Supporting Information

Auxiliary ligand-controlled supramolecular assembly of three Cd(II) coordination polymers based on a (E)-3-(quinolin-4-yl) acrylic acid: syntheses, structures and photoluminescent properties

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Infrared Spectra

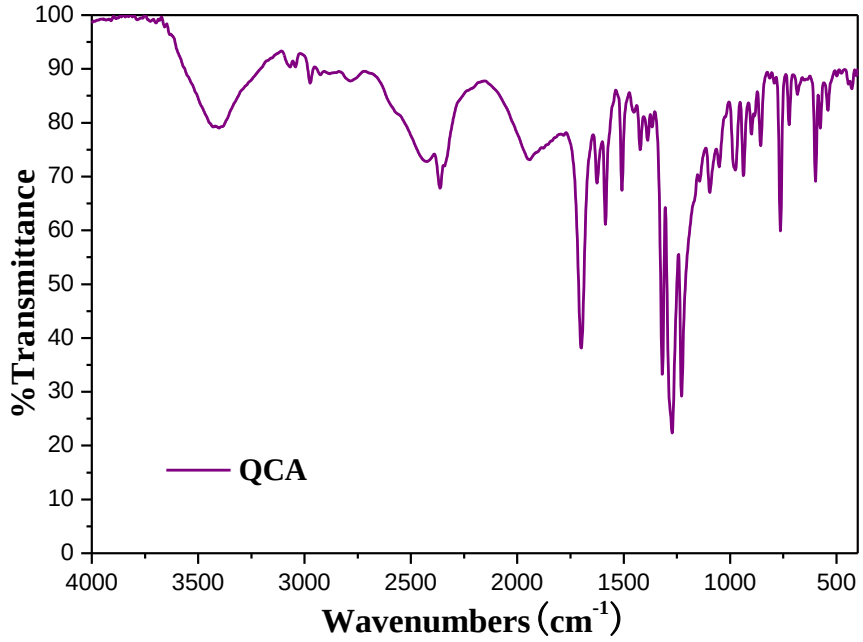

Fig. S1 IR spectrum picture of QCA ligand.

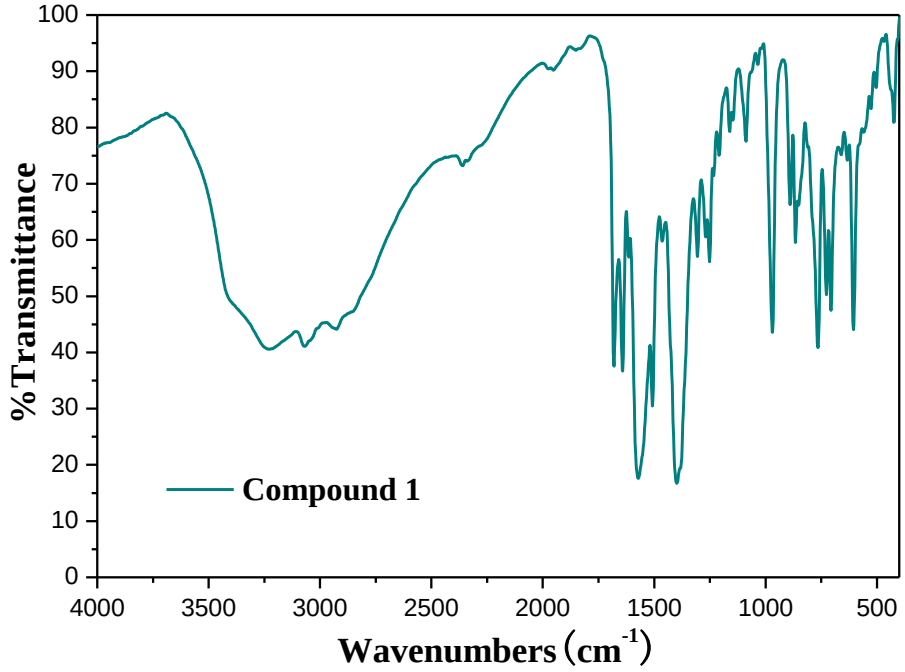

Fig. S2 IR spectrum picture of compound **1**.

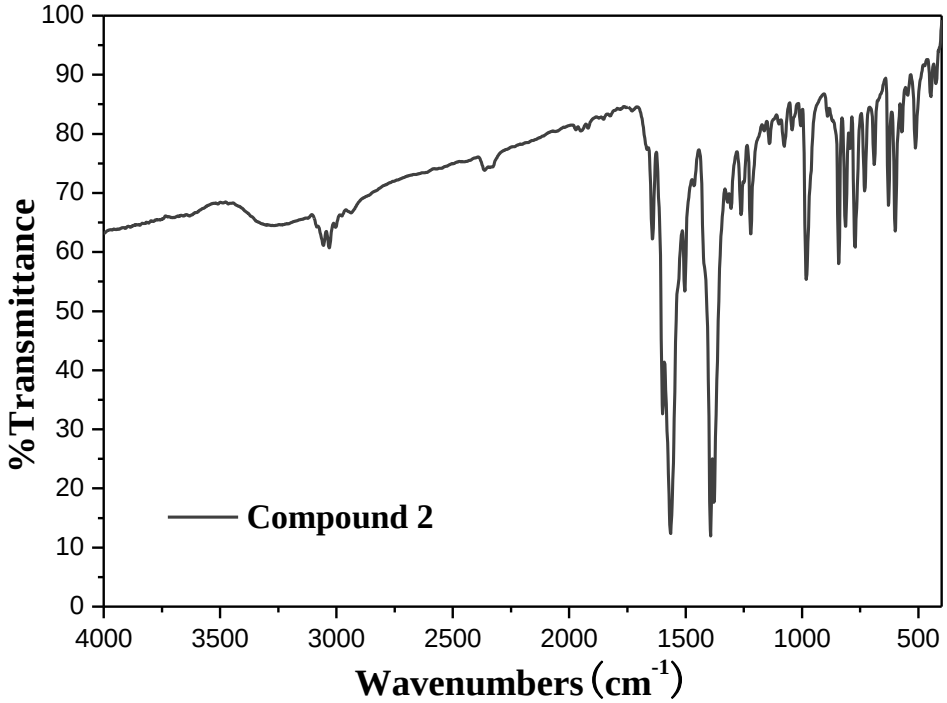

Fig. S3 IR spectrum picture of compound **2**.

