*Supplementary Materials:*

# Difunctional Zn-Based Metal-Organic Frameworks: Chemical Conversion of $CO_2$ and Luminescent Recognition for Secnidazole

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**Table S1** crystal data and structure refinement for compound **1**.

| | **1** |
|---|---|
| Empirical formula | $C_{26}H_{35}N_7O_7Zn$ |
| Formula weight | 618.71 |
| Temperature/K | 123.0(3) |
| Crystal system | Trigonal |
| Space group | *R*-3 |
| *a*/Å | 31.4046(18) |
| *b*/Å | 31.4046(18) |
| *c*/Å | 14.9137(8) |
| *α*/° | 90 |
| *β*/° | 90 |
| *γ*/° | 120 |
| V, Å$^3$ | 12738.0(16) |
| *Z* | 18 |
| $\rho_{calc}$g/cm$^3$ | 1.032 |
| $\mu$/mm$^{-1}$ | 0.892 |
| *F*(000) | 5868.0 |
| 2*θ* range for data collection/° | 6.2325 to 50.014 |
| Reflections collected | 8818 |
| $R_{int}$ | 0.0315 |
| Goodness-of-fit on $F^2$ | 1.038 |
| Final *R* indexes [I>=2σ (I)] | $R_1$ = 0.0398, $wR_2$ = 0.0902 |
| Final R indexes [all data] | $R_1$ = 0.0557, $wR_2$ = 0.0987 |
| Δ*ρ*max/min (e Å$^{-3}$) | 0.382/-0.281 |

**Table S2** Selected bond lengths (Å) and bond angles (°) for compound **1**.

| *Bond distances* | | | |
|---|---|---|---|
| Zn(1)-O(4) | 1.944(2) | C(11)-C(10)#3 | 1.397(4) |
| Zn(1)-O(1) | 1.950(2) | C(8)-C(9)#4 | 1.397(4) |
| Zn(1)-N(4)#1 | 1.998(2) | C(10)-C(11)#5 | 1.397(4) |
| Zn(1)-N(1) | 2.000(2) | C(9)-C(8)#6 | 1.397(4) |
| N(4)-Zn(1)#2 | 1.998(2) | | |
| *Bond Angles* | | | |
| O(4)-Zn(1)-O(1) | 137.80(10) | N(3)-N(4)-Zn(1)#2 | 123.01(18) |
| O(4)-Zn(1)-N(4)#1 | 109.02(9) | C(10)-C(11)-C(10)#3 | 118.4(3) |
| O(4)-Zn(1)-N(1) | 98.21(9) | C(9)-C(8)-C(9)#4 | 118.2(3) |
| O(1)-Zn(1)-N(4)#1 | 97.08(9) | C(11)-C(10)-C(11)#5 | 121.5(3) |
| O(1)-Zn(1)-N(1) | 105.20(9) | C(8)-C(9)-C(8)#6 | 121.8(3) |
| N(4)#1-Zn(1)-N(1) | 107.11(10) | | |

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+1/3, -x+2/3, z-1/3 #2 -y+2/3, x-y+1/3, z+1/3

