Supplementary Material (ESI) for Dalton Transactions

An interpenetrated bioactive nonlinear optical MOF containing coordinated quinolone-like drug and Zn(II) for pH-responsive release

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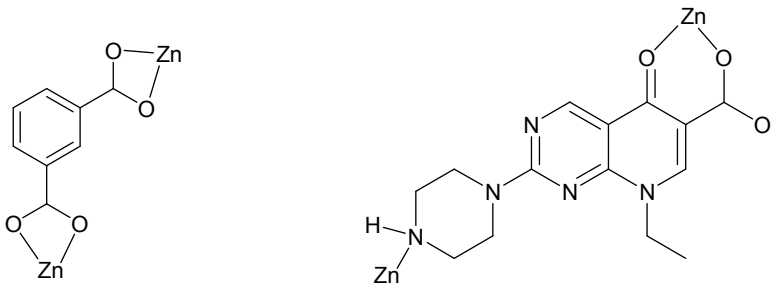
Experimental

Structure determination



Scheme S1. The coordination modes of ppa (a) and 1,3-bdc (b) ligands in **1.**

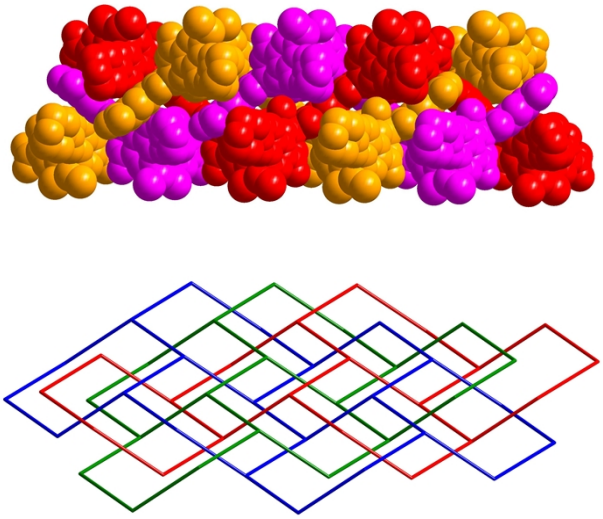


Figure S1. A schematic illustration of the 3-fold interpenetrated **hcb** network in **1**.

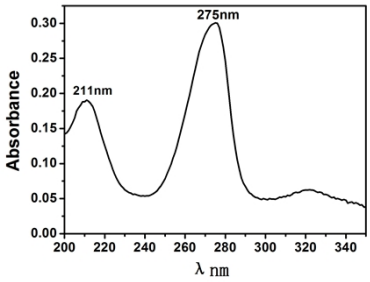


Figure S2. UV-vis spectroscopy of mixture solution in pH 2.0.

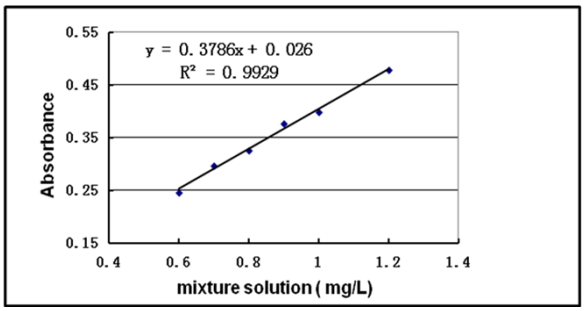
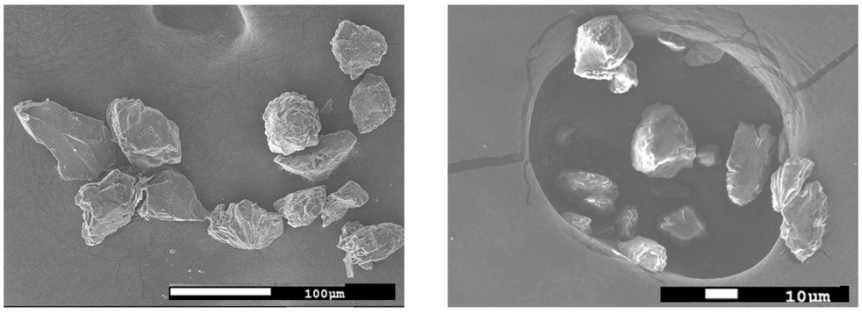


Figure S3. Standard curve of mixture solution in pH 2.0.



(a) **(b)**

Figure S4. SEM micrograph of compound **1** (a) particle size ranges 80−63 μm of **1**; (b) particle size ranges 25−40 μm of **1**.

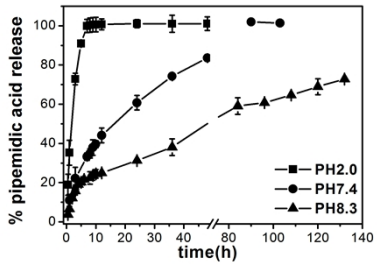


Figure S5. pH-responsive release of pipemidic acid from compound **1**(particle size ranges 80−63 μm) under simulated physiological conditions.