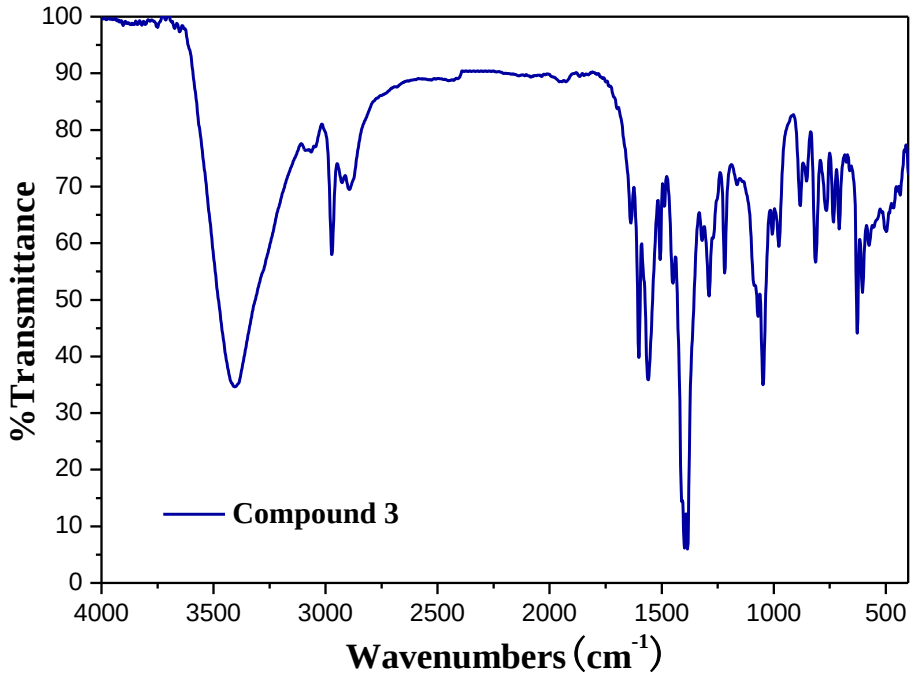

Fig. S4 IR spectrum picture of compound **3**.

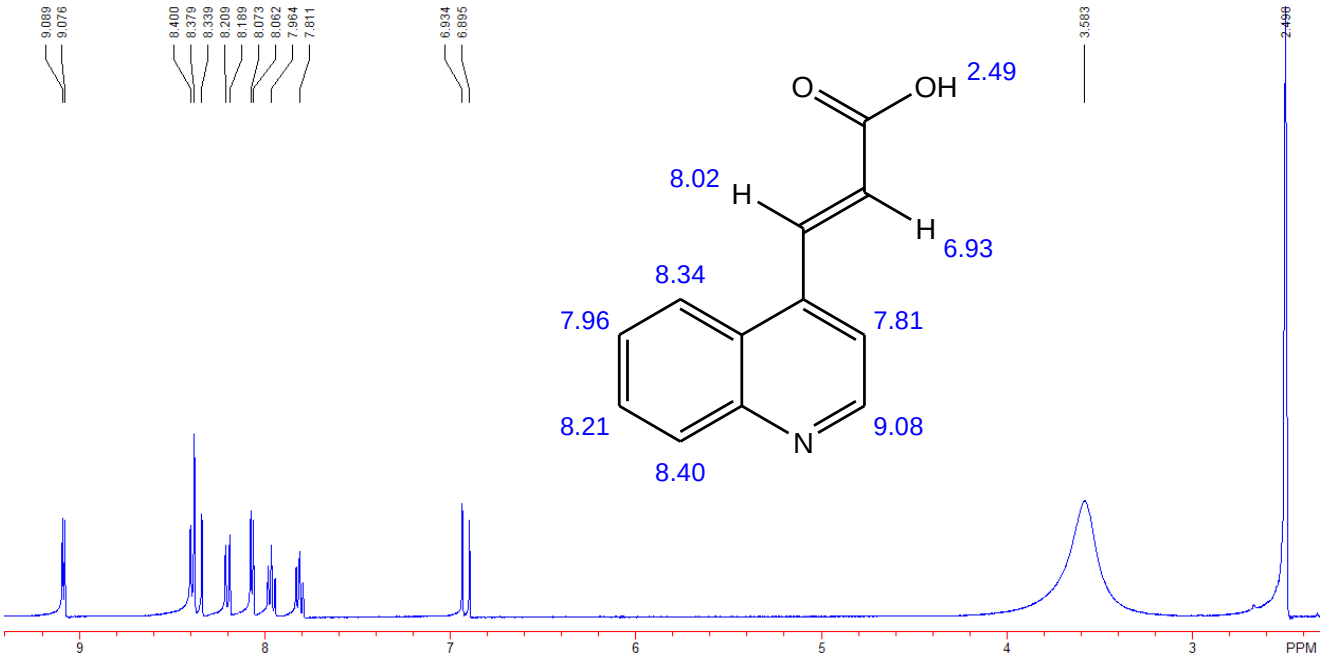

Fig. S5 ^{1}H NMR spectra of QCA ligand in d_6-DMSO solution.