#3 -x+y, -x+1, z #4 -y+1, x-y, z #5 -y+1, x-y+1, z

#6 -x+y+1, -x+1, z

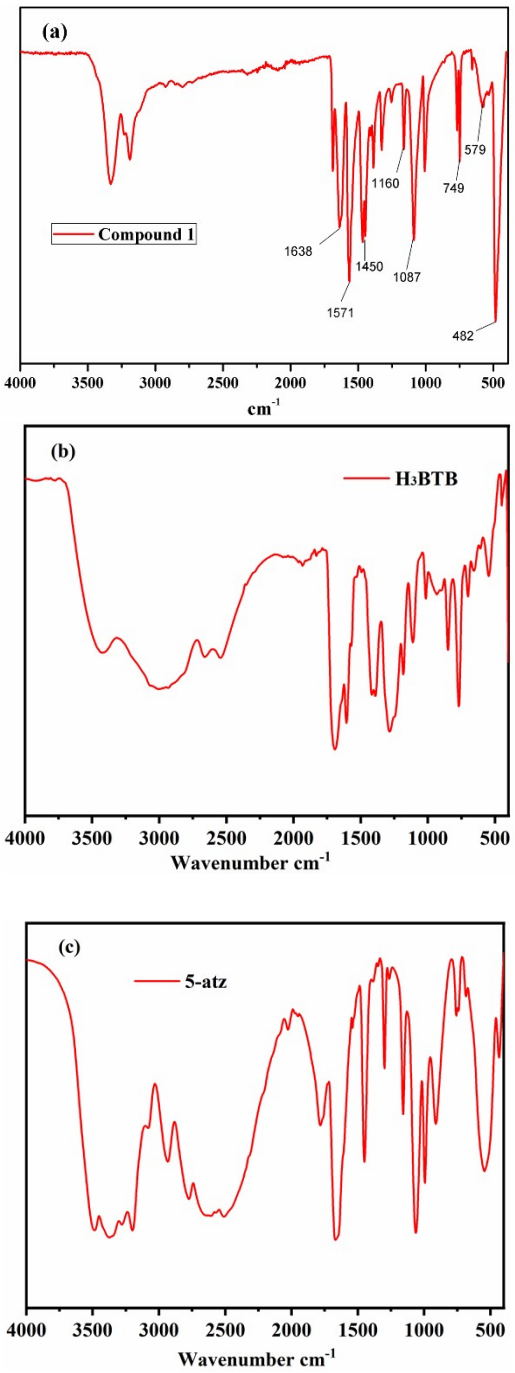



**Fig. S1** The FT-IR spectrum of compound **1** (a), $H_3BTB$ (b) and 5-atz (c). Some main IR ($cm^{-1}$) of compound **1**: 1638 (vs), 1571 (vs), 1450 (s), 1160 (m), 1087 (vs), 749 (s), 579 (w), 482 (vs).

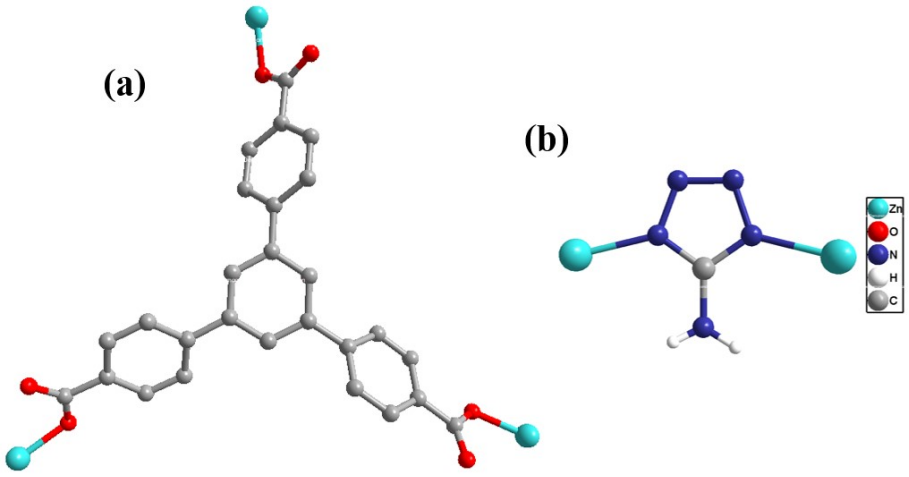



**Fig. S2** The coordination modes of organic ligands: (a) for $H_3BTB$ and (b) for 5-atz.

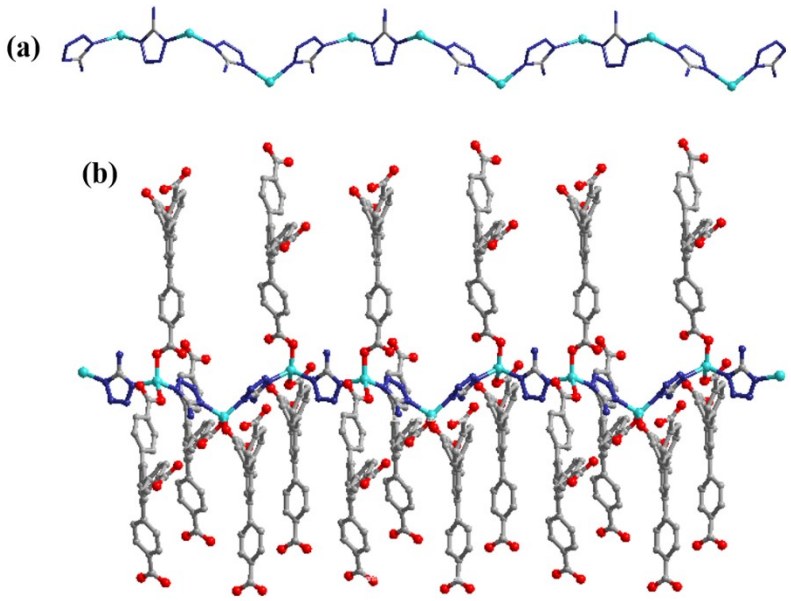



**Fig. S3** (a) The zigzag type 1D chains made from $Zn^{2+}$ ions and 5-atz ligands. (b) The 3D pillar-chain structure built from 1D chains and $H_3BTB$ ligands.

