# Supporting Information

## Three new coordination polymers based on bis(4-(4H-1,2,4-triazol-4-yl)phenyl)methane: syntheses, structures, multiresponsive luminescent sensitive detection for antibiotics and pesticides, and antitumor activities

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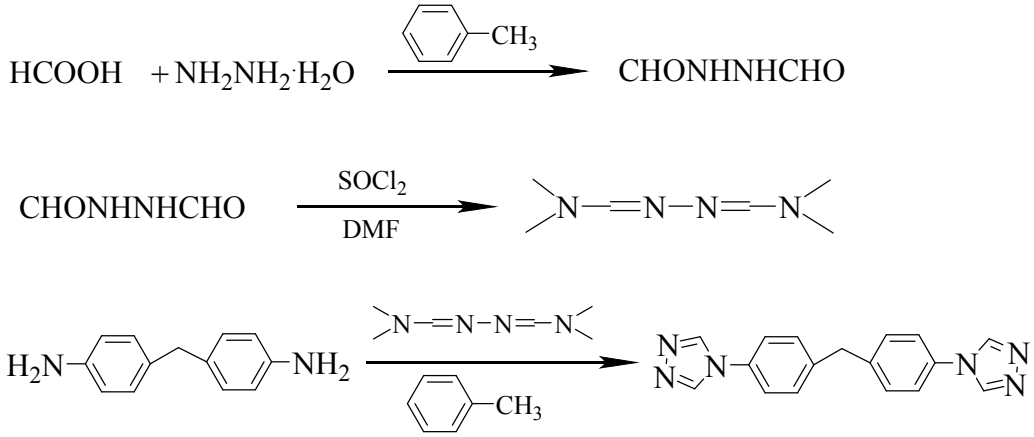
### Synthesis of bis(4-(4H-1,2,4-triazol-4-yl)phenyl)methane (L)




**Scheme S1.** The synthetic route for the ligand.

4,4’-diaminodiphenyl-methane (10 g, 50.38 mmol, 1 equiv) and N'-((dimethylamino)methylene)-N,-Ndimethylformohydrazonamide (23.87 g, 111.35mmol, 2 equiv) in toluene (250 mL) was stirred vigorously and refluxed for 8 h. The pale yellow solid obtained was filtered, and washed with cold EtOH (1 × 3 mL). The solid was dissolved in hot EtOH (30 mL), treated with a pinch of charcoal and filtered. White crystals obtained was separated and dried under vacuum; yield: 21.4g (75%); mp 262 °C. 1H NMR (400 MHz, DMSO-d6) δ 9.08 (s, 4H), 7.61 (d, J = 8.5 Hz, 4H), 7.50 (d, J = 8.6 Hz, 4H), 3.83

(s, 2H).13C NMR (101 MHz, DMSO-d6) δ 141.88, 130.60, 130.48, 129.43, 121.87, 34.51.Chemical Formula: C17H14N6.Exact Mass: 302.13. Elemental Analysis: C, 67.54; H, 4.67; N, 27.80.

**Table S1.** Selected bond distances (Å) and angles (°) for **CP 1**

| **CP 1** | | | |
|---|---|---|---|
| Mo(4)-O(7) | 1.687(8) | Mo(4)-O(3) | 1.755(8) |
| Mo(4)-O(5) | 1.944(8) | Mo(4)-O(2) | 1.961(7) |
| Mo(4)-O(1) | 2.138(7) | Mo(4)-O(1)#1 | 2.377(7) |
| Mo(1)-O(8) | 1.703(8) | Mo(1)-O(9) | 1.715(8) |
| Mo(1)-O(6) | 1.887(8) | Mo(1)-O(2) | 2.009(8) |
| Mo(1)-O(1) | 2.296(8) | Mo(1)-O(5)#1 | 2.398(8) |
| Mo(3)-O(10) | 1.690(9) | Mo(3)-O(11) | 1.711(8) |
| Mo(3)-O(4) | 1.892(8) | Mo(3)-O(5) | 2.000(8) |
| Mo(3)-O(1) | 2.302(7) | Mo(3)-O(2)#1 | 2.355(8) |
| Mo(2)-O(13) | 1.695(9) | Mo(2)-O(12) | 1.699(9) |
| Mo(2)-O(6) | 1.931(8) | Mo(2)-O(4) | 1.946(8) |
| Mo(2)-O(3)#1 | 2.276(8) | Mo(2)-O(1) | 2.518(8) |
| Ag(2)-N(5) | 2.193(12) | Ag(2)-N(9) | 2.205(11) |
| Ag(2)-N(8)#2 | 2.395(11) | Ag(1)-N(7) | 2.242(11) |
| Ag(1)-N(6)#3 | 2.248(11) | Ag(1)-N(10)#2 | 2.331(12) |
| O(7)-Mo(4)-O(3) | 104.9(4) | O(7)-Mo(4)-O(5) | 102.3(4) |
| O(3)-Mo(4)-O(5) | 96.3(3) | O(7)-Mo(4)-O(2) | 100.4(4) |