Table S1 Selected Bond Distances (Å) and Angles (deg) for **1**

Cd(1)-O(1)	2.6170(15)	Cd(1)-O(2)	2.2758(13)
Cd(1)-O(3)	2.2621(14)	Cd(1)-O(4)	2.2858(13)
Cd(1)-O(5)	2.2469(16)	Cd(1)-O(4)#2	2.8561(14)
Cd(1)-N(2)	2.3957(16)		
O(2)-Cd(1)-O(4)	136.58(5)	O(2)-Cd(1)-O(1)	52.73(5)
O(2)-Cd(1)-N(2)	91.05(6)	O(3)-Cd(1)-O(2)	124.01(5)
O(3)-Cd(1)-O(4)	98.20(5)	O(3)-Cd(1)-N(2)	87.13(6)
O(3)-Cd(1)-O(1)	176.39(5)	O(4)-Cd(1)-N(2)	101.73(5)
O(4)-Cd(1)-O(1)	84.75(5)	O(5)-Cd(1)-O(2)	87.03(6)
O(5)-Cd(1)-O(3)	92.21(6)	O(5)-Cd(1)-O(1)	86.17(6)
O(5)-Cd(1)-O(4)	81.10(6)	O(5)-Cd(1)-N(2)	177.16(6)
N(2)-Cd(1)-O(1)	94.33(5)	C(13)-N(2)-Cd(1)	112.88(13)
C(22)-N(2)-Cd(1)	129.46(13)	C(1)-O(1)-Cd(1)	84.67(12)
C(1)-O(2)-Cd(1)	100.04(12)	C(23)-O(3)-Cd(1)	107.50(12)
C(23)#4-O(4)-Cd(1)	144.82(13)		

#2 Symmetry code: x, -y+1/2, z+1/2 #4 Symmetry code: x, -y+1/2, z-1/2

Table S2 Selected Bond Distances (Å) and Angles (°) for **2**

Cd(1)-O(1)	2.258(3)	Cd(1)-O(1)#1	2.258(3)
Cd(1)-O(2)#3	2.366(3)	Cd(1)-O(2)#4	2.366(3)
Cd(1)-N(3)	2.367(5)	Cd(1)-N(2)	2.379(4)
O(2)-Cd(1)#4	2.366(3)		
O(1)-Cd(1)-O(1)#1	170.42(16)	O(1)-Cd(1)-O(2)#3	87.09(11)
O(1)#1-Cd(1)-O(2)#3	92.20(12)	O(1)-Cd(1)-O(2)#4	92.20(12)
O(1)#1-Cd(1)-O(2)#4	87.09(11)	O(2)#3-Cd(1)-O(2)#4	171.49(13)
O(1)-Cd(1)-N(3)	94.79(8)	O(1)#1-Cd(1)-N(3)	94.79(8)
O(2)#3-Cd(1)-N(3)	94.26(7)	O(2)#4-Cd(1)-N(3)	94.26(7)
O(1)-Cd(1)-N(2)	85.21(8)	O(1)#1-Cd(1)-N(2)	85.21(8)
O(2)#3-Cd(1)-N(2)	85.74(7)	O(2)#4-Cd(1)-N(2)	85.74(7)
C(13)-N(2)-Cd(1)	121.3(2)	C(13)#1-N(2)-Cd(1)	121.3(2)
C(18)#5-N(3)-Cd(1)	121.7(2)	C(18)#6-N(3)-Cd(1)	121.7(2)
C(1)-O(1)-Cd(1)	131.4(3)	C(1)-O(2)-Cd(1)#4	144.5(3)
N(3)-Cd(1)-N(2)	180.000(1)		

#1 Symmetry code: -x, y, -z+3/2 #2 Symmetry code: x, y+1, z #3 Symmetry code: x, -y, z+1/2
#4 Symmetry code: -x, -y, -z+1 #5 Symmetry code: x, y-1, z #6 Symmetry code: -x, y-1, -z+3/2

Table S3 Selected Bond Distances (Å) and Angles (deg) for **3**

Cd(1)-O(1)	2.391(8)	Cd(1)-O(2)	2.422(7)
Cd(1)-O(3)	2.372(8)	Cd(1)-O(4)	2.250(8)
Cd(1)-N(3)	2.325(8)	Cd(1)-N(4)	2.350(9)
Cd(1)-N(5)	2.372(9)		
N(3)-Cd(1)-N(4)	90.2(3)	N(3)-Cd(1)-N(5)	173.2(3)
N(3)-Cd(1)-O(1)	92.2(3)	N(3)-Cd(1)-O(2)	93.3(3)
N(3)-Cd(1)-O(3)	91.3(3)	N(3)-Cd(1)-O(4)	87.0(3)
N(4)-Cd(1)-N(5)	95.3(3)	N(4)-Cd(1)-O(1)	136.6(3)
N(4)-Cd(1)-O(2)	82.2(3)	N(4)-Cd(1)-O(3)	82.4(3)
N(4)-Cd(1)-O(4)	134.9(3)	N(5)-Cd(1)-O(1)	86.5(3)
N(5)-Cd(1)-O(2)	91.4(3)	N(5)-Cd(1)-O(3)	85.5(3)
N(5)-Cd(1)-O(4)	86.2(3)	O(1)-Cd(1)-O(2)	54.4(2)
O(1)-Cd(1)-O(4)	88.5(3)	O(2)-Cd(1)-O(4)	142.9(2)
O(3)-Cd(1)-O(2)	163.9(2)	O(3)-Cd(1)-O(4)	52.8(3)
C(1)-O(1)-Cd(1)	93.2(6)	C(1)-O(2)-Cd(1)	92.1(7)
C(13)-O(3)-Cd(1)	96.2(6)	C(13)-O(4)-Cd(1)	90.7(6)
C(25)-N(3)-Cd(1)	118.2(7)	C(27)-N(3)-Cd(1)	123.4(7)
C(28)-N(4)-Cd(1)	121.0(8)	C(32)-N(4)-Cd(1)	123.5(8)
C(33)-N(5)-Cd(1)	119.5(7)	C(37)-N(5)-Cd(1)	122.4(8)

Crystal Structure

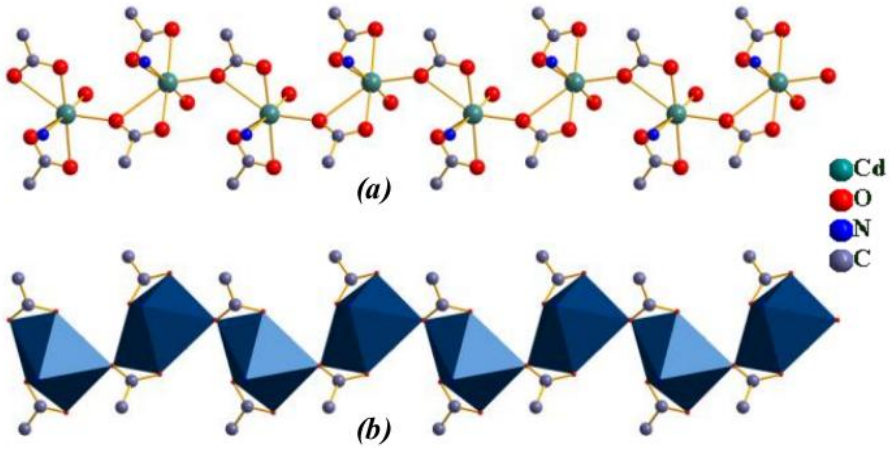

Fig. S6 (a) View of **1**, showing extended chain of Cd(II) ions. (b) A polyhedral presentation of extended chain of Cd(II) ions.

