Electronic Supplementary Information

Three metal complexes with a pyridyl schiff base: cytotoxicity, migration and mechanism of apoptosis

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Contents:

Table S1 Selected Bond Lengths (Å) and Bond Angles (°) in **1-3**

			1		
Cu1—N2	1.942(3)	Cu1—N7	1.994(3)	Cu1—O3	2.288(3)
Cu1—O1	1.957(3)	Cu1—N4	2.039(3)	Cu2—N6	1.939(3)
Cu2—O2	1.974(3)	Cu2—N8	2.060(4)		
Cu2—N3	2.014(3)	Cu2—O6	2.236(3)		
N2—Cu1—O1	79.37(12)	N2—Cu1—N7	158.68(13)	O1—Cu1—N7	95.06(12)
N2—Cu1—N4	80.56(13)	O1—Cu1—N4	159.63(13)	N7—Cu1—N4	104.95(13)
N2—Cu1—O3	98.25(12)	O1—Cu1—O3	90.17(11)	N7—Cu1—O3	102.37(12)
N4—Cu1—O3	89.25(11)	N6—Cu2—O2	78.57(12)	N6—Cu2—N3	154.78(14)
O2—Cu2—N3	94.75(12)	N6—Cu2—N8	80.33(13)	O2—Cu2—N8	158.79(11)
N3—Cu2—N8	105.30(13)	N6—Cu2—O6	122.81(12)	O2—Cu2—O6	102.29(11)
N3—Cu2—O6	82.30(11)	N8—Cu2—O6	87.43(12)		
			2		
Cd1—N3	2.288(2)	Cd1—O5	2.341(2)	Cd1—N4	2.349(3)
Cd1—O2	2.381(2)	Cd1—N2	2.410(2)	Cd1—O6	2.456(2)
Cd1—O3	2.631(2)				
N3—Cd1—O5	136.28(8)	N3—Cd1—N4	112.47(9)	O5—Cd1—N4	106.16(8)
N3—Cd1—O2	81.55(8)	O5—Cd1—O2	120.63(8)	N4—Cd1—O2	87.40(8)
N3—Cd1—N2	89.61(8)	O5—Cd1—N2	84.96(8)	N4—Cd1—N2	69.85(8)
O2—Cd1—N2	150.32(8)	N3—Cd1—O6	96.22(8)	O5—Cd1—O6	53.94(8)
N4—Cd1—O6	148.90(8)	O2—Cd1—O6	85.12(8)	N2—Cd1—O6	124.15(8)
N3—Cd1—O3	130.61(8)	O5—Cd1—O3	74.33(7)	N4—Cd1—O3	80.83(8)
O2—Cd1—O3	50.66(7)	N2—Cd1—O3	137.62(8)	O6—Cd1—O3	71.12(7)
			3		
Eu1—O1	2.373(3)	Eu1—O9'	2.394(3)	Eu1—O9	2.394(3)
Eu1—O8	2.394(3)	Eu1—O2	2.454(3)	Eu1—O6	2.494(3)
Eu1—N2	2.512(4)	Eu1—O3	2.533(3)	Eu1—O5	2.537(3)
Eu1—N4	2.606(4)	Eu1—N5	2.916(4)	Eu1—N6	2.953(4)
Eu1—H9A	2.8102				
O1—Eu1—O9'	87.63(11)	O1—Eu1—O9	87.63(11)	O1—Eu1—O8	150.76(11)
O9'—Eu1—O8	81.47(11)	O9—Eu1—O8	81.47(11)	O1—Eu1—O2	79.42(11)
O9'—Eu1—O2	148.87(11)	O9—Eu1—O2	148.87(11)	O8—Eu1—O2	122.11(11)
O1—Eu1—O6	82.86(10)	O9'—Eu1—O6	126.26(11)	O9—Eu1—O6	126.26(11)
O8—Eu1—O6	81.97(11)	O2—Eu1—O6	80.33(11)	O1—Eu1—N2	62.80(11)
O9'—Eu1—N2	77.48(11)	O9—Eu1—N2	77.48(11)	O6—Eu1—N2	138.47(11)
O8—Eu1—N2	138.97(12)	O2—Eu1—N2	71.41(12)	O1—Eu1—O3	125.84(11)
O9'—Eu1—O3	146.21(11)	O9—Eu1—O3	146.21(11)	O8—Eu1—O3	70.75(11)
O2—Eu1—O3	51.41(11)	O6—Eu1—O3	69.32(11)	N2—Eu1—O3	111.46(11)
O1—Eu1—O5	73.72(10)	O9'—Eu1—O5	75.43(11)	O9—Eu1—O5	75.43(11)
O8—Eu1—O5	77.30(11)	O2—Eu1—O5	126.23(11)	O6—Eu1—O5	51.10(10)
N2—Eu1—O5	129.06(11)	O3—Eu1—O5	115.10(11)	O1—Eu1—N4	125.97(11)
O9'—Eu1—N4	83.01(12)	O9—Eu1—N4	83.01(12)	O8—Eu1—N4	79.66(11)
O2—Eu1—N4	82.05(12)	O6—Eu1—N4	142.29(11)	N2—Eu1—N4	63.21(12)
O3—Eu1—N4	73.60(12)	O5—Eu1—N4	150.39(11)	O1—Eu1—N5	103.09(11)
O9'—Eu1—N5	159.30(11)	O9—Eu1—N5	159.30(11)	O8—Eu1—N5	96.25(11)