| | | | |
|---|---|---|---|
| O(3)-Mo(4)-O(2) | 96.8(3) | O(5)-Mo(4)-O(2) | 149.8(3) |
| O(7)-Mo(4)-O(1) | 98.7(3) | O(3)-Mo(4)-O(1) | 156.4(3) |
| O(5)-Mo(4)-O(1) | 78.3(3) | O(2)-Mo(4)-O(1) | 78.8(3) |
| O(7)-Mo(4)-O(1)#1 | 173.7(3) | O(3)-Mo(4)-O(1)#1 | 81.2(3) |
| O(5)-Mo(4)-O(1)#1 | 78.4(3) | O(2)-Mo(4)-O(1)#1 | 76.9(3) |
| O(1)-Mo(4)-O(1)#1 | 75.3(3) | O(8)-Mo(1)-O(9) | 103.6(4) |
| O(8)-Mo(1)-O(6) | 102.0(4) | O(9)-Mo(1)-O(6) | 100.9(4) |
| O(8)-Mo(1)-O(2) | 99.3(4) | O(9)-Mo(1)-O(2) | 97.7(4) |
| O(6)-Mo(1)-O(2) | 147.4(3) | O(8)-Mo(1)-O(1) | 96.2(3) |
| O(9)-Mo(1)-O(1) | 159.6(4) | O(6)-Mo(1)-O(1) | 79.2(3) |
| O(2)-Mo(1)-O(1) | 74.2(3) | O(8)-Mo(1)-O(5)#1 | 165.8(3) |
| O(9)-Mo(1)-O(5)#1 | 87.9(4) | O(6)-Mo(1)-O(5)#1 | 83.6(3) |
| O(2)-Mo(1)-O(5)#1 | 70.5(3) | O(1)-Mo(1)-O(5)#1 | 71.8(3) |
| O(10)-Mo(3)-O(11) | 104.2(4) | O(10)-Mo(3)-O(4) | 101.5(4) |
| O(11)-Mo(3)-O(4) | 100.6(4) | O(10)-Mo(3)-O(5) | 98.2(4) |
| O(11)-Mo(3)-O(5) | 99.6(4) | O(4)-Mo(3)-O(5) | 147.2(3) |
| O(10)-Mo(3)-O(1) | 95.0(4) | O(11)-Mo(3)-O(1) | 160.3(4) |
| O(4)-Mo(3)-O(1) | 79.0(3) | O(5)-Mo(3)-O(1) | 73.4(3) |
| O(10)-Mo(3)-O(2)#1 | 164.7(3) | O(11)-Mo(3)-O(2)#1 | 89.0(4) |
| O(4)-Mo(3)-O(2)#1 | 83.3(3) | O(5)-Mo(3)-O(2)#1 | 71.6(3) |
| O(1)-Mo(3)-O(2)#1 | 71.4(3) | O(13)-Mo(2)-O(12) | 105.3(5) |

| | | | |
|---|---|---|---|
| O(13)-Mo(2)-O(6) | 103.4(4) | O(12)-Mo(2)-O(6) | 98.3(4) |
| O(13)-Mo(2)-O(4) | 104.2(4) | O(12)-Mo(2)-O(4) | 97.0(4) |
| O(6)-Mo(2)-O(4) | 143.5(3) | O(13)-Mo(2)-O(3)#1 | 89.5(4) |
| O(12)-Mo(2)-O(3)#1 | 165.3(4) | O(6)-Mo(2)-O(3)#1 | 78.1(3) |
| O(4)-Mo(2)-O(3)#1 | 78.7(3) | O(13)-Mo(2)-O(1) | 158.6(4) |
| O(12)-Mo(2)-O(1) | 96.1(4) | O(6)-Mo(2)-O(1) | 72.9(3) |
| O(4)-Mo(2)-O(1) | 72.7(3) | O(3)#1-Mo(2)-O(1) | 69.2(3) |
| N(5)-Ag(2)-N(9) | 149.7(4) | N(5)-Ag(2)-N(8)#2 | 106.2(4) |
| N(9)-Ag(2)-N(8)#2 | 104.1(4) | N(7)-Ag(1)-N(6)#3 | 152.6(4) |
| N(7)-Ag(1)-N(10)#2 | 105.2(4) | N(6)#3-Ag(1)-N(10)#2 | 102.2(4) |

Symmetry Code:#1 -x+3/2,-y+3/2,-z+2,#2 x+1/2,-y+1/2,z+1/2,#3 x+1/2,-y+3/2,z+1/2,#4 x-1/2,-y+3/2,z-1/2,#5 x-1/2,-y+1/2,z-1/2.