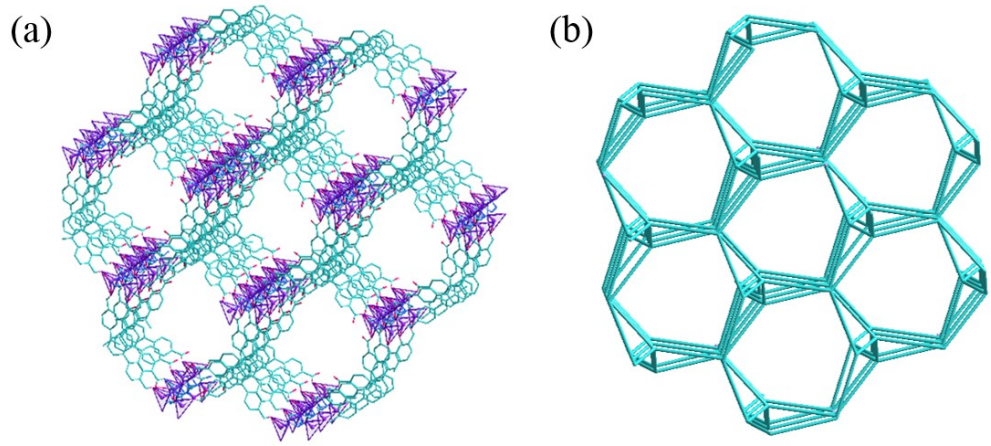



**Fig. S4** (a) A set of 3D interpenetrating framework of **1** and (b) its corresponding topological network.

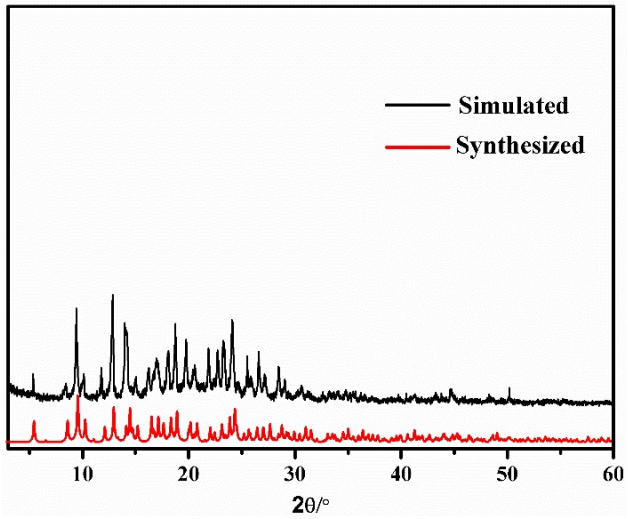



**Fig. S5** The PXRD patterns of the simulated and synthesized samples for compound **1**.

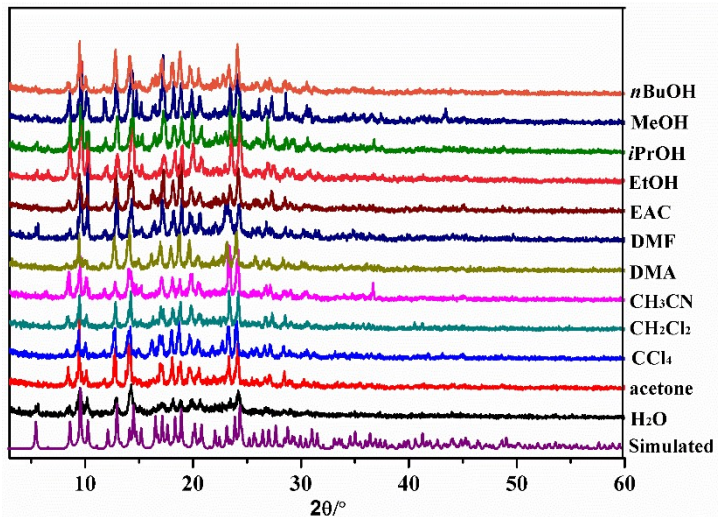



**Fig. S6** The PXRD patterns for compound **1** immersing in various common solvents.

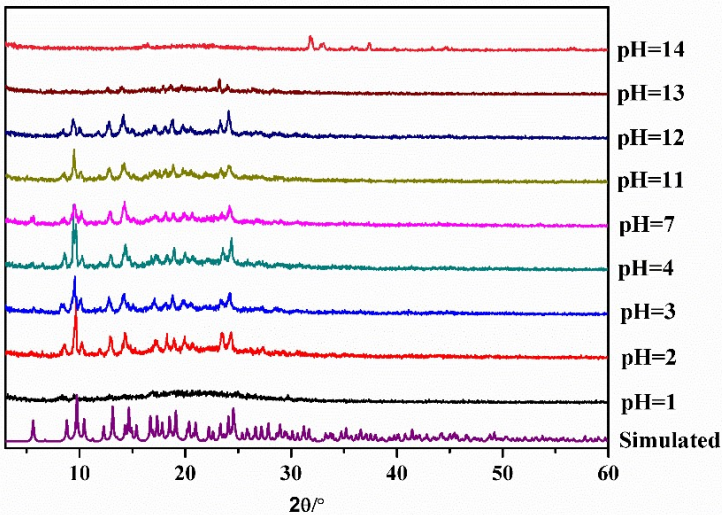



**Fig. S7** The PXRD patterns for compound **1** in various solutions from pH 2 to 13.

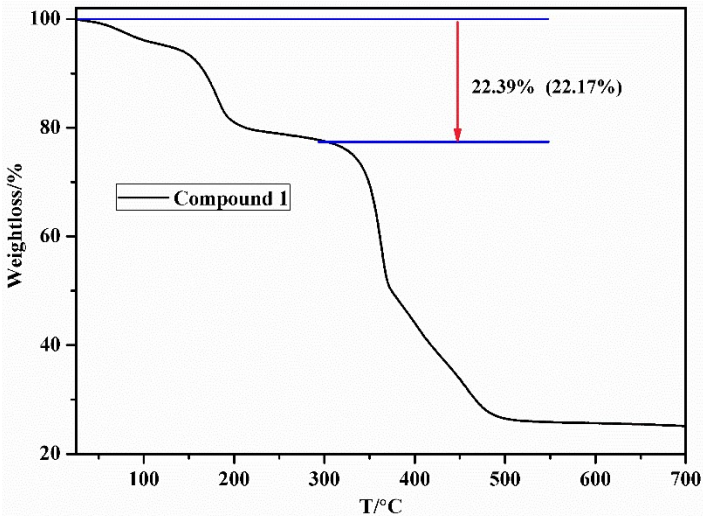
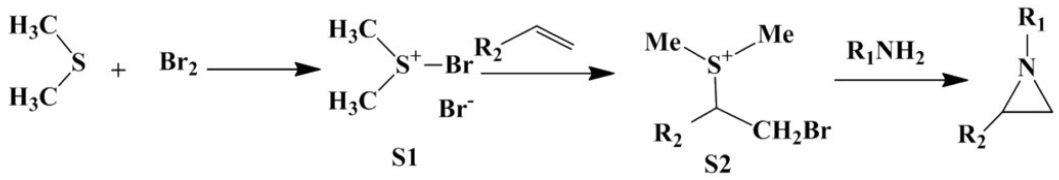



**Fig. S8** TG curve for compound **1**.




**Scheme 1** Preparation of aziridines.

Typical procedure for the synthesis of aziridines was described as following (**Scheme S1**): Firstly, bromine (0.2 mol, 32.0 g) in dry $CH_2Cl_2$ (40 mL) was slowly dropped over 30 min to 40 mL $CH_2Cl_2$ solution of dimethyl sulfide (0.2 mol, 12.4 g) in ice-salt baths. Light orange crystals of bromodimethyl sulfonium bromide gradually generated during the process, and the orange crystals **S1** were completely obtained and collected by filtration. Yield: 80%.

Secondly, olefin (160 mmol) was slowly dropped to 160 mL $CH_3CN$ solution of **S1** (160 mmol, 35.56 g) in ice-salt baths. The solution was stirred for 2h after the addition of olefin was completed. The white solid **S2** gradually generated during the process. The crystals **S2** was collected by filtration, dried under vacuum. Yield: 30-38.6 %.

Thirdly, a solution of amine (20-50 mmol) was slowly added into a stirred solution of compound **S2** (10 mmol) in 20 mL water at r.t., and the resulting mixture was stirred overnight. Then the mixture was slowly dropped into 20 mL of saturated brine, extracted with diethyl ether (3×20 mL), dried with anhydrous $Na_2SO_4$ overnight and the solvent evaporated under reduced pressure. Aziridines were obtained by distillation under reduced pressure. Yield: 85-100 %.

**Table S3** The ICP result of compound **1** after catalytic recycling (filter liquor).

| | Compound **1** ($Zn^{2+}$) |
|---|---|
| after catalytic recycling ($M^{2+}$ of filter liquor) | 0.25% |

