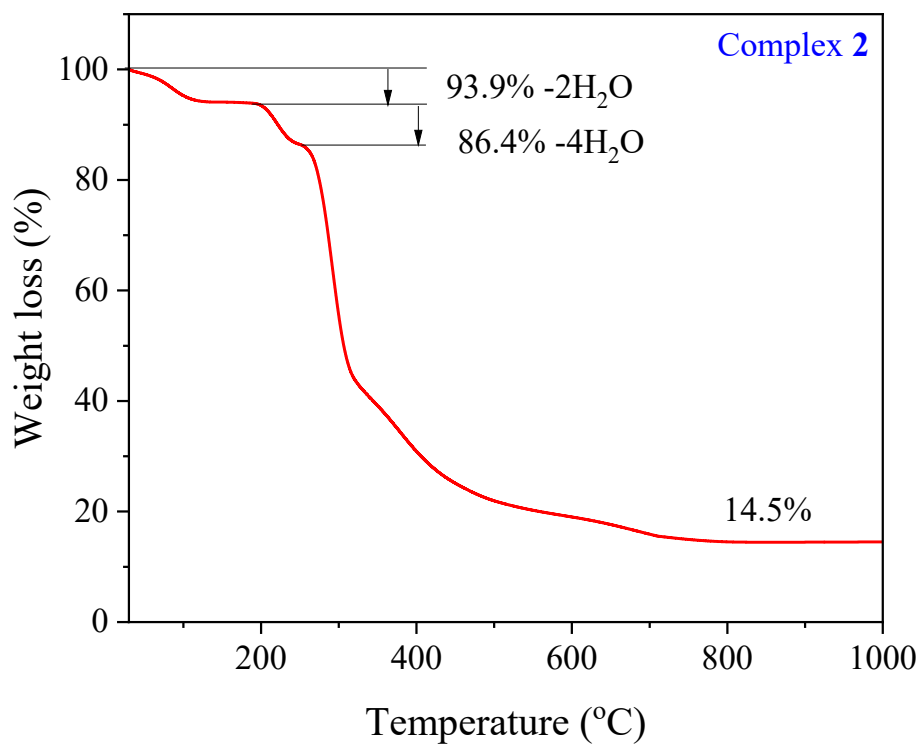


Fig. S6 Thermogravimetric analysis curve of complex **2**

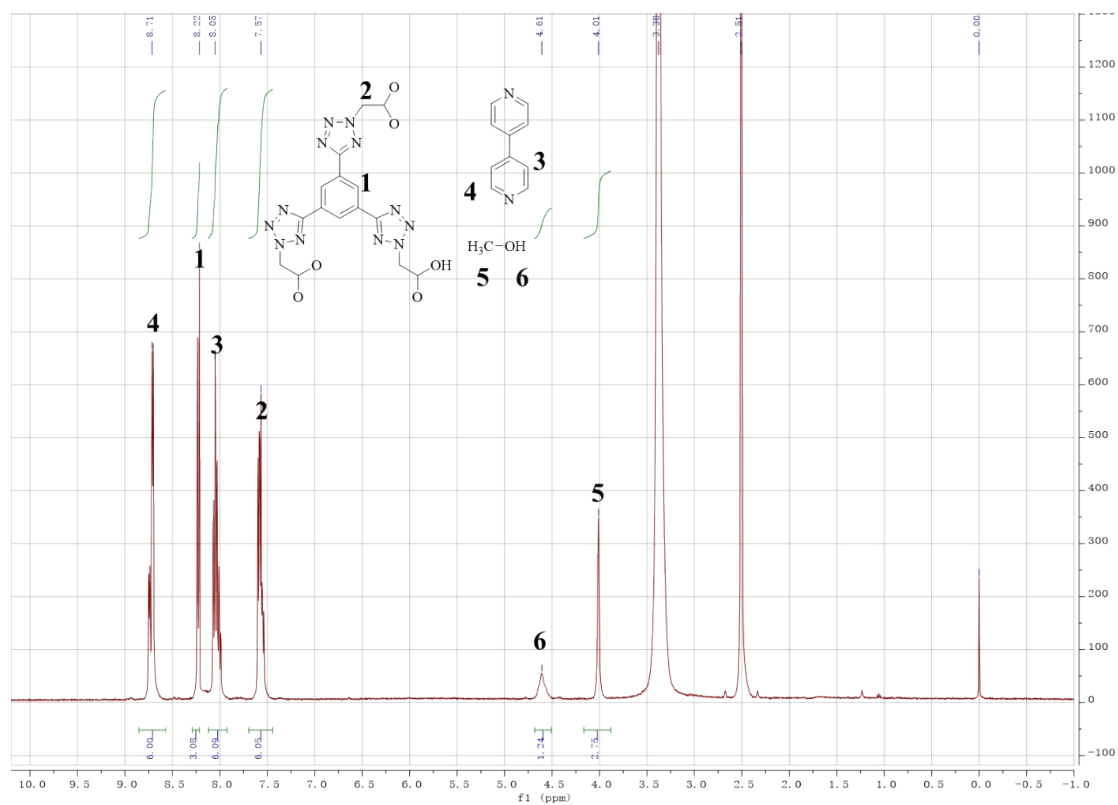