**Table S2.** Selected bond distances (Å) and angles (°) for **CP 2**

| **CP 2** | | | |
|---|---|---|---|
| Zn(1)-O(2) | 1.9430(13) | Zn(1)-O(4) | 1.9499(13) |
| Zn(1)-N(4)#1 | 2.0020(15) | Zn(1)-N(1) | 2.0484(15) |
| O(2)-Zn(1)-O(4) | 111.17(6) | O(2)-Zn(1)-N(4)#1 | 115.08(6) |
| O(4)-Zn(1)-N(4)#1 | 119.59(7) | O(2)-Zn(1)-N(1) | 112.22(6) |
| O(4)-Zn(1)-N(1) | 96.46(6) | N(4)#1-Zn(1)-N(1) | 99.82(6) |

Symmetry Code:#1-x+2,-y,-z+2,#2 -x+1,-y+1,-z+1,#3 -x+2,-y+2,-z+1,#4 -x+2-y+2,-

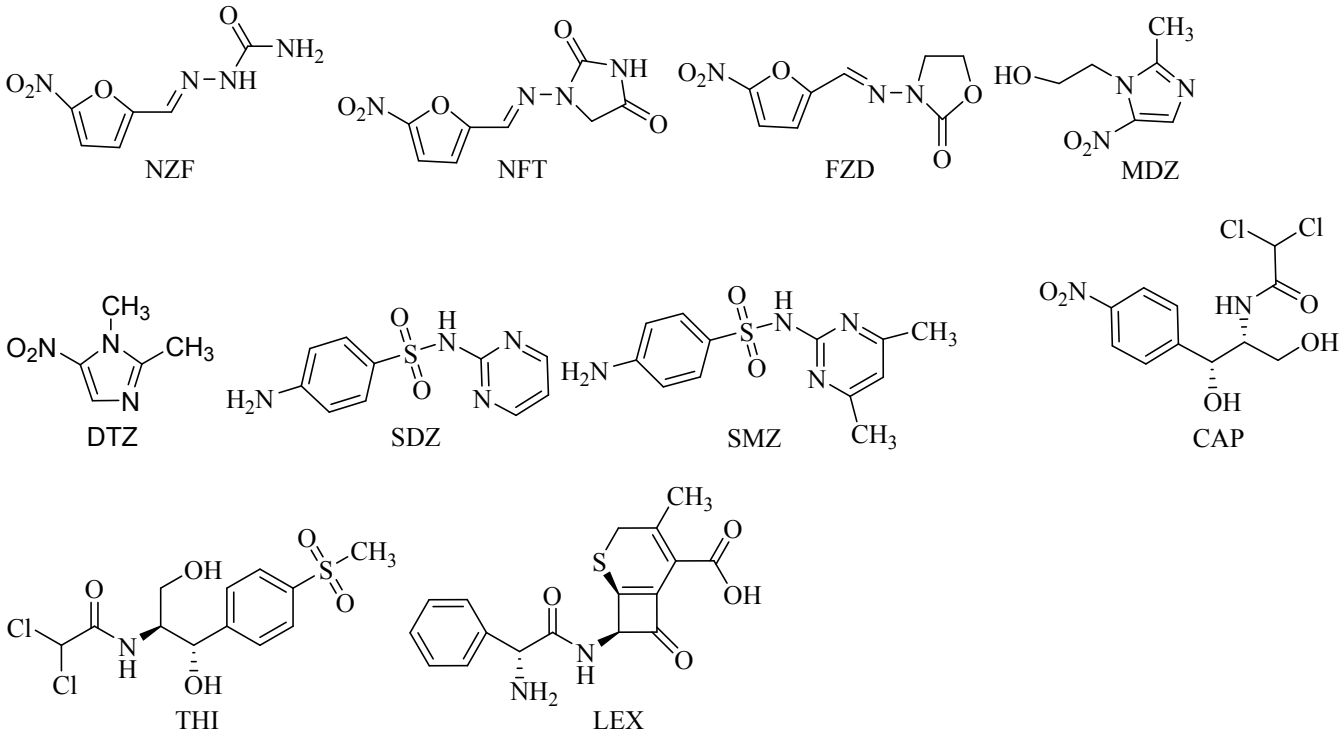
z+2,#5 -x+3,-y,-z+2.