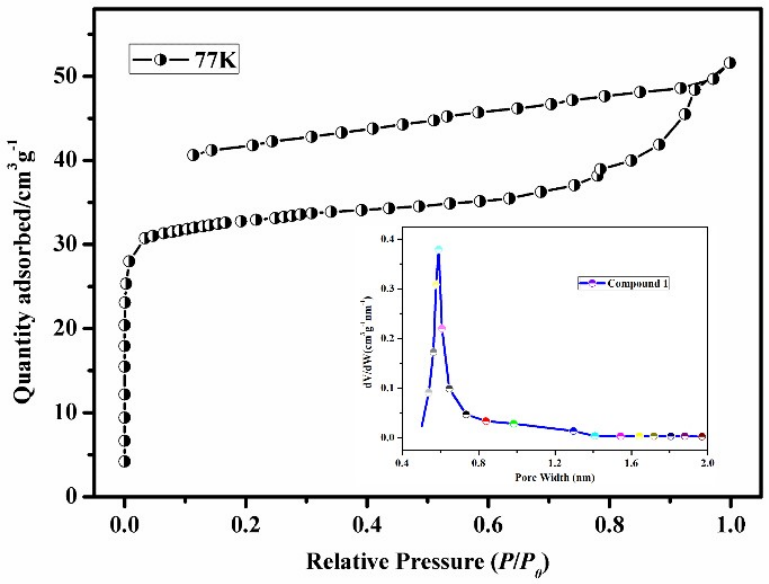



**Fig. S9** The $N_2$ adsorption of compound **1** at 77 K and pore size distribution.

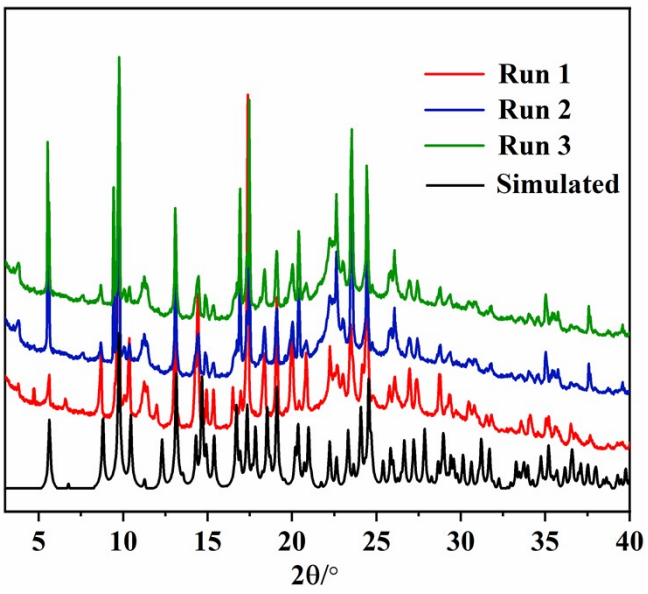



**Fig. S10** The PXRD patterns of recycled **1** after five catalytic recycles.

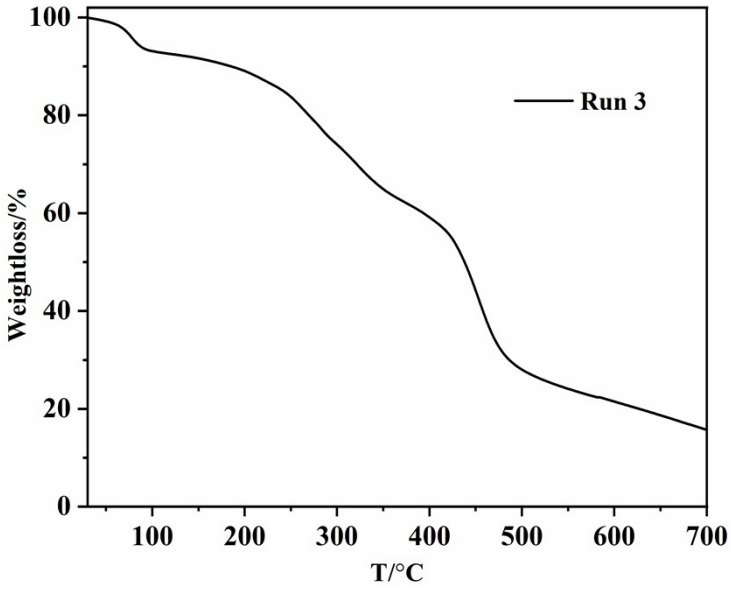



**Fig. S11** The TG curve of compound **1** after five catalytic recycling in $CO_2$ cycloaddition is unchanged in comparison with the one of synthesized **1**.