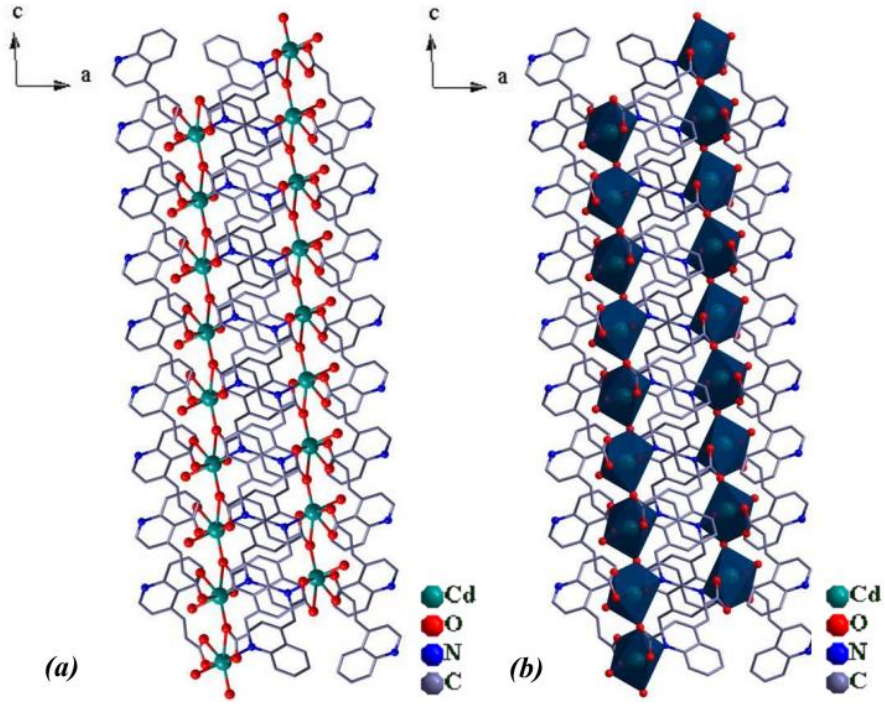

Fig. S7 (a) 2D undulated layer structure and (b) polyhedral presentation of 2D undulated layer structure of **1** viewed down from *b* axis.

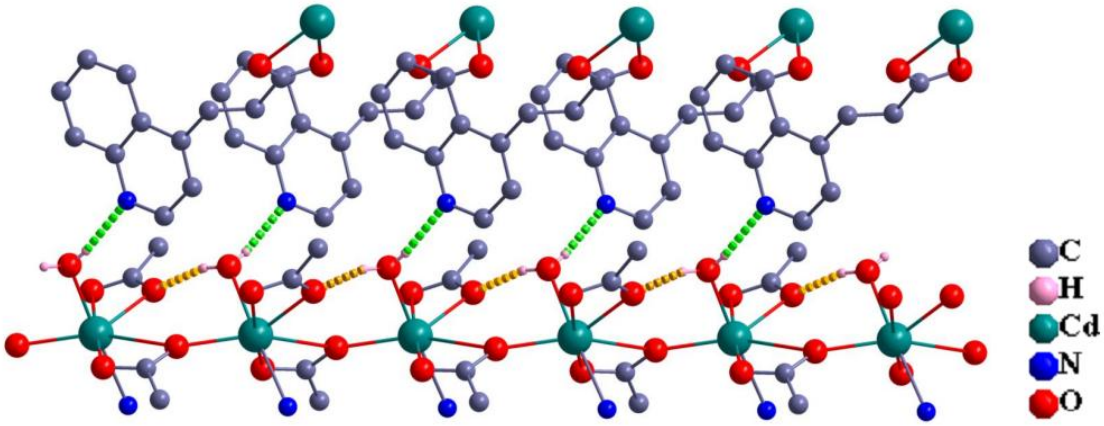

Fig. S8 Intermolecular (green) and intramolecular (orange) hydrogen-bonding details in compound **1**. Green: O5-H50···N1A: 2.0379 Å, 2.7394 Å, 171.322 °(A Symmetry code: -x, y+1/2, -z+3/2.) Orange: O5-H51···O2B: 1.8004 Å, 2.7016 Å, 161.329 °(B Symmetry code: x, -y+1/2, z-1/2).

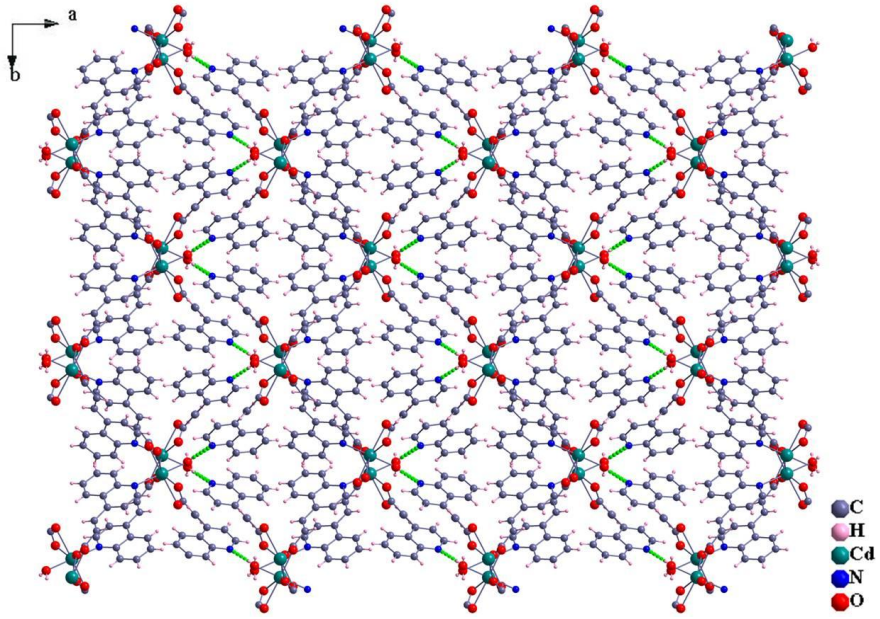

Fig. S9 The 3D stacking structure picture of **1** assembled from intermolecular hydrogen-bonding interactions viewed down from *c* axis.