**Table S3.** Selected bond distances (Å) and angles (°) for **CP 3**

| **CP 3** | | | |
|---|---|---|---|
| Cd(1)-O(1) | 2.2424(18) | Cd(1)-N(2) | 2.322(2) |
| Cd(1)-O(2)#1 | 2.3282(19) | Cd(1)-N(5)#2 | 2.341(2) |
| Cd(1)-N(6)#3 | 2.355(2) | Cd(1)-N(3)#1 | 2.386(2) |
| O(1)-Cd(1)-N(2) | 113.76(7) | O(1)-Cd(1)-O(2)#1 | 156.93(7) |
| N(2)-Cd(1)-O(2)#1 | 88.98(7) | O(1)-Cd(1)-N(5)#2 | 99.93(8) |
| N(2)-Cd(1)-N(5)#2 | 89.96(7) | O(2)#1-Cd(1)-N(5)#2 | 83.13(8) |
| O(1)-Cd(1)-N(6)#3 | 92.58(9) | N(2)-Cd(1)-N(6)#3 | 85.65(8) |
| O(2)#1-Cd(1)-N(6)#3 | 85.06(8) | N(5)#2-Cd(1)-N(6)#3 | 167.47(8) |
| O(1)-Cd(1)-N(3)#1 | 77.99(7) | N(2)-Cd(1)-N(3)#1 | 167.70(7) |
| O(2)#1-Cd(1)-N(3)#1 | 79.09(7) | N(5)#2-Cd(1)-N(3)#1 | 91.53(8) |
| N(6)#3-Cd(1)-N(3)#1 | 90.33(8) | | |

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

## Detection of antibiotics




## Detection of pesticide

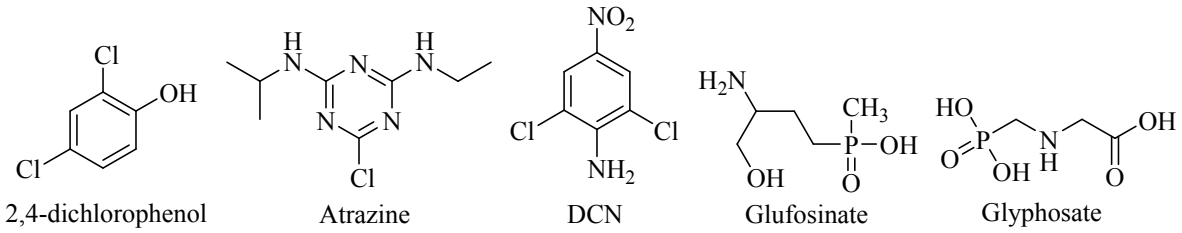



**Table S4**. HOMO and LUMO energies for the selected antibiotics calculated by the calculation formula (-|4.78+x|eV)

| Analytes | HUMO (eV) | LUMO (eV) | Band Gap (eV) |
|---|---|---|---|
| NZF | -6.36 | -4.1 | 2.26 |
| NFT | -6.53 | -4.27 | 2.26 |

| | | | |
|---|---|---|---|
| MDZ | -6.51 | -3.83 | 2.68 |
| DTZ | -6.5 | -3.7 | 2.8 |
| SDZ | -5.98 | -3.36 | 2.62 |
| SMZ | -6.05 | -3.12 | 2.93 |
| CAP | -6.43 | -3.91 | 2.52 |
| THI | -6.58 | -3.27 | 3.31 |
| LEX | -6.44 | -3.49 | 2.95 |
| FZD | -6.75 | -4.14 | 2.61 |

**Table S5.** HOMO and LUMO energies for the selected pesticides calculated by the calculation formula (-|4.78+x|eV)

| **Analytes** | **HUMO (eV)** | **LUMO (eV)** | **Band Gap (eV)** |
|---|---|---|---|
| 2,4-dichlorophenol | -6.32 | -2.57 | 3.75 |
| Atrazine | -6.43 | -2.54 | 3.89 |
| DCN | -6.63 | -3.84 | 2.79 |
| Glufosinate | -6.45 | -4.18 | 2.27 |
| Glyphosate | -6.45 | -2.46 | 3.99 |

