

Supplementary Information-

I₃⁻ Entrapped Cationic Zn(II) Coordination Polymer: Selective Detection and Dose-Dependent Photocatalytic Degradation of Roxithromycin

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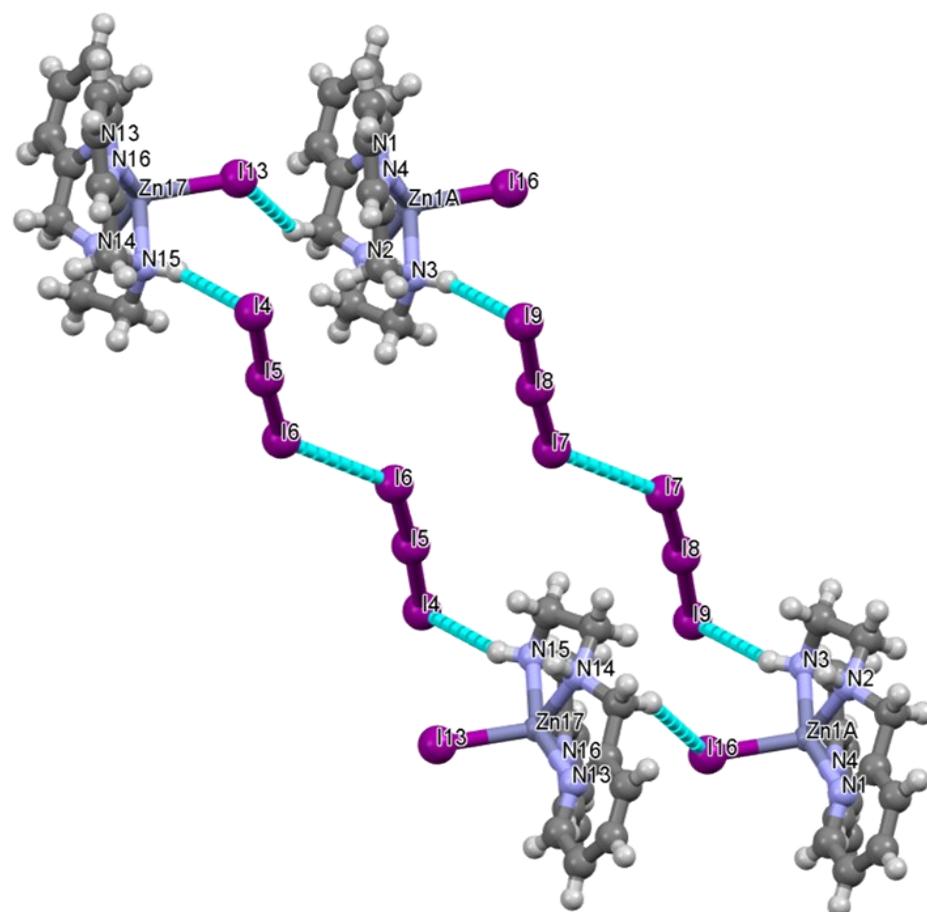


Fig. S1. One-dimensional polymeric non-covalent interaction of Zinc-CP along with crystallography b-axis