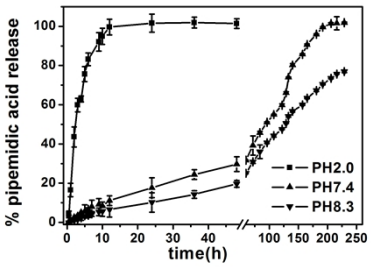


Figure S6. pH-responsive release of pipemidic acid from compound **1**(tablets) under simulated physiological conditions.

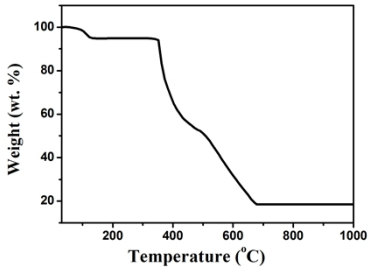


Figure S7. TGA curves of **1.**

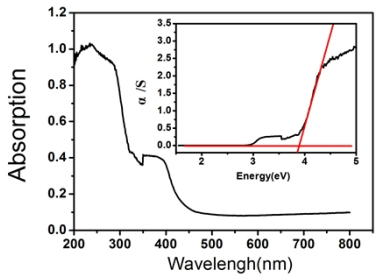


Figure S8. The UV−vis diffuse reflectance of **1**.

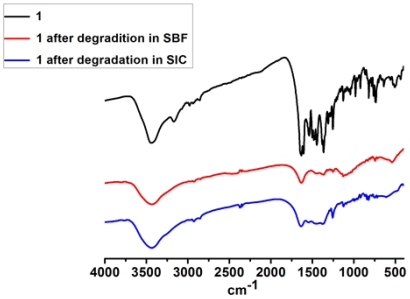


Figure S9. IR spectrum of compound **1** berfore and after release tests**.**

Table S1. The half life of different particle sizes of **1**.

Simulated physiological conditions / Particle size	SGF	SBF	SIC
25−40μm	1.5h	7h	18h
63−80μm	2h	18h	72 h
tablets	3h	96h	129h

Table S2. Crystal data and structure refinements for compound **1.**

Complex	**1**
Molecular formula	$C_{36}H_{38}Zn_2N_{10}O_{13}$
M	949.50
Crystal system	monoclinic
Space group	*Cc*
a (Å)	21.383(5)
b (Å)	18.940(5)
c (Å)	9.587(2)
α(°)	90
β (°)	94.379(8)
γ(°)	90
V (Å^3)	3871.4(17)
Z	4
$\rho_{calc,}$(g cm^{-3})	1.629
μ, (mm^{-1})	1.320
F(000)	1952
Reflections collected	7974
Independent reflections	5886
R_1[a] [I> 2σ(I)]	0.0477
wR_2[b] [I> 2σ(I)]	0.1234
R_1 (all data)	0.0633
wR_2 (all data)	0.1294

R_1[a]=$\sum||F_o|-|F_c||/\sum|F_o|$, wR_2[b]= $[\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S3. Selected bond lengths (Å) and angles (º) for **1.**

1

Zn(2)-O(7)	2.320(7)	Zn(2)-O(6)	2.054(6)	Zn(2)-N(5a)	2.052(5)
Zn(2)-O(10b)	1.986(4)	Zn(2)-O(8b)	1.965(5)	Zn(1)-O(3)	2.011(4)
Zn(1)-O(1)	2.006(4)	Zn(1)-O(4)	1.978(5)	Zn(1)-N(6)	2.087(5)
Zn(1)-O(1W)	2.366(6)	N(5)-Zn(2c)	2.052(5)	O(10)-Zn(2d)	1.986(4)
O(8)-Zn(2d)	1.965(5)				
O(6)-Zn(2)-O(7)	58.7(2)	N(5a)-Zn(2)-O(7)	88.8(2)	N(5a)-Zn(2)-O(6)	139.6(2)
O(10b)-Zn(2)-O(7)	159.2(2)	O(10b)-Zn(2)-O(6)	101.9(2)	O(10b)-Zn(2)-N(5a)	104.7(19)
O(8b)-Zn(2)-O(7)	100.3(2)	O(8b)-Zn(2)-O(6)	104.8(2)	O(8b)-Zn(2)-N(5a)	104.2(2)
O(8b)-Zn(2)-O(10b)	91.74(19)	O(3)-Zn(1)-N(6)	104.6(2)	O(3)-Zn(1)-O(1W)	77.78(19)
O(1)-Zn(1)-O(3)	88.16(18)	O(1)-Zn(1)-N(6)	99.0(2)	O(1)-Zn(1)-O(1W)	162.6(2)
O(4)-Zn(1)-O(3)	150.04(19)	O(4)-Zn(1)-O(1)	97.91(19)	O(4)-Zn(1)-N(6)	103.4(2)
O(4)-Zn(1)-O(1W)	89.6(2)	N(6)-Zn(1)-O(1W)	94.5(2)		

Symmetry codes: a) -1/2+x,1/2-y,3/2+z; b) 1/2+x,1/2+z,3/2+z; c) 1/2+x,1/2-y,-3/2+z; d) -1/2+x,1/2-y,-3/2+z.