Fig. S7 ^1H NMR spectrum of complex **1**

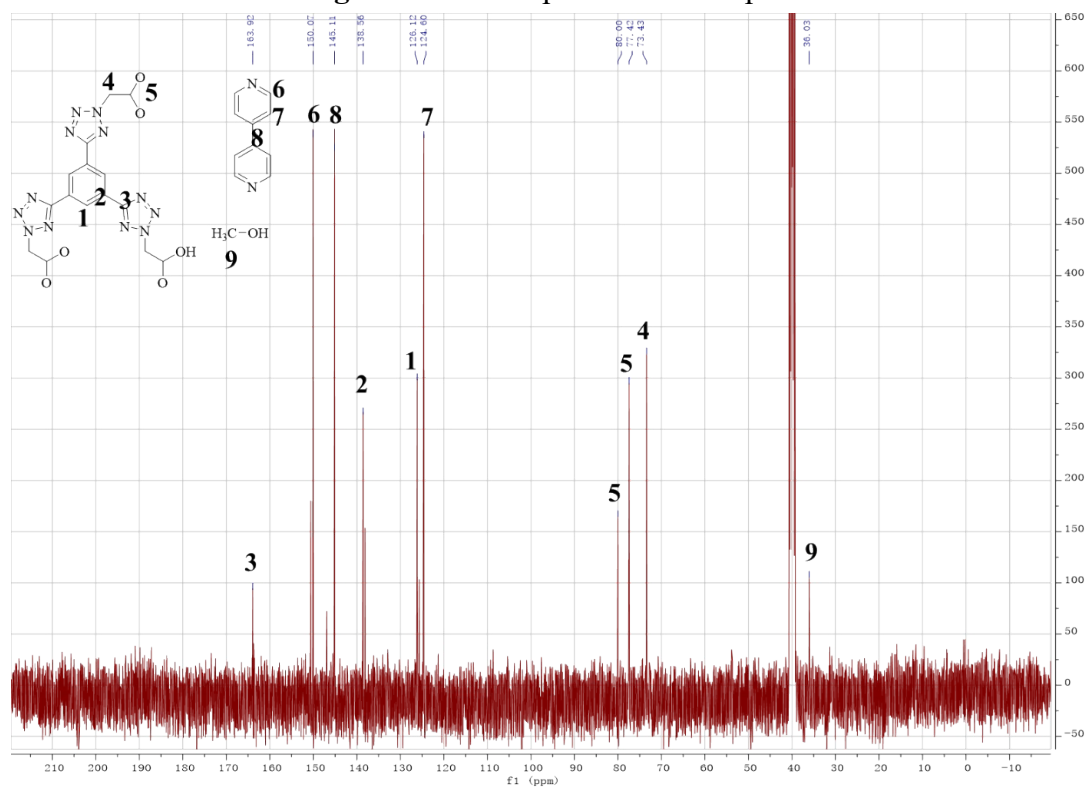


Fig. S8 ^{13}C NMR spectrum of complex **1**