O2—Eu1—N5	25.88(11)	O6—Eu1—N5	73.26(10)	N2—Eu1—N5	91.57(11)
O3—Eu1—N5	25.53(11)	O5—Eu1—N5	124.35(10)	N4—Eu1—N5	76.36(12)
O1—Eu1—N6	77.13(10)	O9'—Eu1—N6	100.45(11)	O9—Eu1—N6	100.45(11)
O8—Eu1—N6	78.30(11)	O2—Eu1—N6	103.99(11)	O6—Eu1—N6	25.95(10)
N2—Eu1—N6	139.90(11)	O3—Eu1—N6	92.54(11)	O5—Eu1—N6	25.15(10)
N4—Eu1—N6	156.88(11)	N5—Eu1—N6	99.20(11)	O1—Eu1—H9A	71.6
O9—Eu1—H9A	16.4	O8—Eu1—H9A	94.2	O2—Eu1—H9A	142.1
O6—Eu1—H9A	118.6	N2—Eu1—H9A	73.8	O3—Eu1—H9A	162.5
O5—Eu1—H9A	68.2	N4—Eu1—H9A	95.5	N5—Eu1—H9A	165.3
N6—Eu1—H9A	93				

Table S2 IC_{50} values of different complexes

Metal	complex	parameter	value	cell line	Ref
Cd	Cd	IC_{50}（μM）	36.91±0.47， 23.01±1.28， 36.96±0.75，	A549， MCF-7 HT29	1
	Cd	IC_{50}（μg/μL）	4.55 1.45	HT116 HepG-2	2
	Cd	ID_{50}（μg/mL）	12 15	ADLD HeLa	3
	[Cd(L)Cl_2(H_2O)]	IC_{50}（μM）	410±31	A549	4
	[CdL(CH3COO)(H2O2)]	IC_{50}（μM）	0.3485 0.3369	HepG2 MCF-7	5
Eu	$EuL_2(H_2O)\cdot 4H_2O$	IC_{50}（μM）	45.85 44.37	HeLa HCT116	6
	complex **2**	IC_{50}（μM）	27.36±3.02	HeLa	7
	6	IC_{50}（μM）	50.22±1.00 >100 41.77±2.42 >100 61.48±1.94 >100	BEL-7402 NCL-H460 MGC80-3 Hep-G2 HeLa T-24	8
Cu	Cu(Cl_2-L_1)NO_3	IC_{50}（μM）	18.1±1.78 4.2±2.2 29.9±6.86	HCT116 A2780 MCF7	9
	1	IC_{50}（μM）	60.00±0.29 25.00±1.17 30.00±0.58	A549 MCF-7 HeLa	10
	[Cu(btacn)$_2$]·(ClO_4)$_2$	IC_{50}（μM）	5.17±0.39 2.28±0.44	HeLa HepG-2	11
	ATRs-Cu	IC_{50}（μg/mL）	14.20 6.10	HepG-2 HCT116	12

	1	IC_{50}（μM）	53.52±6.4	A549	13

Ref 1 Ligand: 2,6-bis(2-benzimidazolyl)pyridine

Ref 2 Ligand:(ahpv), where ahp = 2-amino-3-hydrox-ypyridine and v = 3-methoxysalicylaldehyde (o-vanillin)

Ref 3 Ligand:2,6-bis[1-(4-amino-1,2,3,6-tetra-hydro-1,3-dimethyl-2,6-dioxopyrimidin-5-yl)imino]eth-ylpyridine

Ref 4 Ligand:(N-[(phenylcarbamothioyl)amino]pyridine-3-carboxamide)

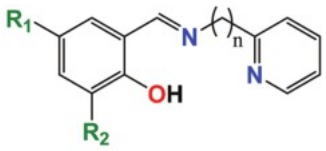
Ref 5 Ligand:(Z)-(2-((1,3-diphenyl-1H-pyrazol-4-yl)methylene)-hydrazinyl)(pyridin-2-ylamino)methanethiol

Ref 6 Ligand:derived from glycylglycine and 4-nitrobenzaldehyde

Ref 7 Ligand:1,10(1,4-phenylene-bis [methylene])-bis (pyridine-3-carboxylicaicd)

Ref 8 Ligand:2-((2-(pyridin-2-yl) hydrazono)methyl)quinolin-8-ol

Ref 9 Ligand:

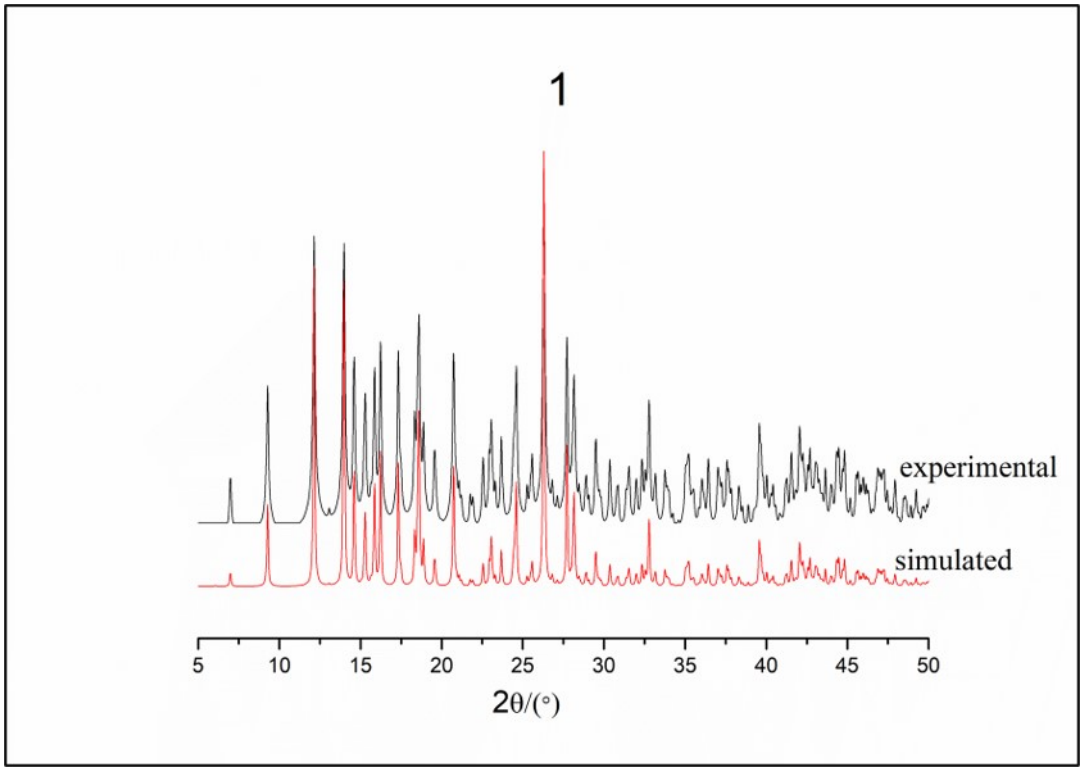


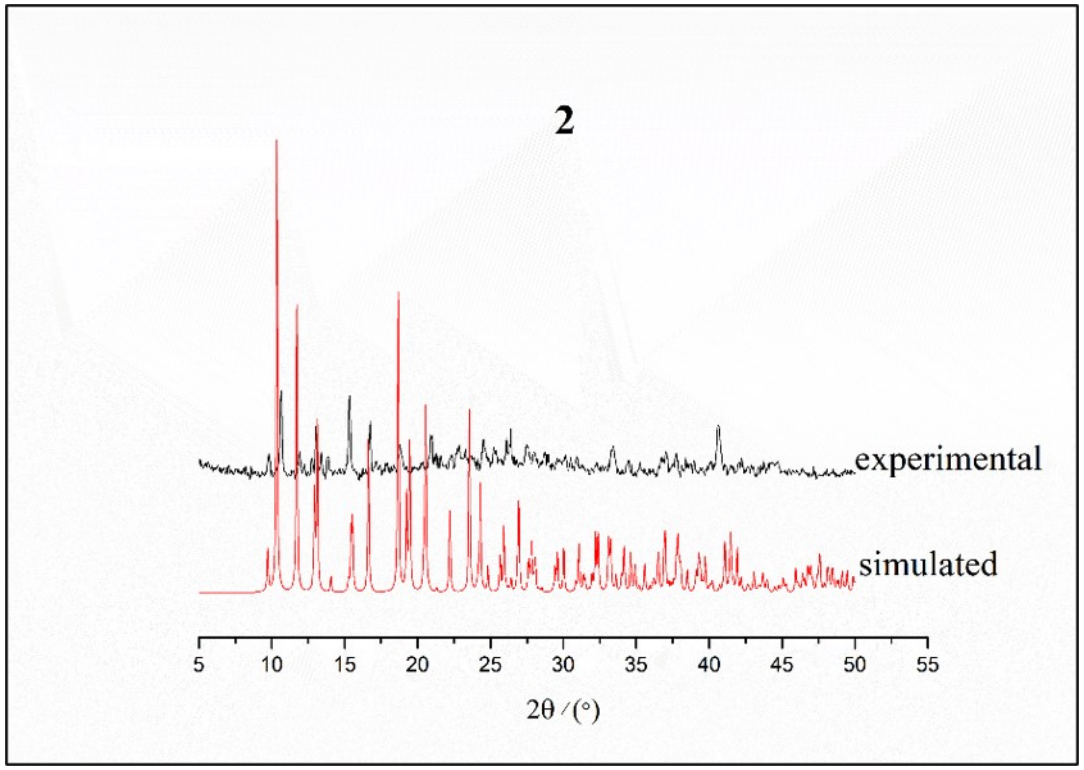
(R1=R2=Cl)