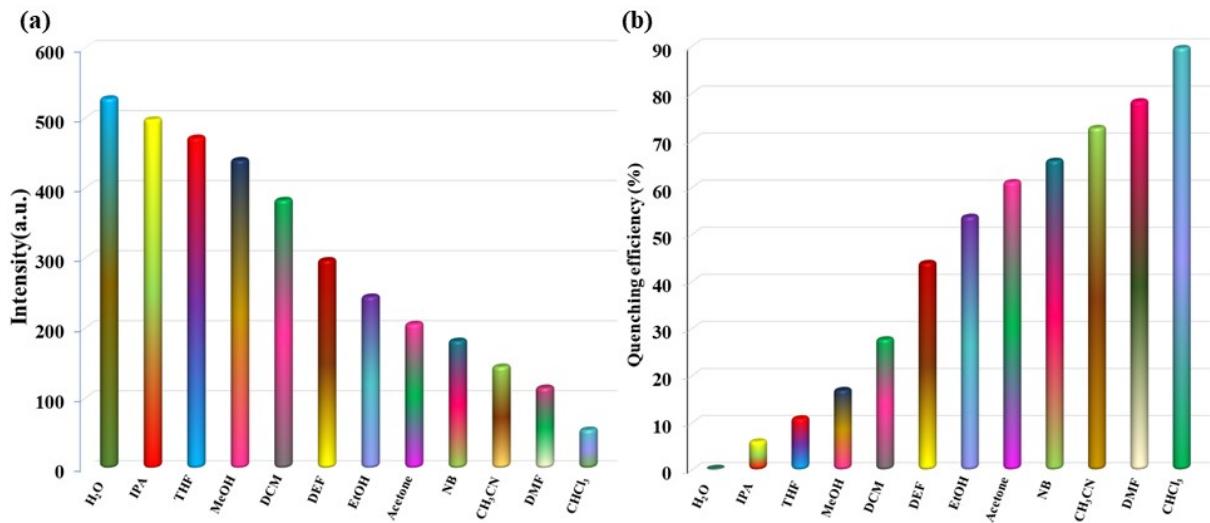


Fig. S2. (a) The levels of fluorescence intensity exhibited by **Zinc-CP** in the presence of different organic solvents; and (b) The relative quenching efficiencies of **Zinc-CP** dispersed in aqueous solutions containing specific solvents.

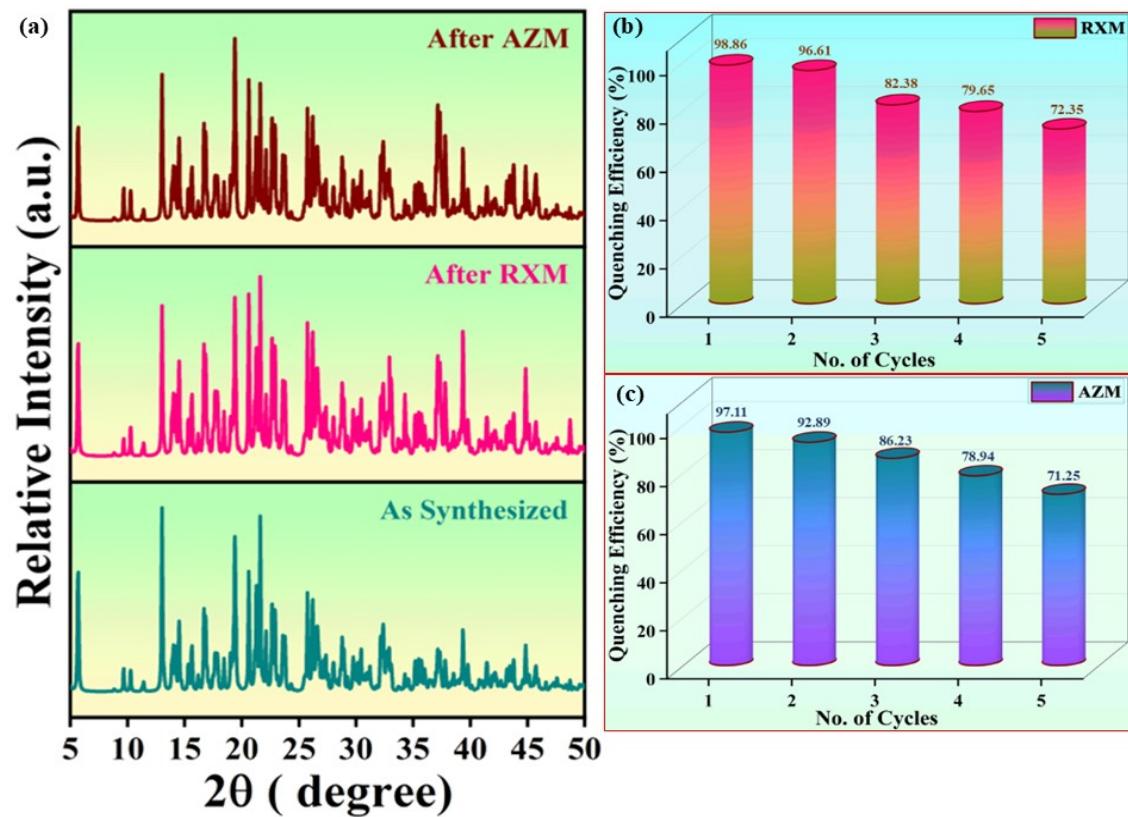


Fig. S3. (a) PXRD pattern of **Zinc-CP** after luminescence detection of antibiotics RXM and AZM (b) Quenching efficiency (%) of **Zinc-CP** over the course of five cycles and (c) Quenching efficiency (%) of **Zinc-CP** over the course of five cycles.