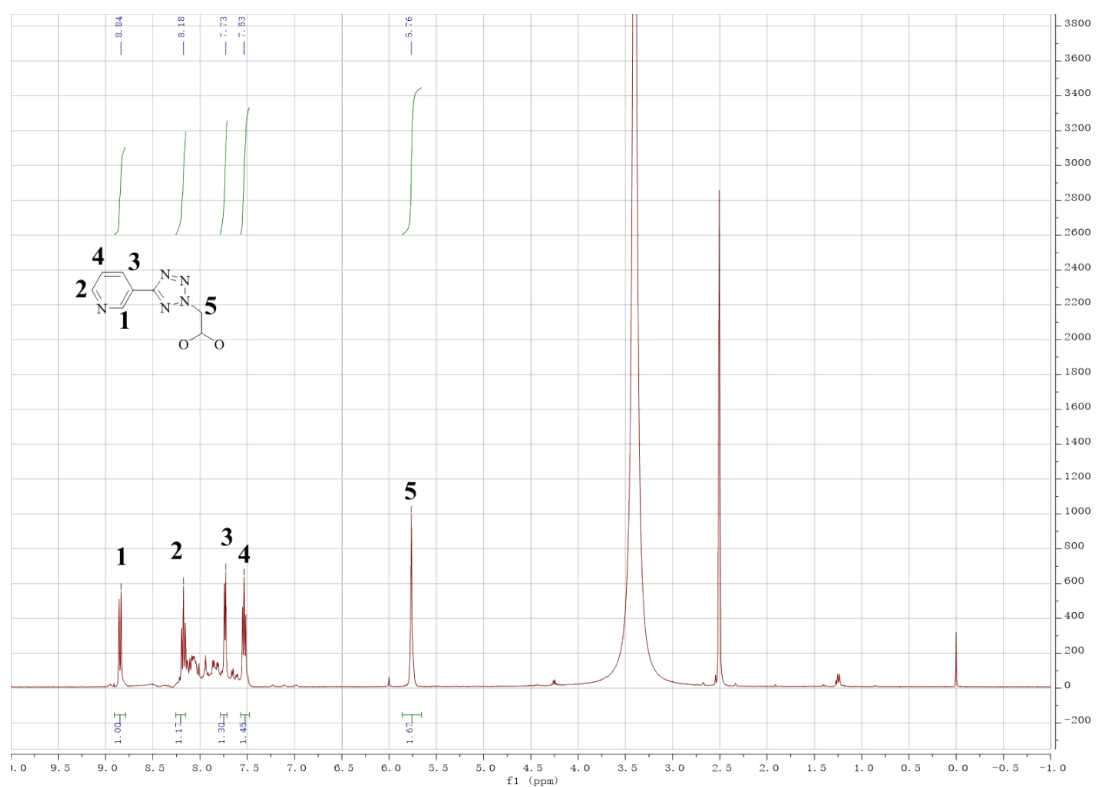


Fig. S9 ^1H NMR spectrum of complex 2

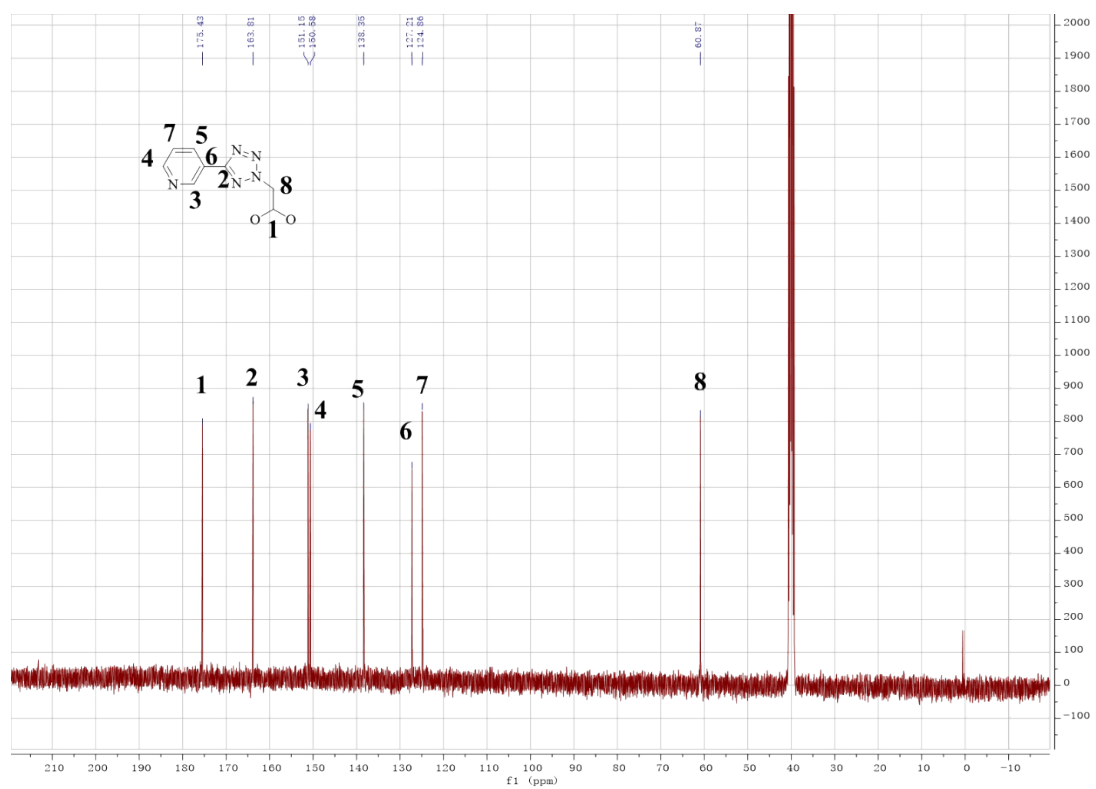