Ref 10 Ligand: 5-[(pyridin-2-ylmethylene)-amino]-pentan-1-ol)

Ref 11 Ligand: 1,4,7-triazacyclononane-derivative,4-benzyloxy-benzyl-1,4,7-triazacyclononane

Ref 12 Ligand: [4-bromo-2-(thiazole-2-yliminomethyl) phenol]


1
experimental
simulated
5
10
15
20
25
30
35
40
45
50
2θ/(°)


2
experimental
simulated
5
10
15
20
25
30
35
40
45
50
55
2θ /(°)

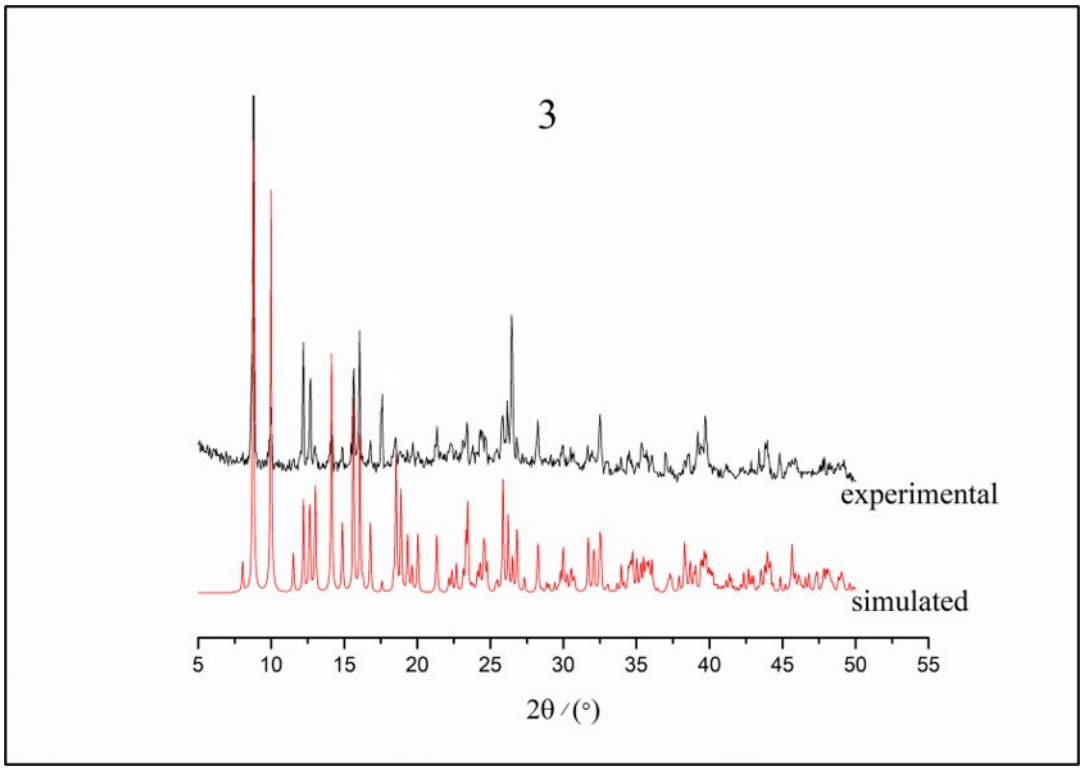
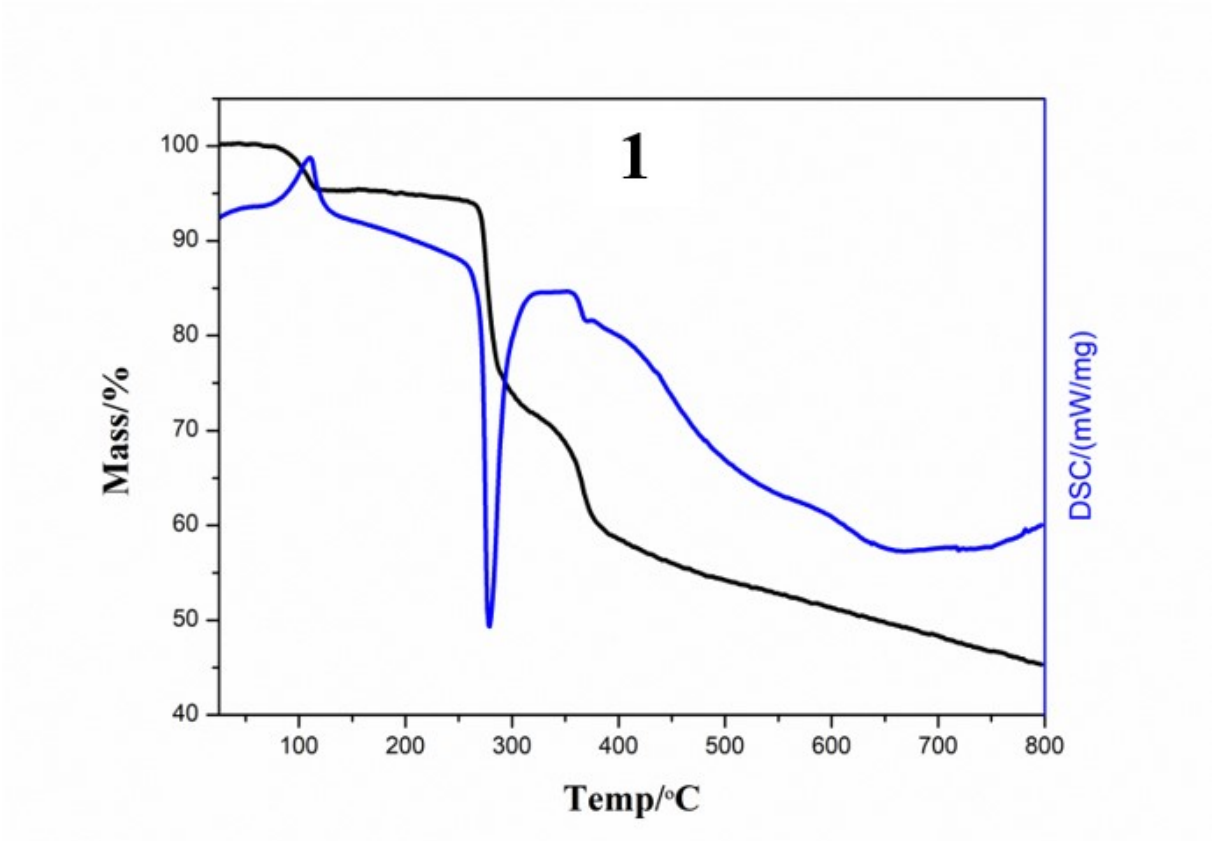