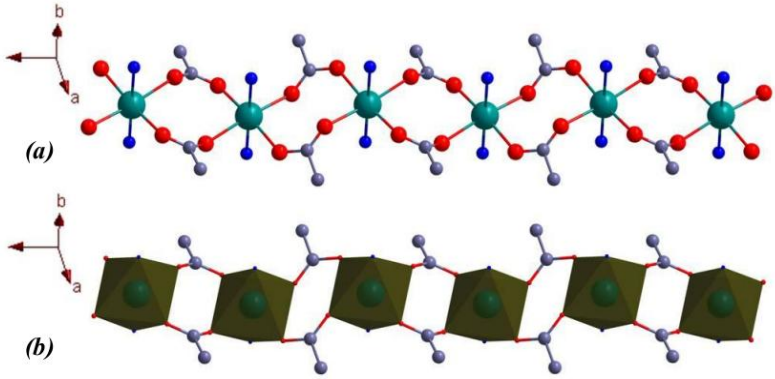

Fig. S10 (a) View of **2**, showing extended chain of Cd(II) ions. (b) A polyhedral presentation of extended chain of Cd(II) ions.

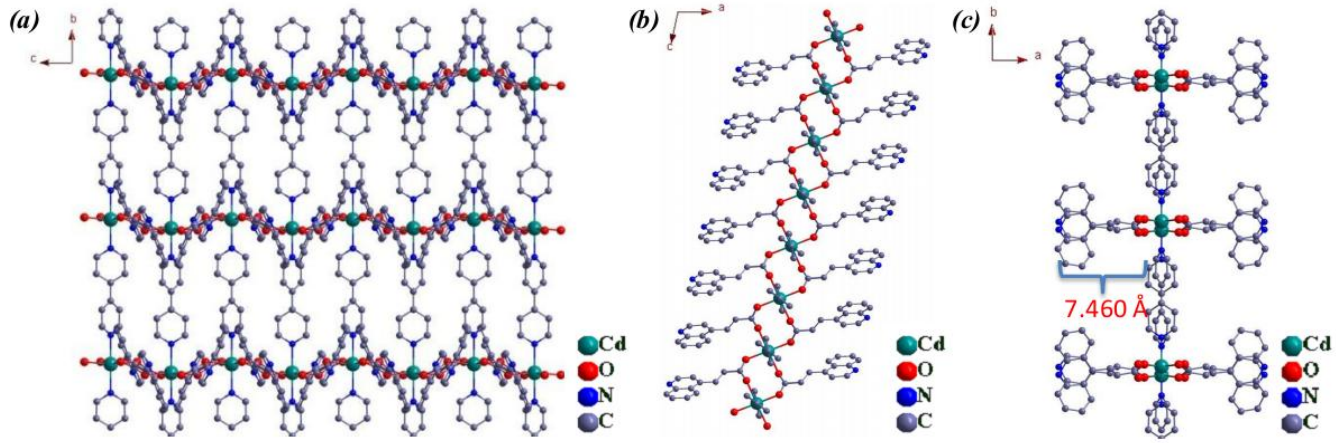

Fig. S11 The 2D structure pictures of compound **2** viewed down from (a) *a*, (b) *b* and (c) *c* axis respectively.

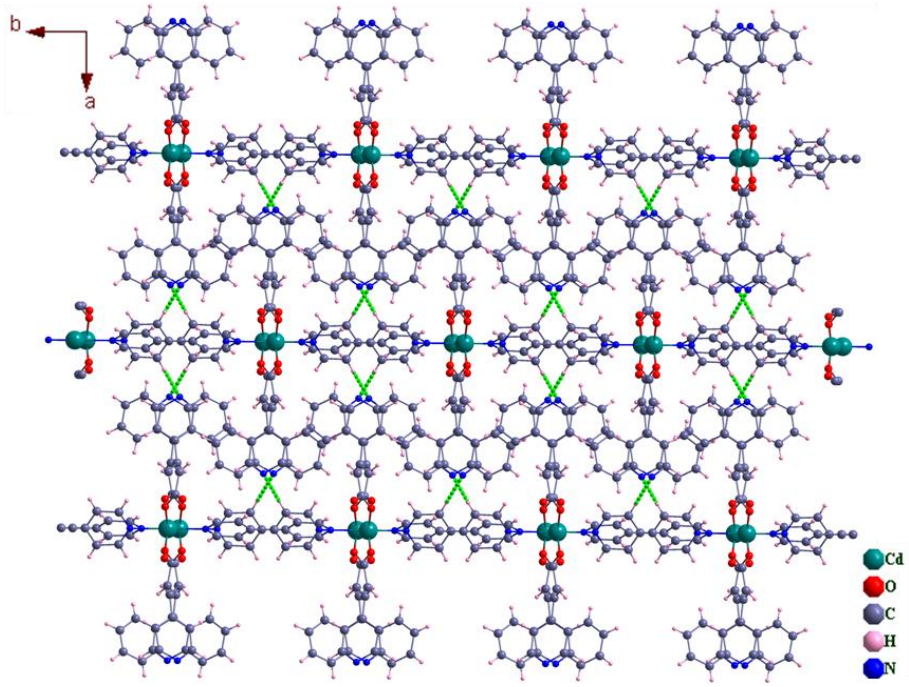

Fig. S12 The 3D structure pictures of complound **2** viewed down from *c* axis.