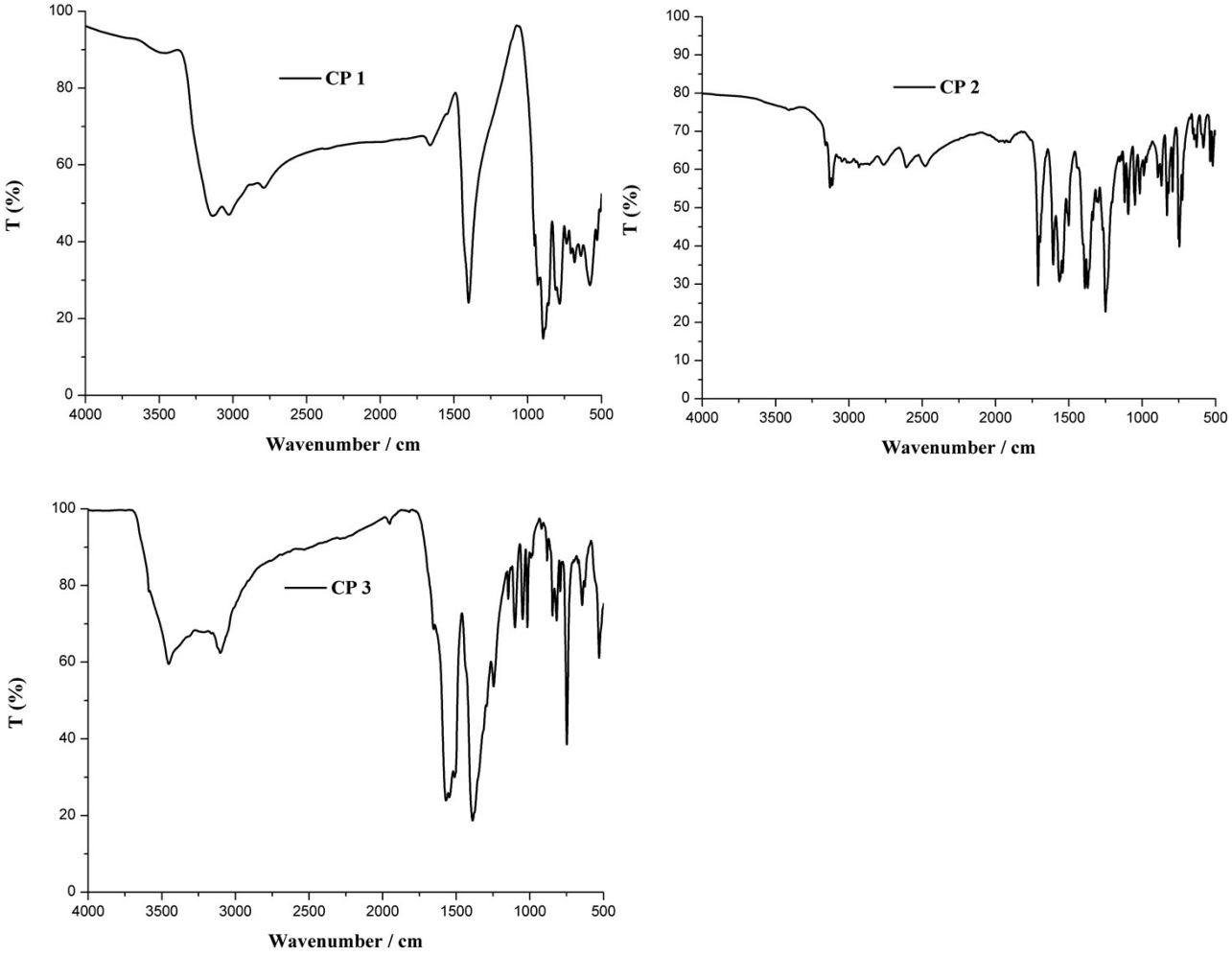
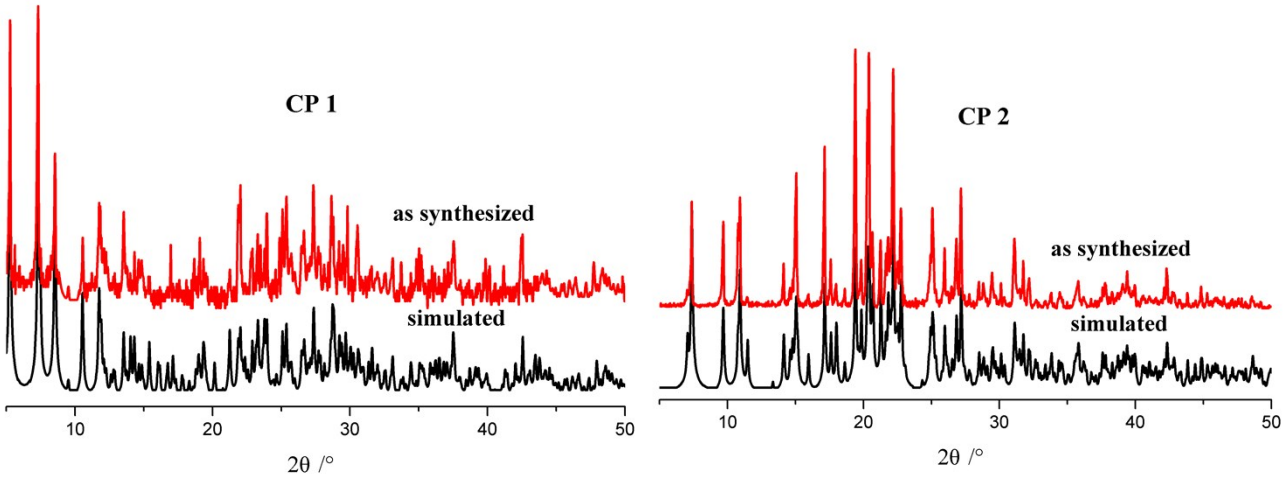