Figure S1 Powder XRD patterns of **1-3**



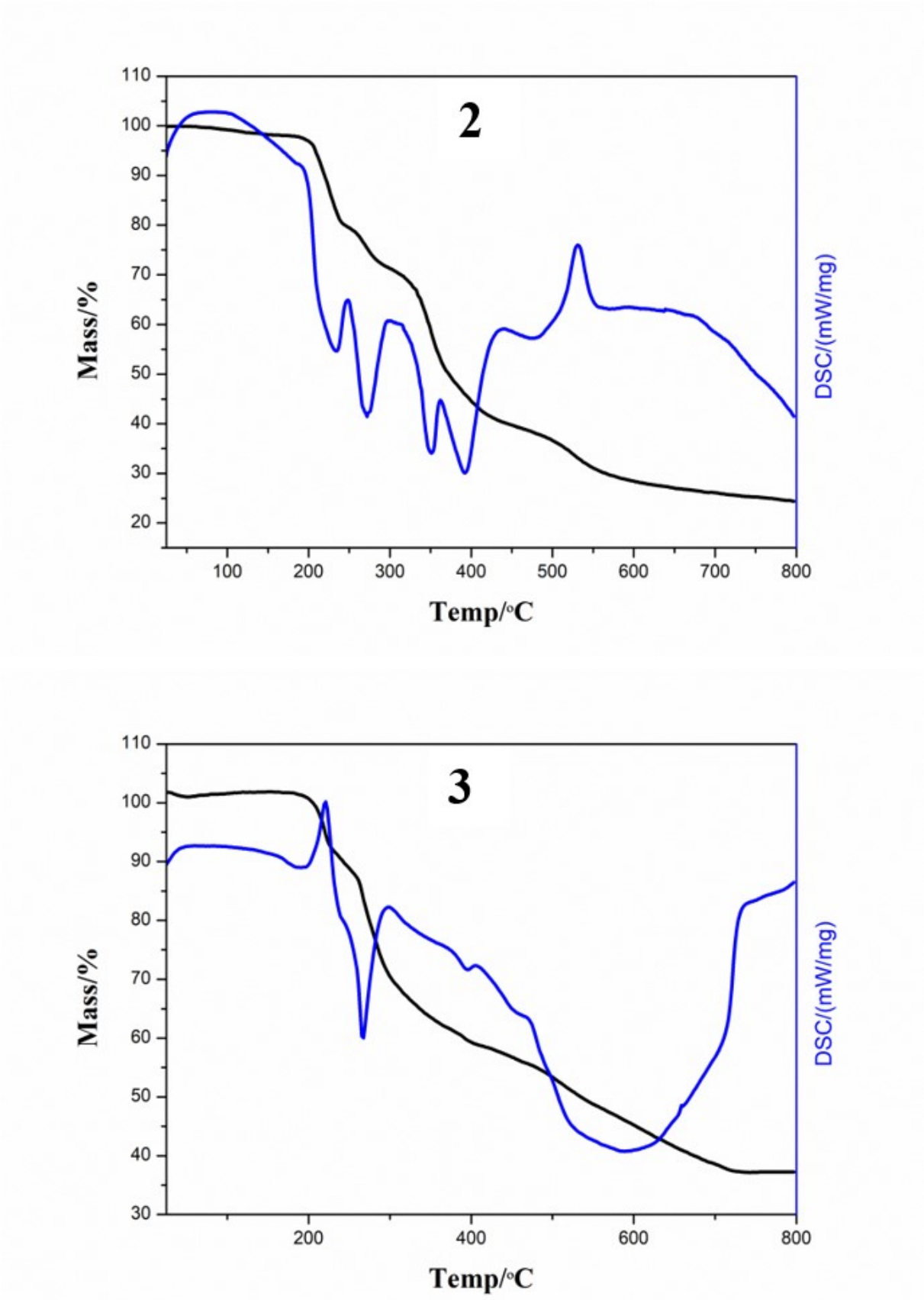