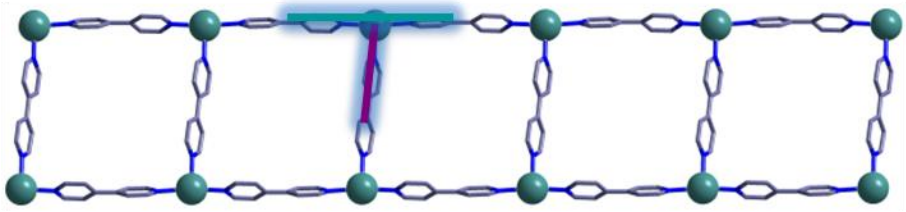

Fig. S13 View of the ladder-like substructure assembled by 4,4'-bipy ligands and Cd(II) ions and the T-shaped node in **3**.

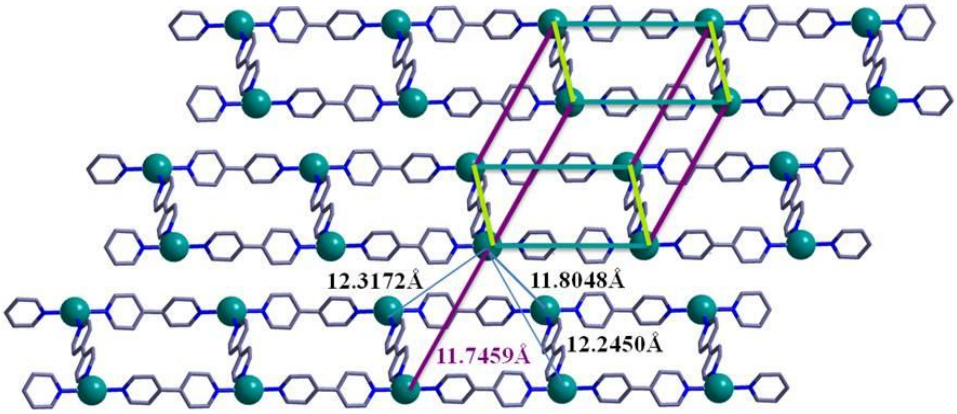

Fig. S14 The picture showing Cd···Cd distances between ladder-like chain in **3**.

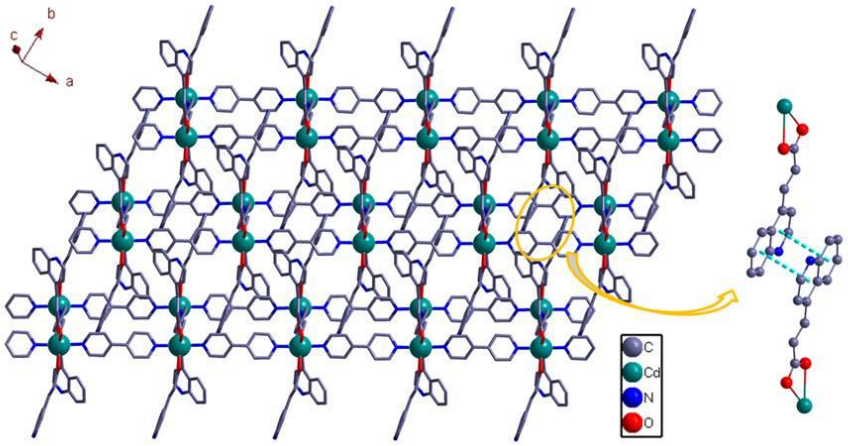

Fig. S15 View of the 2D layered structure formed by π–π stacking and H-bonding interactions of **3**.

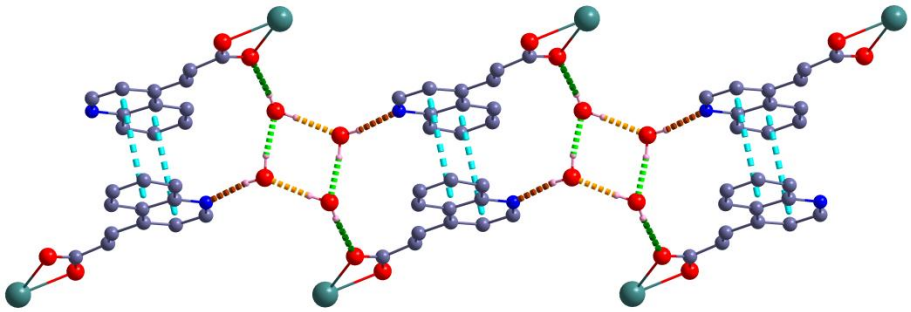

Fig. S16 View of picture of the cyclic water tetramer and its immediate environment as found in **3** (Green: O5-H5B···O6: 1.7642 Å, 2.6091 Å, 170.833 °; Yellow: O6-H6B···O5: 1.8771 Å, 2.7243 Å, 174.620 °; Brown: O5-H5A···N1: 1.9450 Å, 2.2877 Å, 170.779 °; Dark green: O6-H6A···O2: 1.9747 Å, 2.8210 Å, 174.668 °; A Symmetry code: x, y-1, z; B Symmetry code: -x+1/2, -y+1/2, -z).

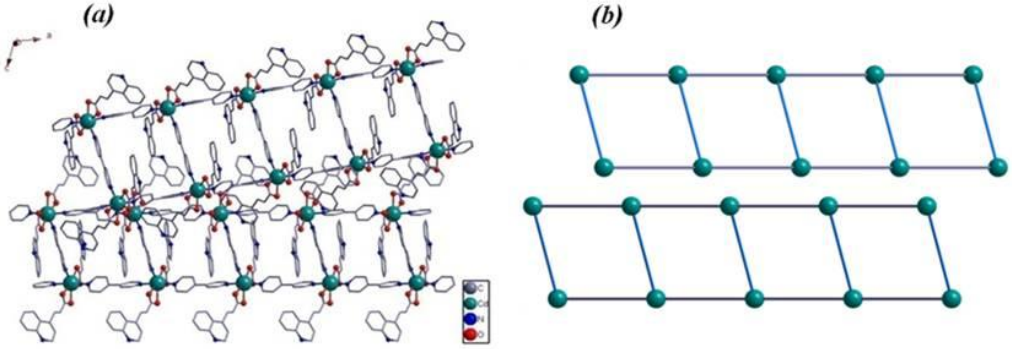

Fig. S17 View of the two intersected 1D ladder-like chains between adjacent 2D layers of **3**.