**Fig. S1** The IR spectra of CP 1-3



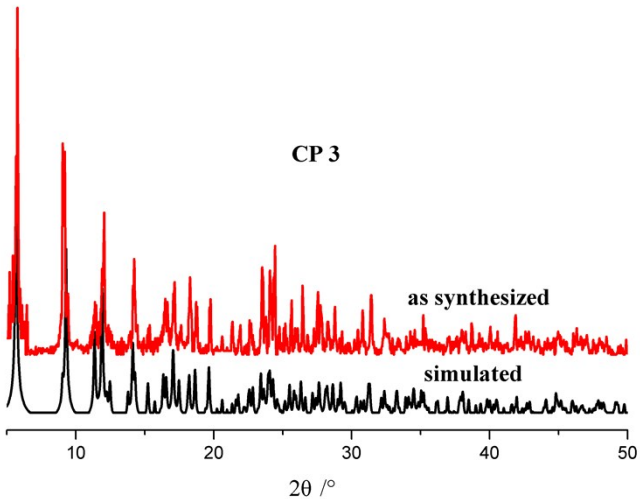



**Fig. S2** PXRD patterns of CP 1-3

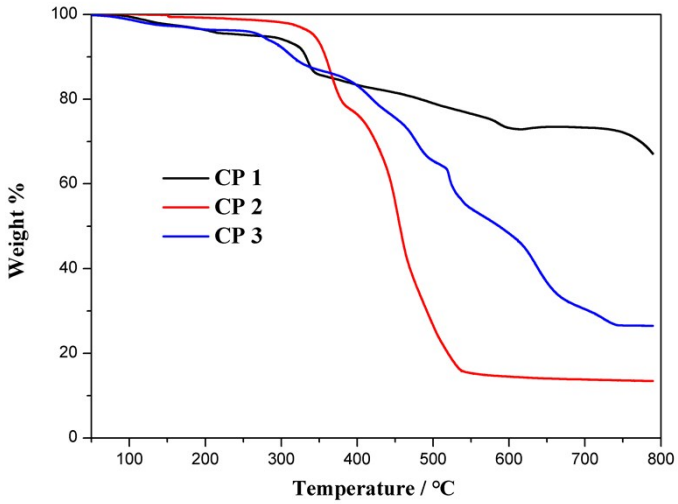



**Fig. S3** The TGA diamgram of CP 1-3

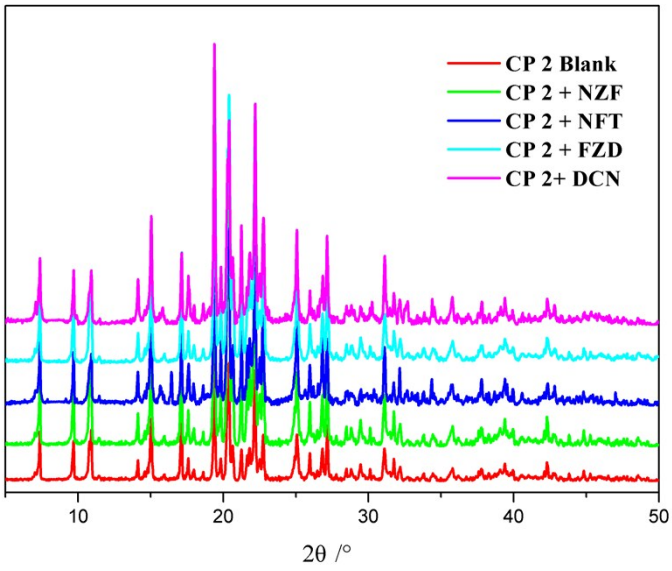



**Fig. S4** PXRD patterns of CP 2 after immersed in the water solution (1.0 mM) with different analytes nitrofurazone (NZF), nitrofurantoin (NFT), furazolidone (FZD) and 2,6-dichloro-4-nitroaniline (DCN)) for 12 hours.