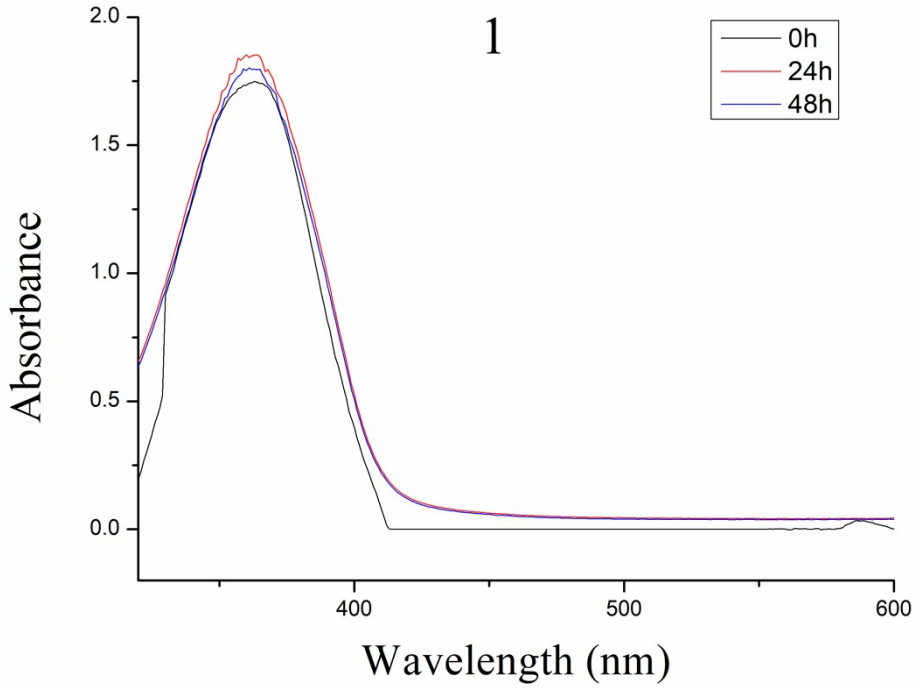
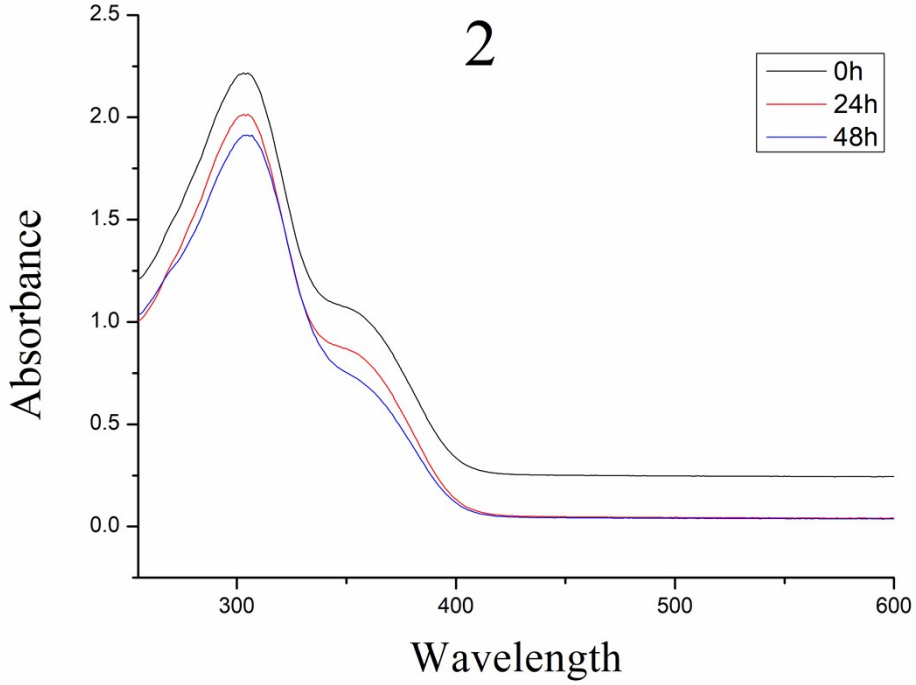
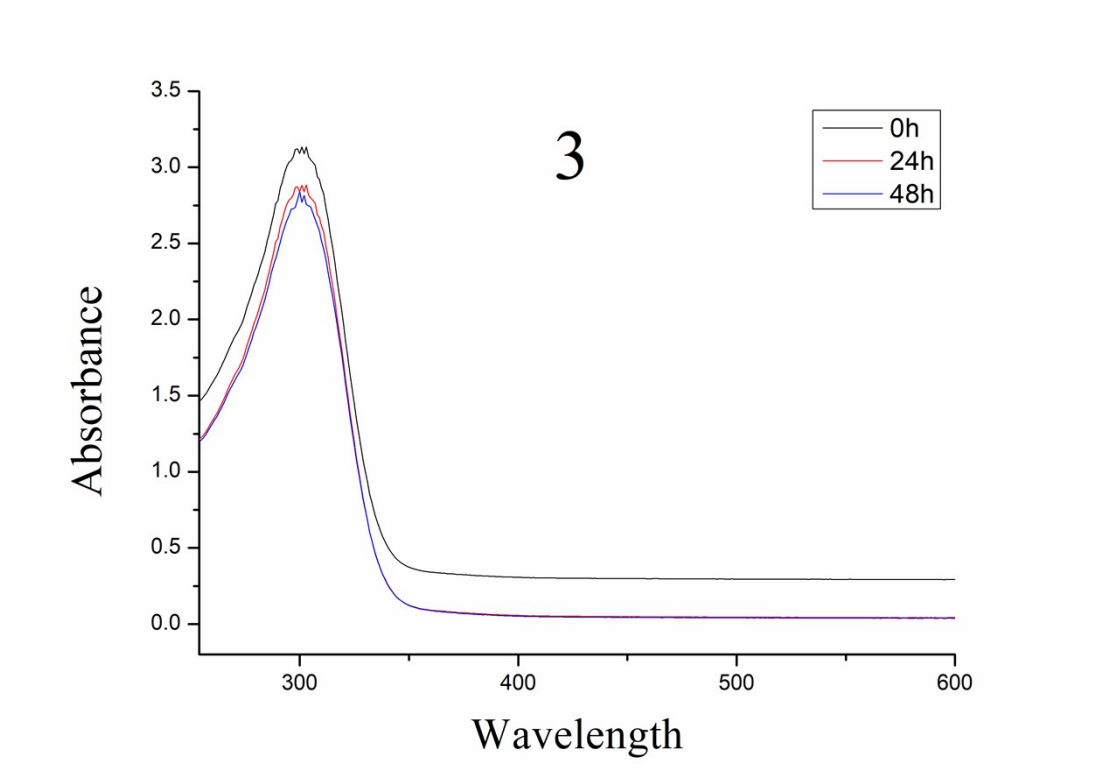