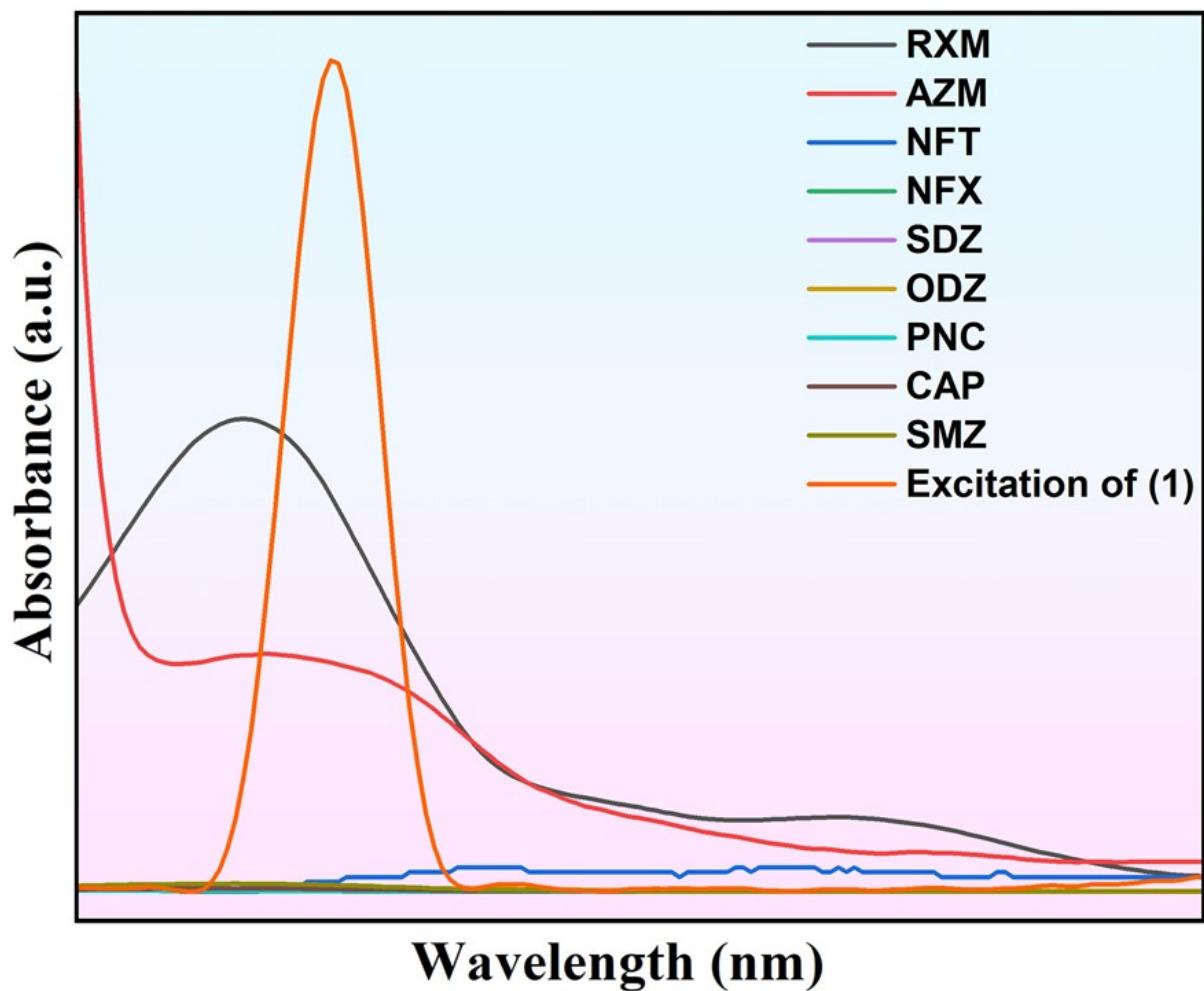


Fig. S4. Spectral overlap between the UV-Vis absorption spectra of Antibiotics (RXM and AZM) with the excitation spectra of Zinc-CP.

