Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Dinuclear Cd(II), Mn(II) and Cu(II) complexes derived from (anthraquinone-1-diyl) benzoate: DNA binding and cleavage studies

5 **Lin Liu,[a,†] Gong-Ming Zhang,[a,†] Ru-Gang Zhu,[*b] Yong-Hui Liu,[b] Hui-Meng Yao,[a] Zheng-Bo Han[*a]**

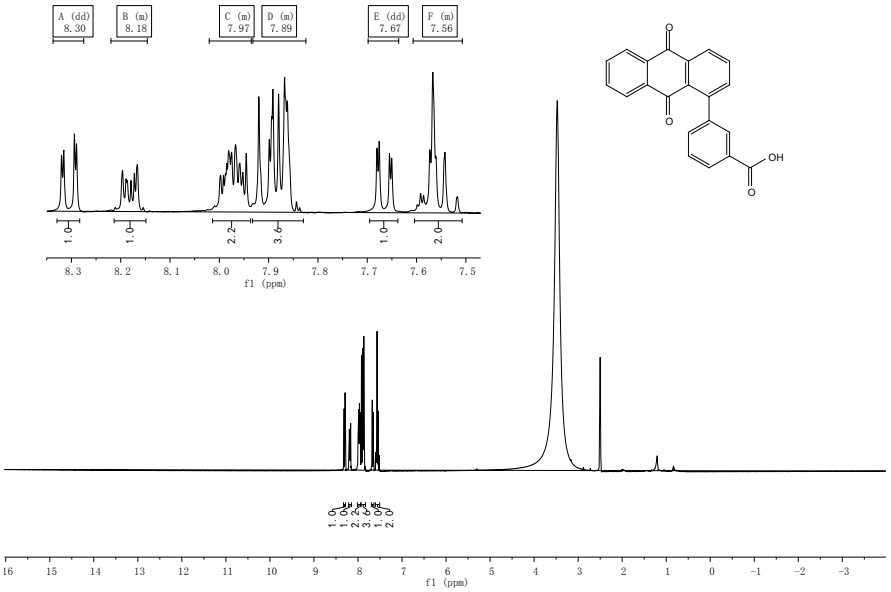
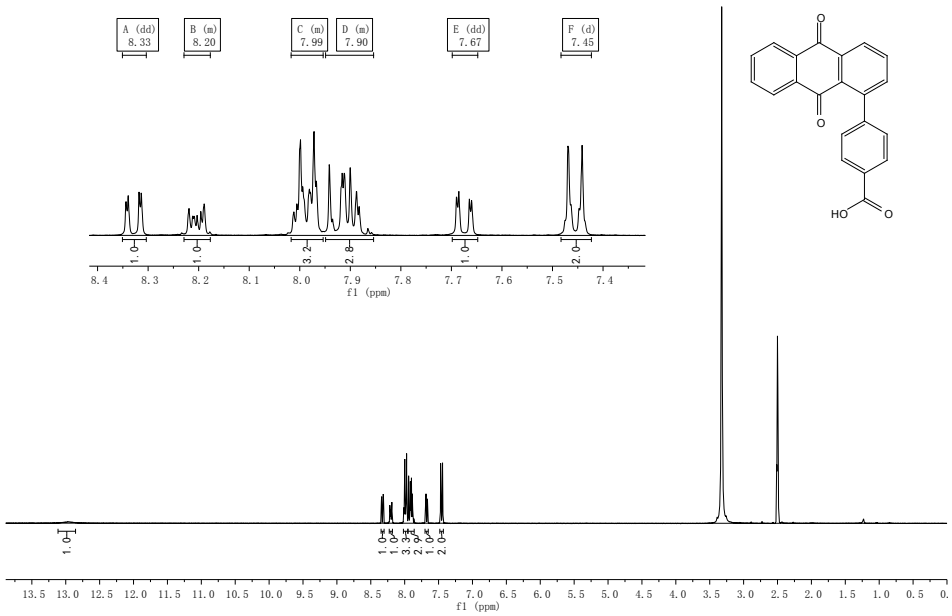


Figure S1. The [1]HNMR of 3-(anthraquinone-1-diyl) methyl benzolic acid



(b)