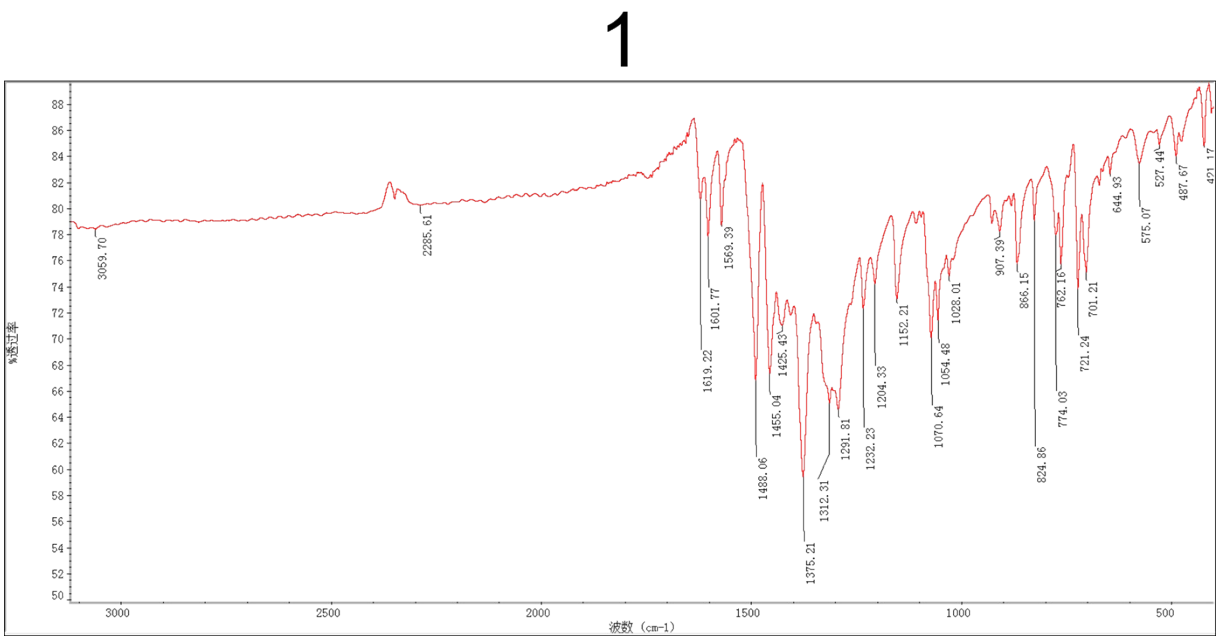
Figure S2 TG-DSC curves of **1-3**


1
0h
24h
48h
Absorbance
Wavelength (nm)
2.0
1.5
1.0
0.5
0.0
400
500
600


2
0h
24h
48h
Absorbance
Wavelength
2.5
2.0
1.5
1.0
0.5
0.0
300