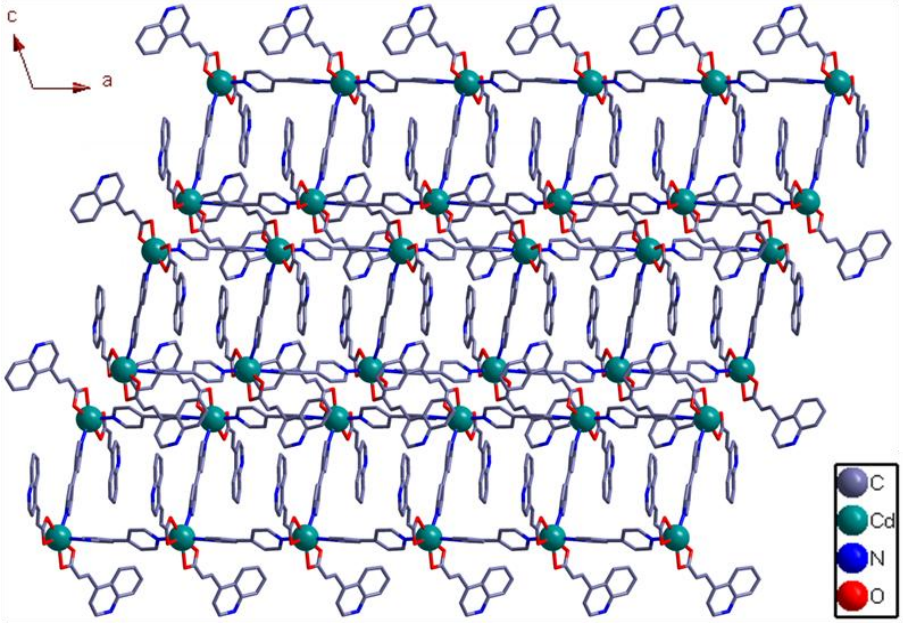

Fig. S18 3D stacking structure picture of **3** viewed down from *b* axis.

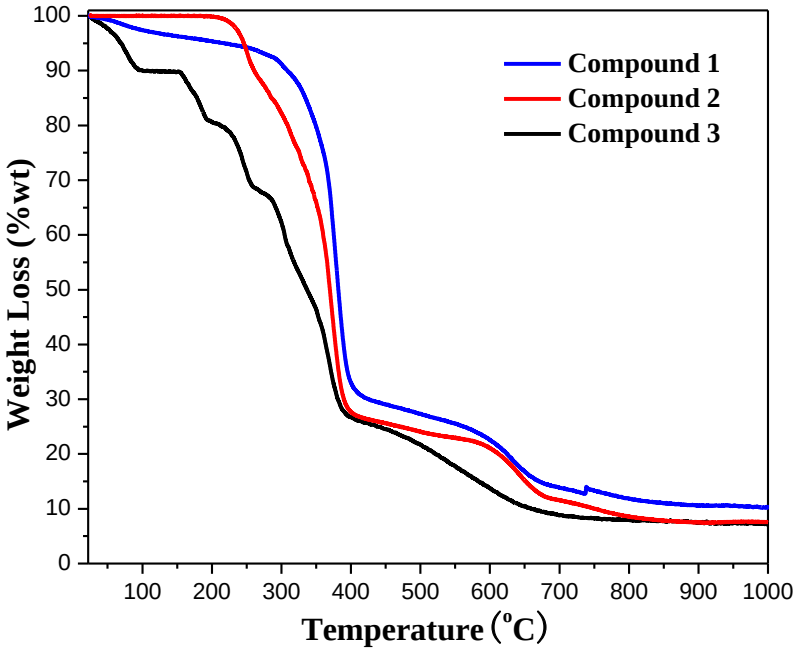

Fig. S19 TGA curve for compounds **1-3**.