Figure S2. The [1]HNMR of 4-(anthraquinone-1-diyl) methyl benzolic acid

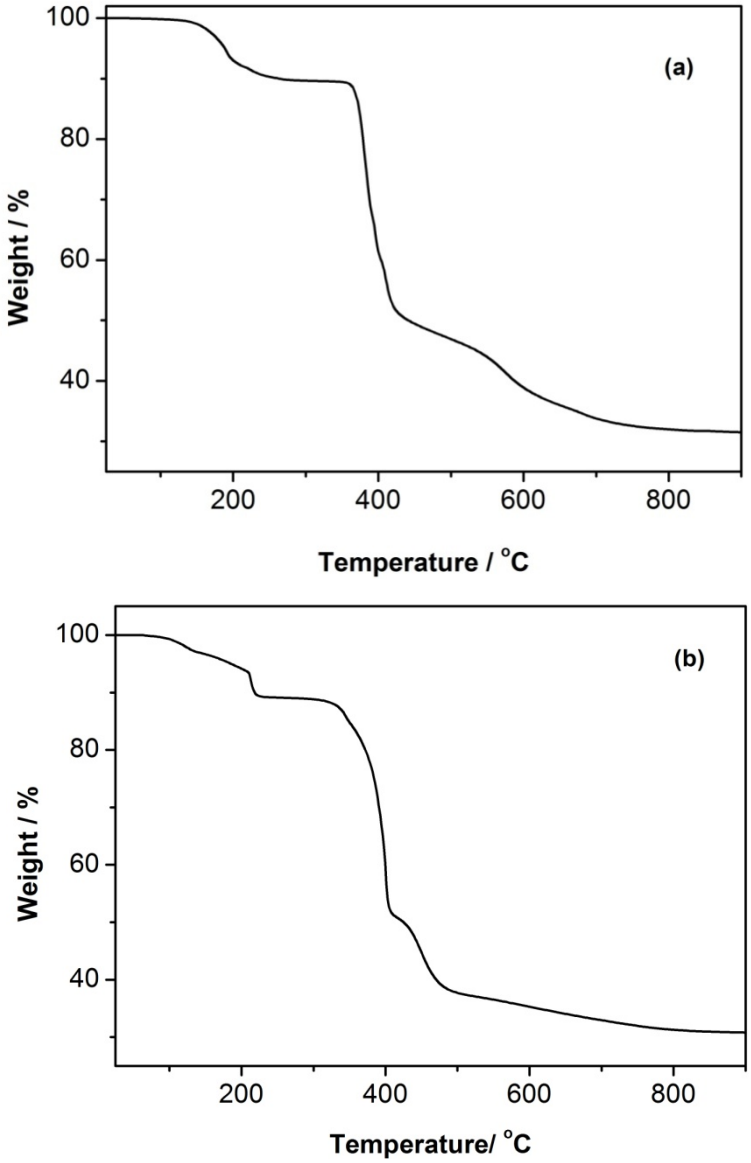


Figure S3. TGA curves of **1**(a) and **3**(b).

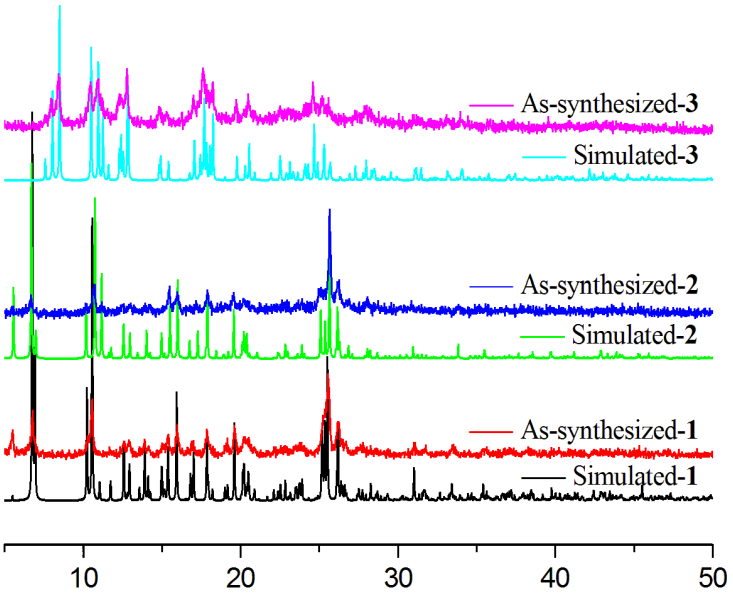


Figure S4. XRPD patterns of simulated and as-synthesized of **1-3**.