400
500
600



FigureS3 Ultraviolet spectrum of **1-3** in buffer solution



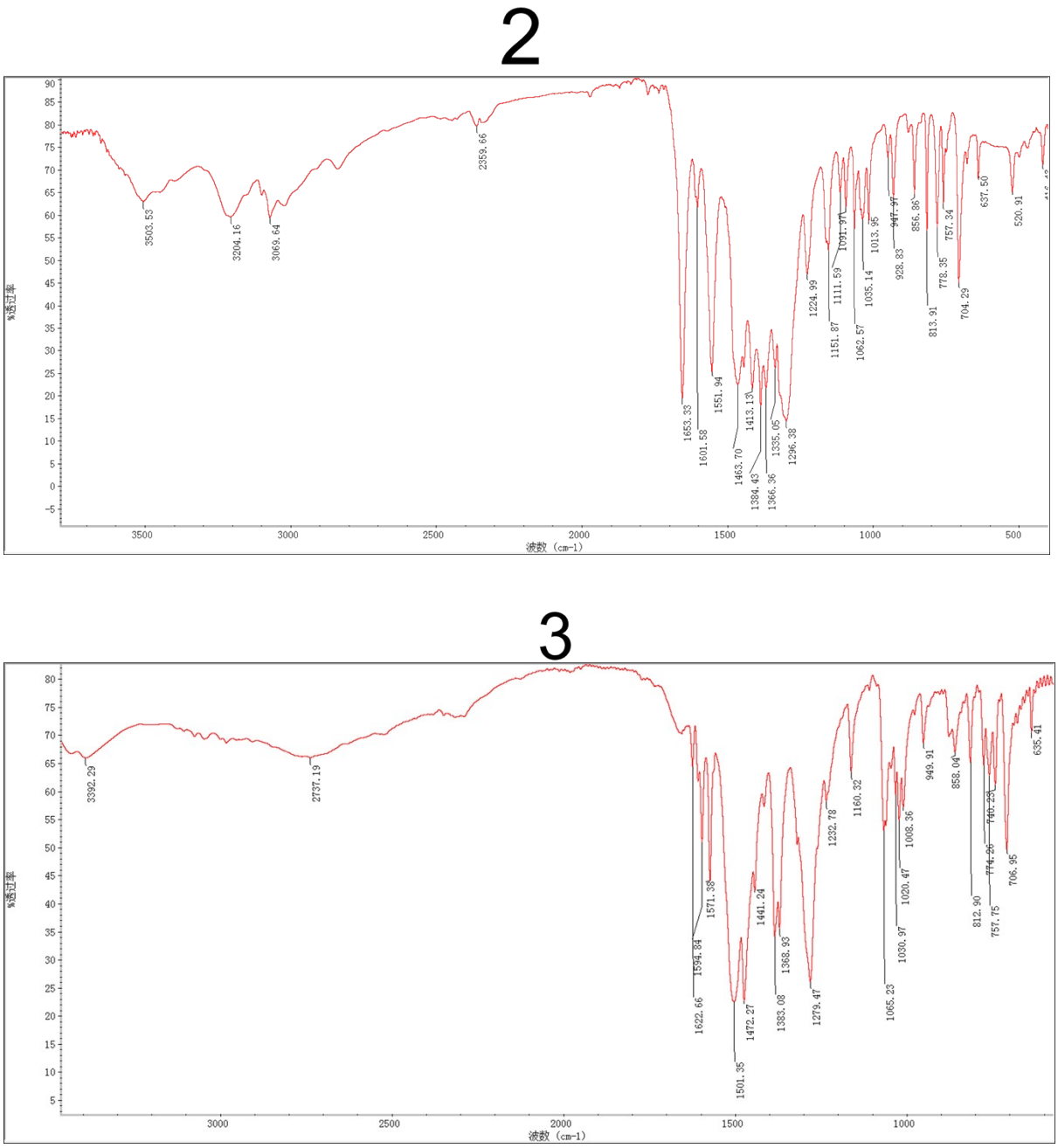


Figure S4 Infrared spectroscopy of **1-3**

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