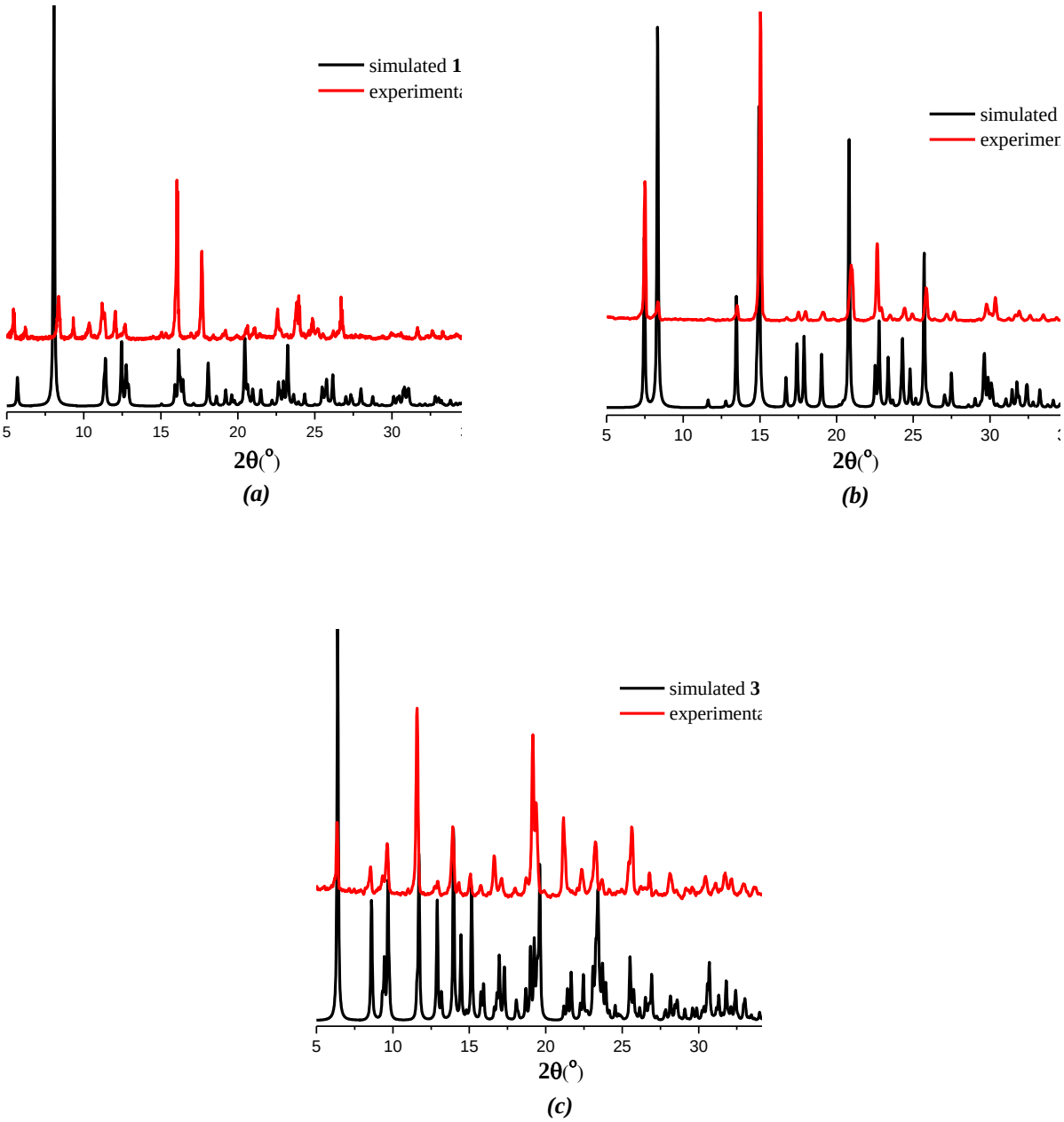

Fig. S20 Experimental and simulated PXRD pattern for (a) **1**, (b) **2** and (c) **3**.

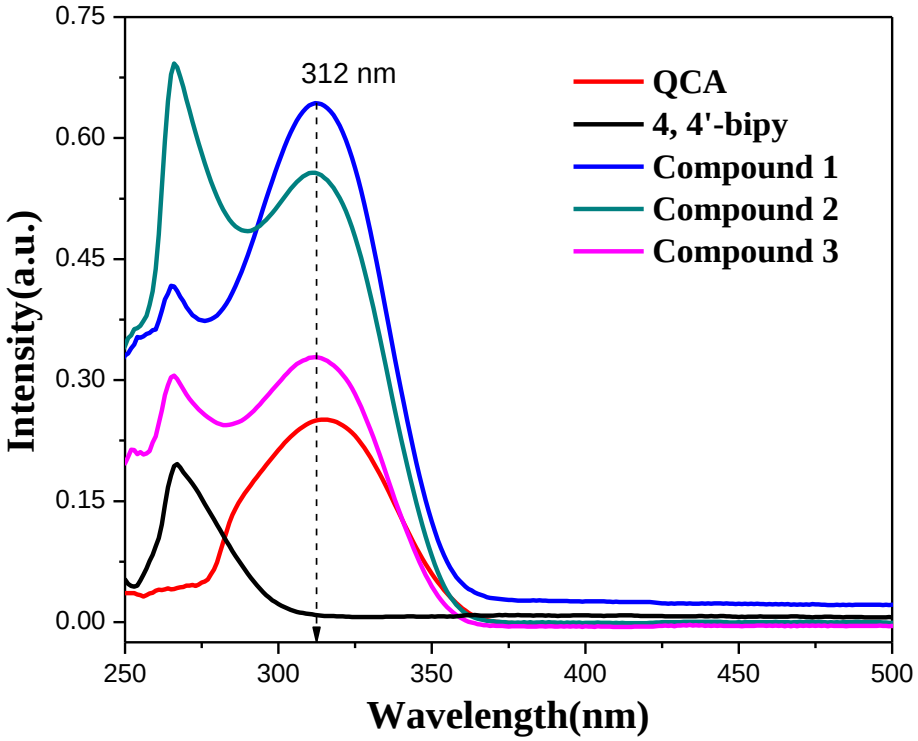

Fig. S21 UV-vis spectra of 4,4′-bipy, QCA and compounds **1-3**.

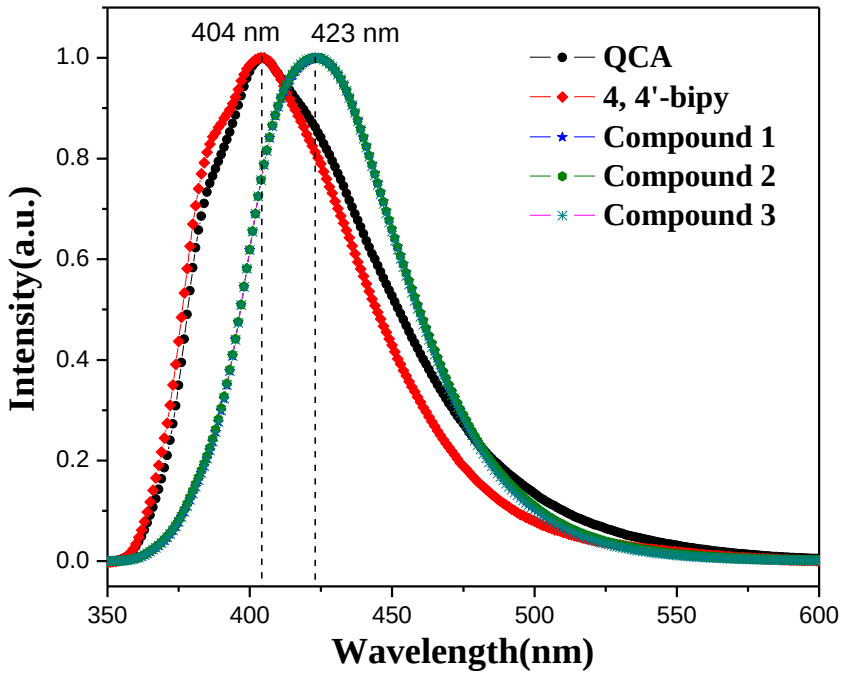

Fig. S22 Luminescent normalized emission spectra for compounds **1-3** and the free QCA and 4,4′-bipy ligands in DMF solution (λ_{ex} = 312 nm).