Table S1 Selected Bond Lengths (Å) and Angles (deg) for **1-3**

		1	
Cd1-O6^{i}	2.274(3)	Cd1-O1	2.467(3)
Cd1-O5	2.292(3)	Cd1-O6	2.625(3)
Cd1-O9	2.303(3)	Cd1-O6i	2.274(3)
Cd1-O2	2.305(3)	Cd1-O5	2.292(3)
Cd1-O1W	2.342(3)		
O6^{i}-Cd1-O5	124.90 (11)	O5-Cd1-O1	82.36 (11)
O6^{i}-Cd1-O9	84.56 (18)	O9-Cd1-O1	93.33 (17)
O5-Cd1-O9	89.15 (16)	O2-Cd1-O1	54.59 (10)
O6^{i}-Cd1-O2	98.20 (11)	O1W-Cd1-O1	87.15 (12)
O5-Cd1-O2	136.90 (10)	O6i-Cd1-O6	73.27 (11)
O9-Cd1-O2	94.84 (15)	O5-Cd1-O6	51.66 (10)
O6^{i}-Cd1-O1W	98.15 (13)	O9-Cd1-O6	85.55 (15)
O5-Cd1-O1W	84.14 (12)	O2-Cd1-O6	171.40 (9)
O9-Cd1-O1W	173.15 (14)	O1W-Cd1-O6	89.21 (12)
O2-Cd1-O1W	91.00 (12)	O1-Cd1-O6	133.99 (10)
O6^{i}-Cd1-O1	152.52 (12)		
Symmetry code: (i) −x+3, −y+1, −z+1.			
		2	
Mn1-O6i	2.082 (3)	Mn1-O2	2.198 (3)
Mn1-O5	2.145 (3)	Mn1-O2W	2.248 (3)
Mn1-O9	2.159 (4)	O5-Mn1-O2W	83.36 (10)
O6^{i}-Mn1-O5	117.14 (11)	O9-Mn1-O2W	170.48 (13)
O6^{i}-Mn1-O9	91.20 (16)	O2-Mn1-O2W	88.93 (11)
O5-Mn1-O9	89.12 (13)	O6^{i}-Mn1-O1	153.12 (11)
O6^{i}-Mn1-O2	97.13 (11)	O5-Mn1-O1	89.73 (10)
O5-Mn1-O2	145.53 (11)	O9-Mn1-O1	90.10 (15)
O9-Mn1-O2	94.03 (14)	O2-Mn1-O1	56.00 (10)
O6^{i}-Mn1-O2W	97.41 (12)	O2W-Mn1-O1	84.05 (12)
Symmetry code: (i) −x+3, −y+1, −z+1.			
		3	
Cu1-O2^{i}	1.962 (2)	Cu1-O1	1.968 (2)
Cu1-O6	1.962 (2)	Cu1-O10A	2.172 (2)
Cu1-O5^{i}	1.967 (2)	Cu1-Cu1^{i}	2.6154 (14)
O2^{i}-Cu1-O6	89.03 (10)	O5^{i}-Cu1-O1	90.59 (9)
O2^{i}-Cu1-O5^{i}	89.29 (9)	O2^{i}-Cu1-O10A	97.20 (9)
O6-Cu1-O5^{i}	168.98 (8)	O6-Cu1-O10A	94.26 (9)
O2^{i}-Cu1-O1	169.00 (8)	O5^{i}-Cu1-O10A	96.75 (9)
O6-Cu1-O1	89.00 (10)	O1-Cu1-O10A	93.74 (9)
Symmetry code: (i) −x+1, −y, −z.			