Fig. S10 ^{13}C NMR spectrum of complex 2

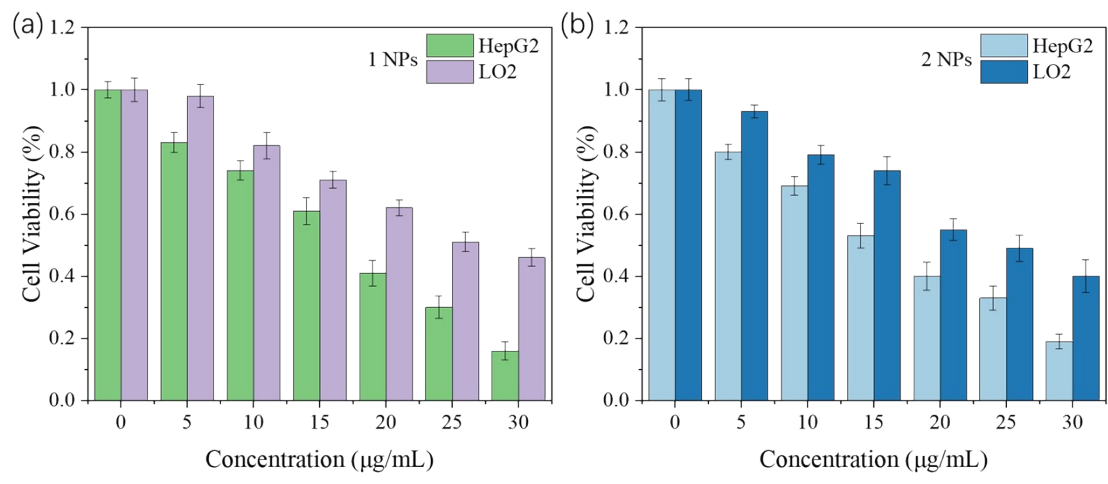


Fig. S11 CCK-8 assay of the NPs of 1-3 for HepG2 and LO2 cells.