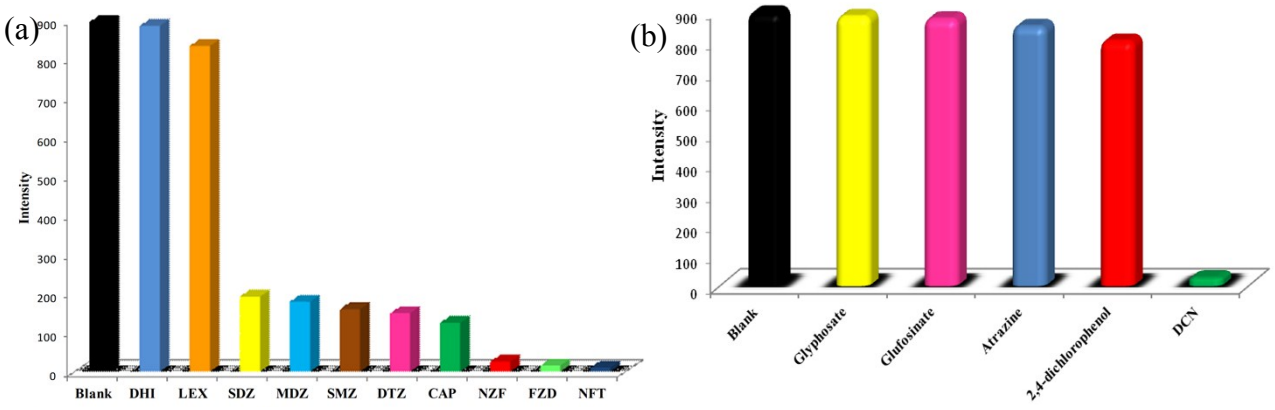



**Fig. S5** (a) Comparison of the fluorescence intensities of CP 2 treated by 0.30 mM different antibiotics. (b) Fluorescence intensities of CP 2 immersed in 0.30 mM DMF solution of different pesticides.