Table S2 Hydrogen bonding geometry (Å, deg) for **1**

D-H···A	D-H	H···A	D···A	∠D-H···A
O1W-H1WA···O(5)^{i}	0.84	2.13	2.854(5)	143
O1W-H1WB···O(1)^{i}	0.85	2.52	2.845(5)	103
C(11)-H(11A)···O(4)^{ii}	0.95	2.55	3.263(6)	132
C(19)-H(19A)···O(3)^{iii}	0.95	2.59	3.310(6)	133
C(24)-H(24A)···O(2)^{iv}	0.95	2.58	3.469(5)	157
C(32)-H(32A)···O(8)^{ii}	0.95	2.57	3.258(6)	129
C(43)-H(43C)···O(9)	0.98	2.35	2.76(2)	104

Symmetry codes：(i) 2-x,1-y,1-z; (ii) -1+x,y,z; (iii) 1+x,y,z (iv) 3-x,1-y,1-z.

Table S3 π-π stacking interaction for **3**

Cg(I) is Plane number I; Alpha is Dihedral Angle between Planes I and J (Deg); Beta is Angle Cg(I)-Cg(J) or Cg(I)-Me vector and normal to plane I (Deg); Gamma is Angle Cg(I)-Cg(J) vector and normal to plane J (Deg); Cg-Cg is Distance between ring Centroids (Ang.); CgI-Perp is Perpendicular distance of Cg(I) on ring J (Ang.); CgJ-Perp is Perpendicular distance of Cg(J) on ring I (Ang.); Slippage is Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang). Cg(3) is the centroid of the C(8)/C(9)/C(10)/C(11)/C(12)/ C(13); Cg(4) is the centroid of the C(12)/C(13)/C(17)/C(16)/C(15)/C(14); Cg(5) is the centroid of the C(15)/C(16)/C(21)/C(20)/C(19)/C(18); Cg(9) is the centroid of the C(35)/C(36)/C(37)/C(38)/C(39)/C(40).

Cg(I)-Cg(J)	Cg-Cg	Alpha	Beta	Gamma	CgI-Perp	CgJ-Perp	Slippage
Cg(3)-Cg(5)^{i}	3.7579	2.30	22.79	22.39	3.474	3.465	
Cg(4)-Cg(4)^{i}	3.7422	0.02	23.45	23.45	3.433	3.433	1.489
Cg(5)-Cg(3)^{i}	3.7579	2.30	22.39	22.79	3.465	3.474	
Cg(5)-Cg(4)^{i}	3.7142	1.42	22.93	21.51	3.455	3.421	
Cg(5)-Cg(9)^{ii}	3.8195	18.52	23.49	9.07	3.772	3.503	

Symmetry codes：(i) 1-x, 3-y, 1-z; (ii) -x, 2-y, 1-z.

Table S4 X-H···Cg interactions (Gamma < 30°) for **3**

X-H···Cg is the distance between the carbon atom and the ring centroid; H-Perp is the perpendicular distance of H from ring; Cg(1) is the centroid of the C(33)/C(34) /C(35) /C(40)/C(41)/C(42) plane.

X-H	Cg	H…Cg	H-Perp	Gamma	X-H…Cg	X…Cg
C(4)-H(14a)	Cg(1)^{i}	2.88 Å	2.64 Å	23.55^{o}	153	3.729(5) Å

Symmetry codes：(i) 1-x, 1-y, -z.

Table S5 Hydrogen bonding geometry (Å, deg) for **3**

D-H···A	D-H	H···A	D···A	∠D-H···A
C(9) -H(9A)···O(7)^{i}	0.93	2.42	3.267(6)	152
C(25) -H(25A)···O(9)^{ii}	0.93	2.58	3.497(5)	168
C(39) -H(39A)···O(8)^{i}	0.93	2.44	3.239(5)	144
C(43) -H(43 C)···O(3)^{iii}	0.96	2.39	3.231(7)	146
C(45) -H(45 A)···O(4)^{iv}	0.93	2.55	3.282(4)	136

Symmetry codes：(i) -x, 1-y, 1-z; (ii) -1+x, y, z (iii) x,-1+y,z (iv) 1-x,2-y,1-z