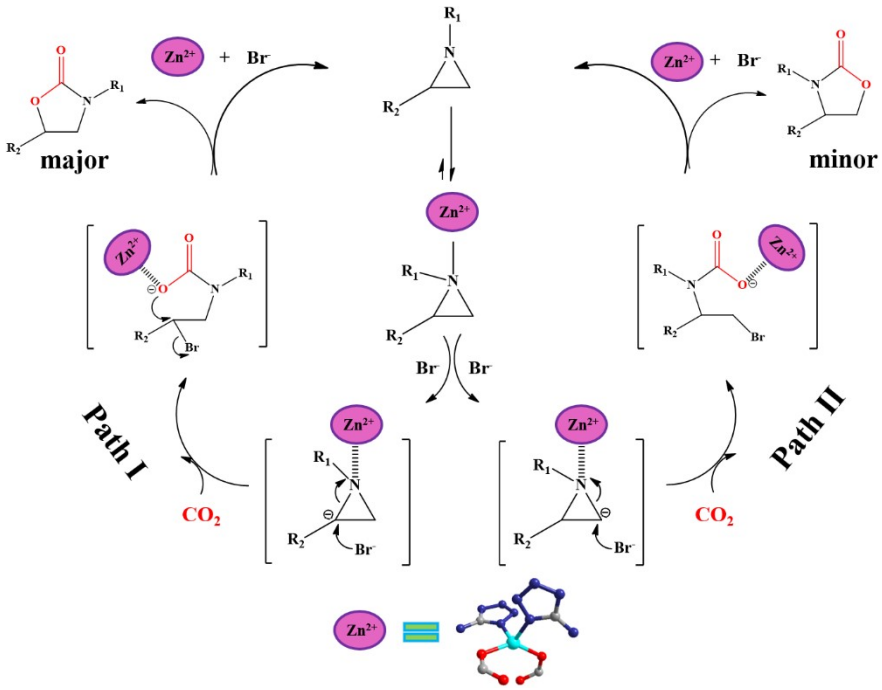



**Fig. S12** The possible mechanism for the cycloaddition of aziridine with $CO_2$ into oxazolidinone.

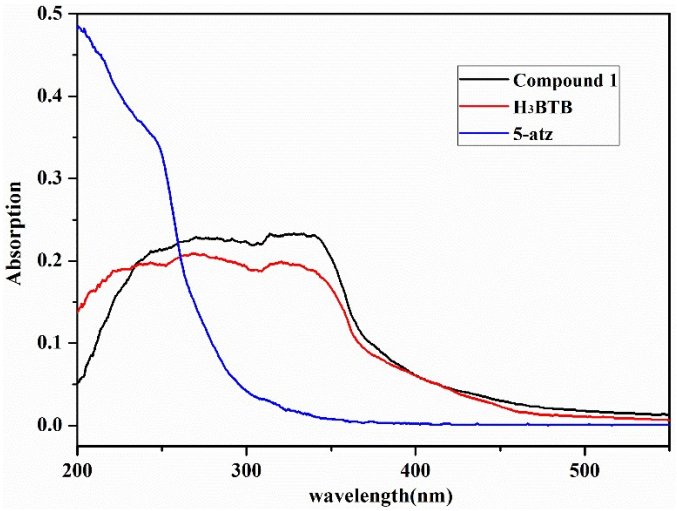



**Fig. S13** The solid-state UV spectra for compound **1** and ligands ($H_3BTB$ and 5-atz). Black: compound **1**; Red: $H_3BTB$; Blue: 5-atz.

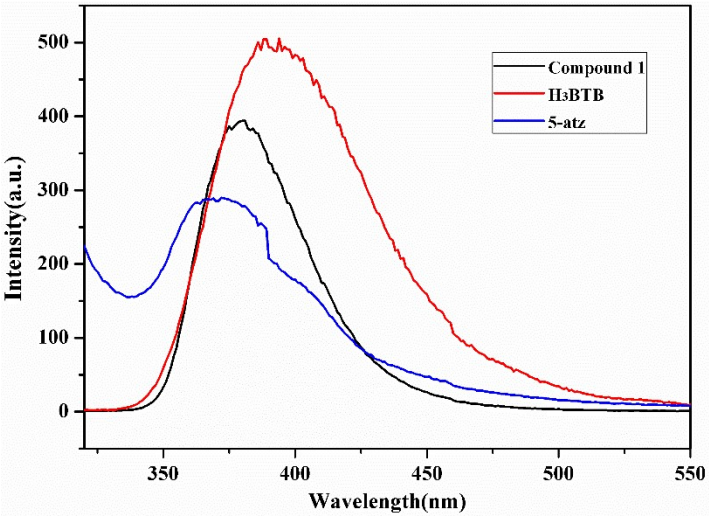



**Fig. S14** The solid-state photoluminescence spectra for compound **1** and ligands ($H_3BTB$ and 5-atz). Black: compound **1**; Red: $H_3BTB$; Blue: 5-atz.

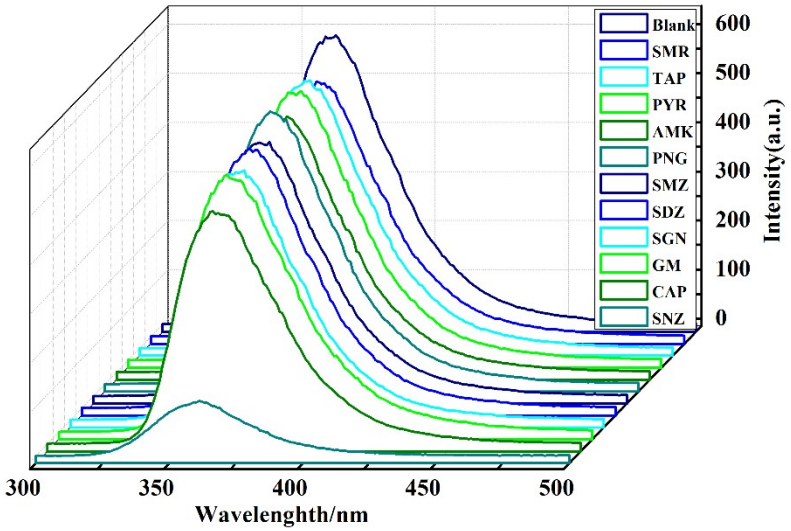
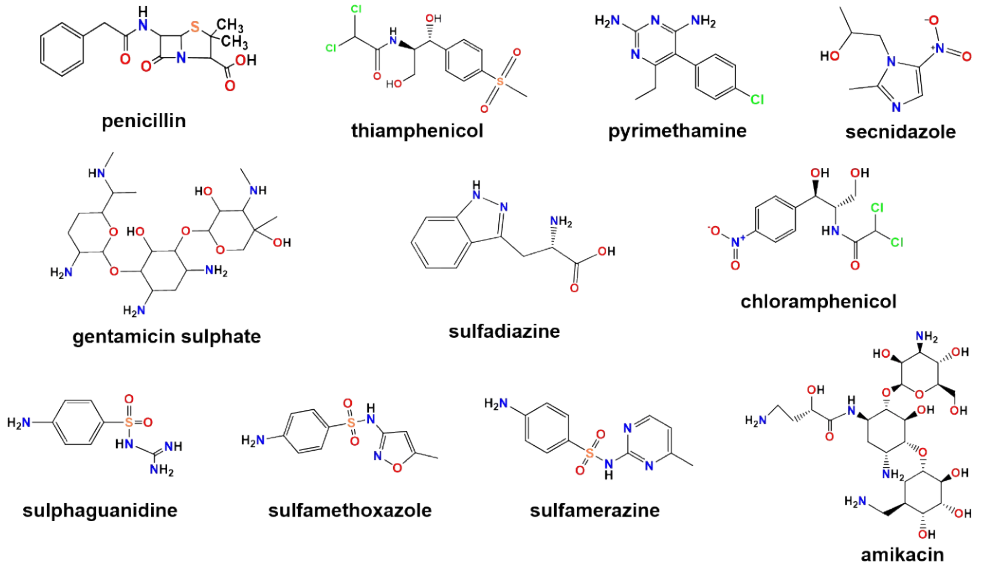