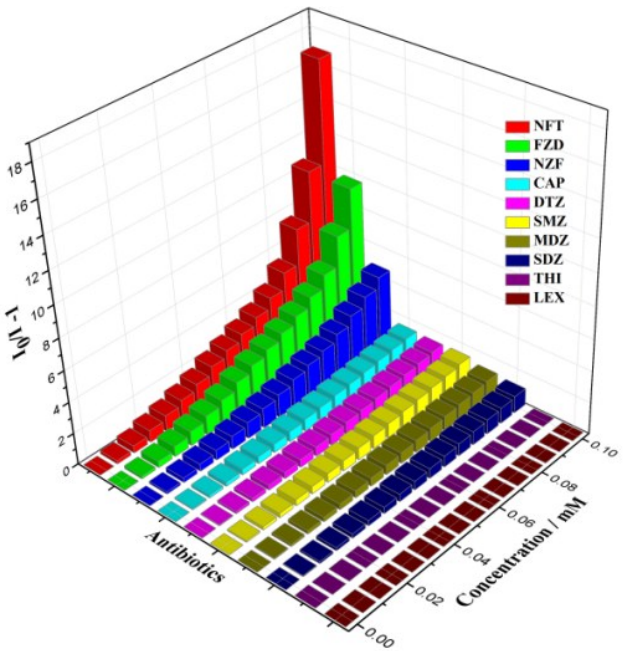



**Fig. S6** Stern–Volmer plots of selected antibiotics of CP 2.

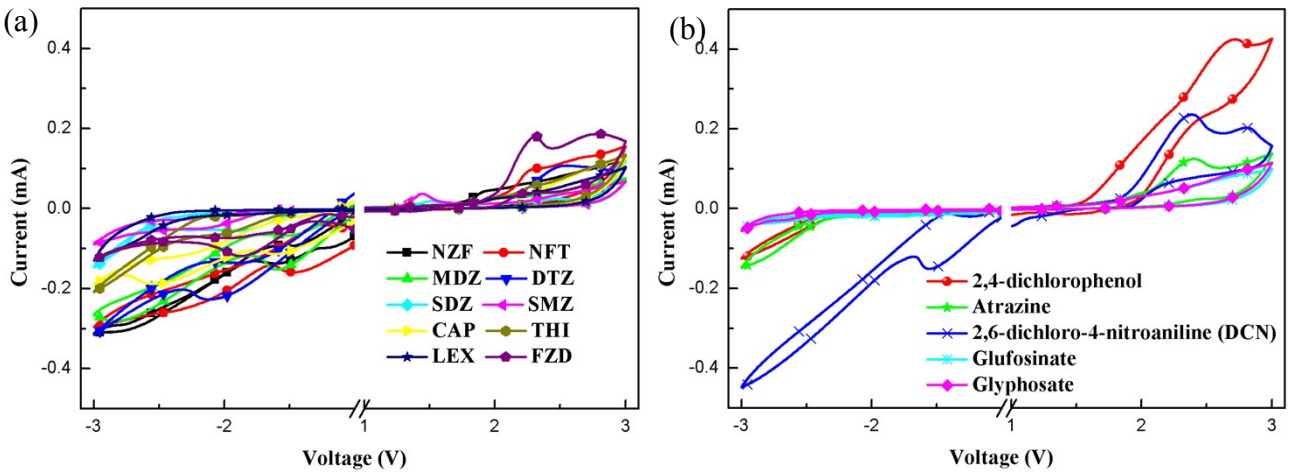



**Fig. S7** Electrochemical map of selected antibiotics (a) and pesticides (b).

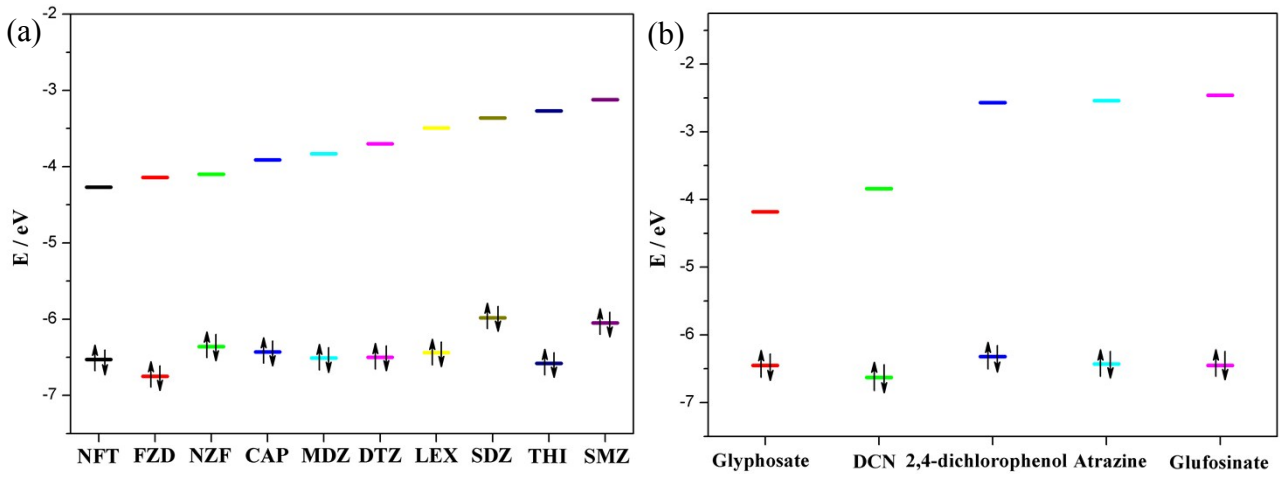



**Fig. S8** HOMO and LUMO energies for the selected antibiotics (a) and pesticides (b) calculated by the calculation formula (-|4.78+x|eV).

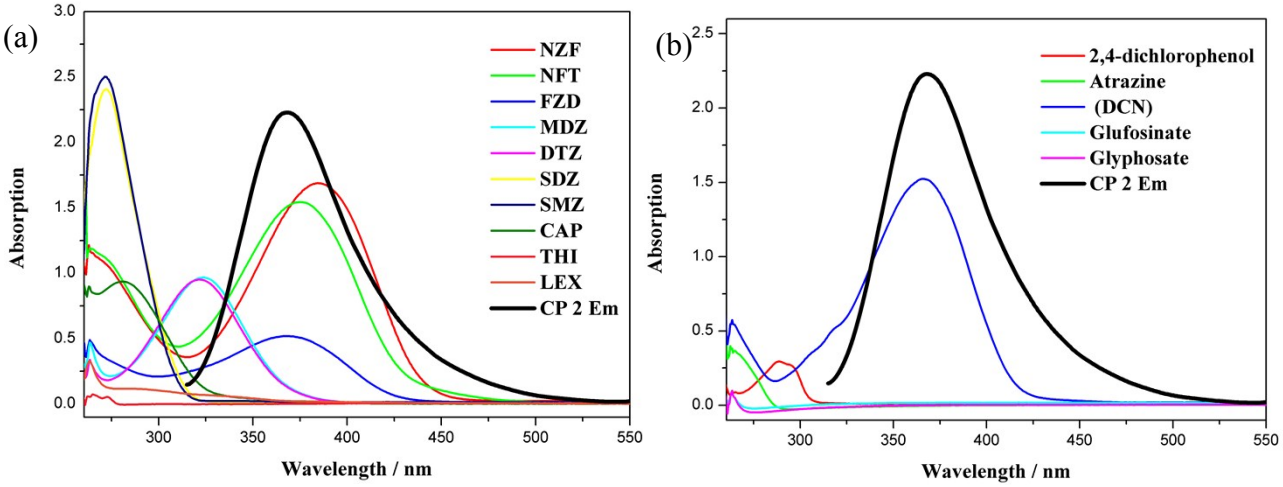



**Fig. S9**. UV-vis absorption spectra of selected antibiotics (a) and pesticides (b) (0.10 mM) and the normalized emission spectra of CP 2 in water.

## References

1. S. S. Han, L. L. Shi, K. Li, S. Zhao, B. L. Li and B. Wu. *RSC Adv.,*2015, **5,** 107166-107178.

2. N. Wang, Y. C. Feng, W. Shi, B. Zhao, P. Cheng, D. Z. Liao and S. P. Yan. *CrystEngComm.,*2012, **14,** 2769-2778.