**Fig. S15** The luminescence spectra of **1** after adding various antibiotics.




**Scheme S2** The structures of various antibiotic molecules.

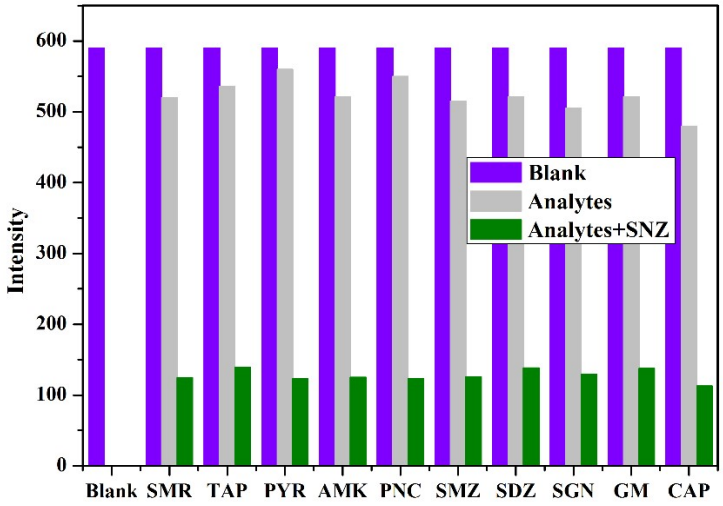



**Fig. S16** Luminescent response of compound **1** towards the other competing antibiotics (500 ppm) or a mixture of competing antibiotics (500 ppm) and target analyte (SNZ, 250 ppm).

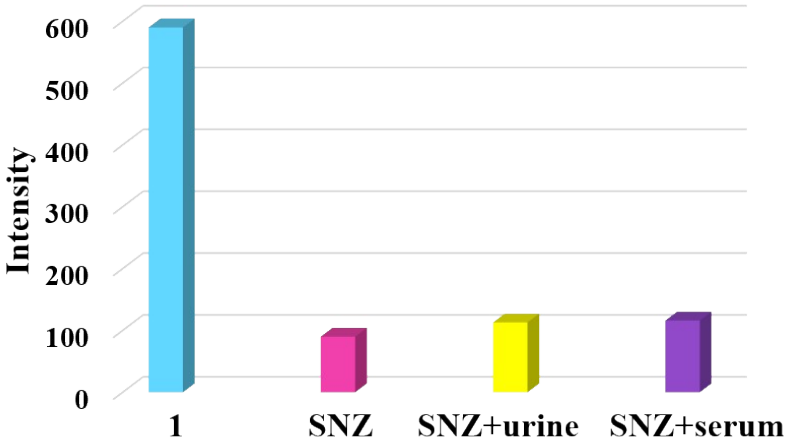



**Fig. S17** Luminescent response of compound **1** towards SNZ (500 ppm) or a mixture of SNZ and urine/serum (500 ppm).

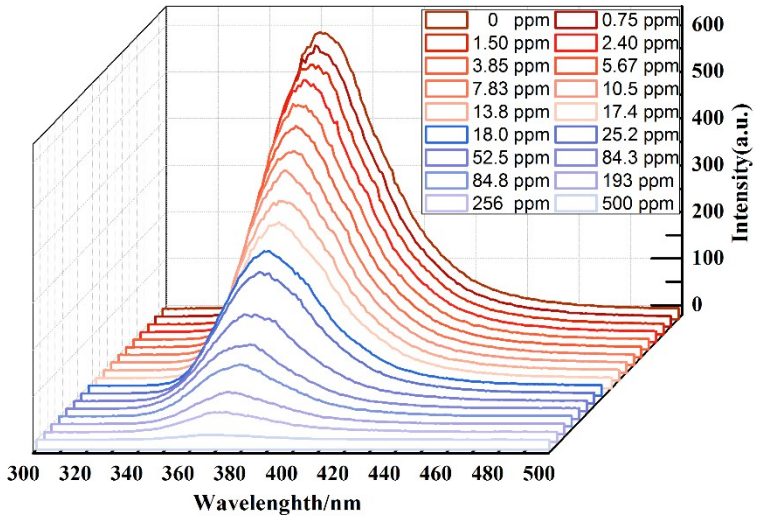



**Fig. S18** Emission spectra of compound **1** dispersed in different concentrations of secnidazole solutions.

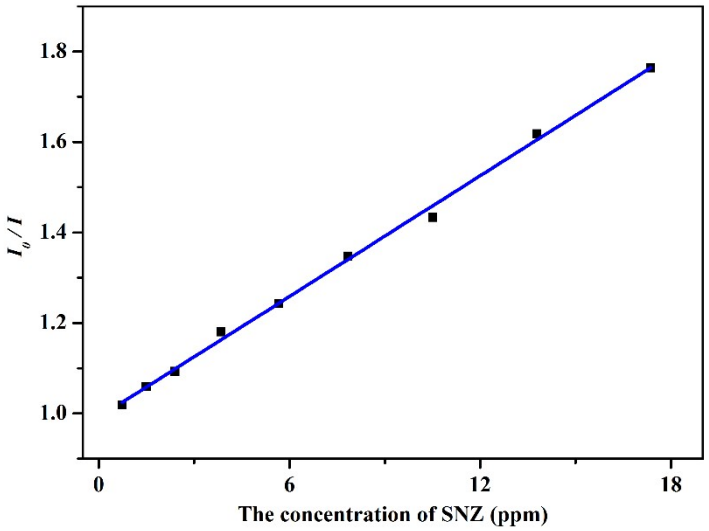



**Fig. S19** Relative luminescence intensity ($I_0/I$) *vs* the concentration of SNZ antibiotic plot.

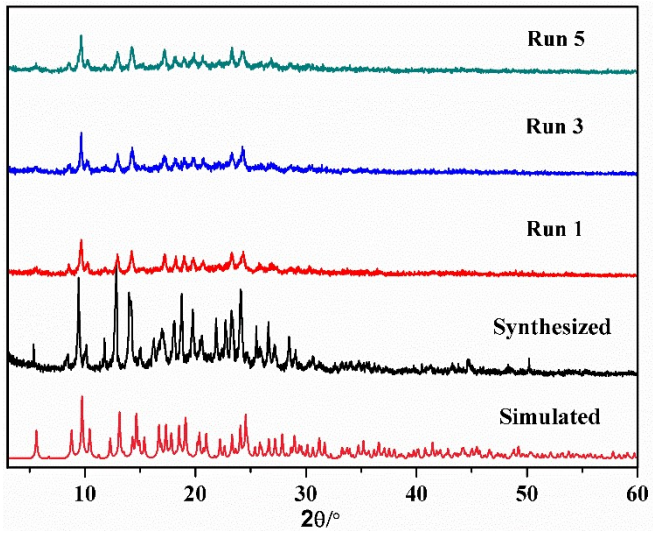



**Fig. S20** The PXRD patterns of compound **1** after luminescent recycling agree well with the synthesized and simulated ones.

**Table S4** The ICP result of reaction mixture filtrate after five recycles for sensing SNZ.

| filter liquor | The leakage of $Zn^{2+}$ |
|---|---|
| After five recycles for sensing SNZ | 0.056% |

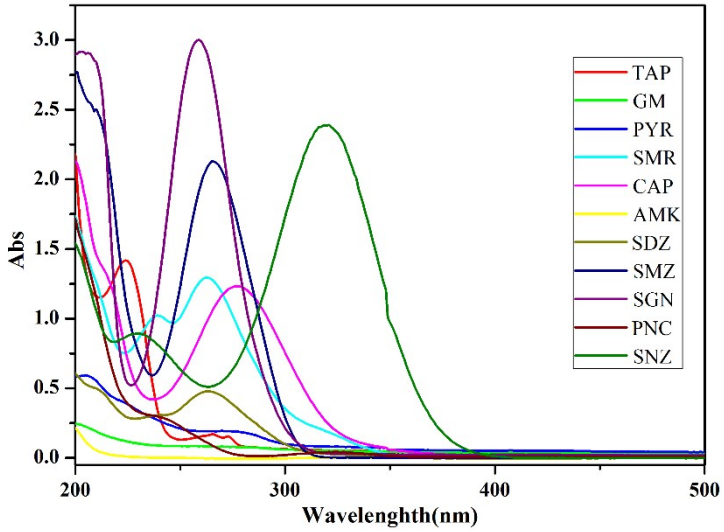



**Fig. S21** UV/Vis absorption spectra of different antibiotics. Concentrations: 45 ppm.