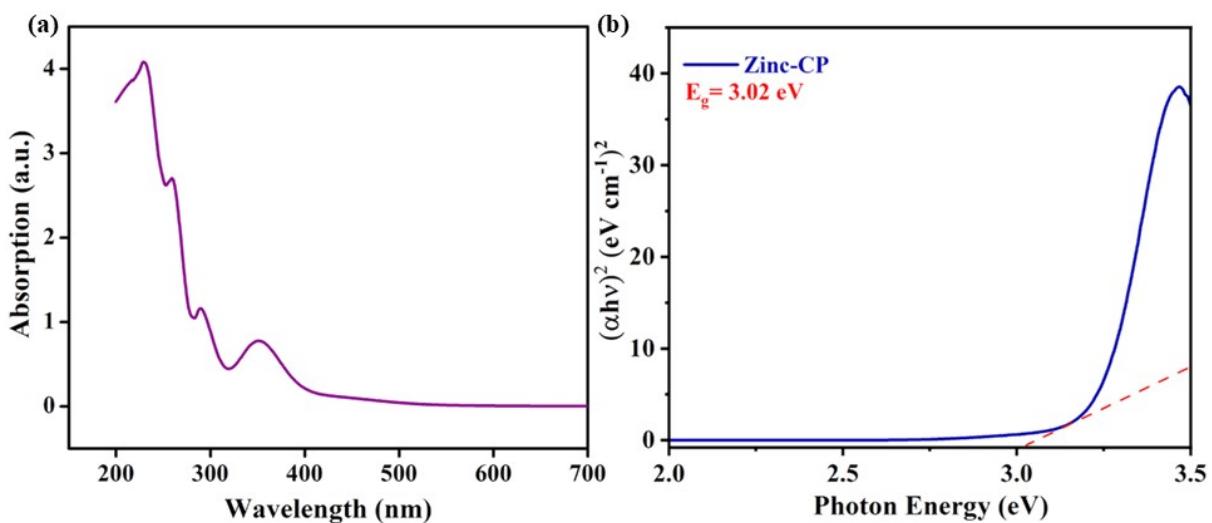


Fig. S5. (a) UV-Visible absorption spectra of Zinc-CP (b) Band gap analysis of Zinc-CP using Tauc Plot $(\alpha h\nu)^2 (\text{eV cm}^{-1})^2$ Vs Energy (eV).

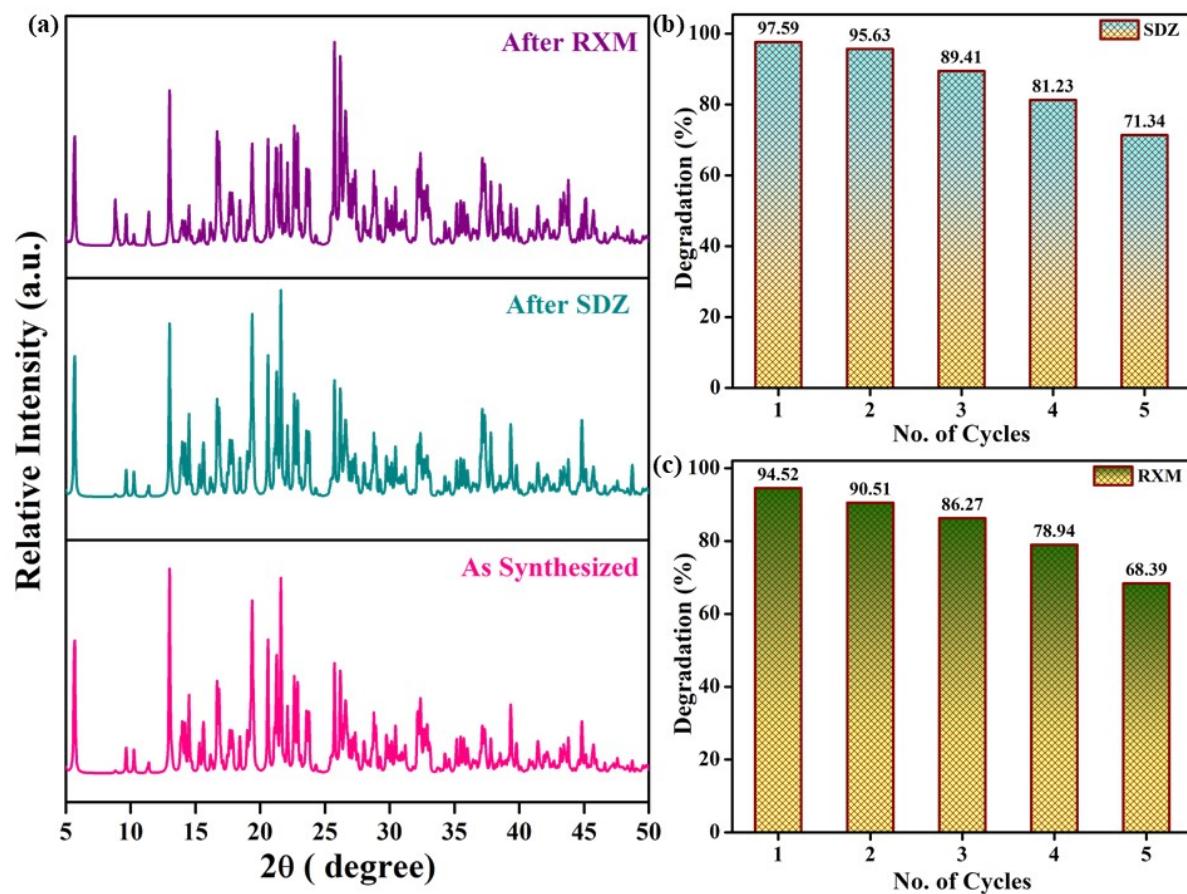


Fig. S6. (a) PXRD pattern of **Zinc-CP** and after photocatalytic degradation of antibiotics SDZ and RXM (b) degradation efficiency of **Zinc-CP** over the course of five cycles and (c) degradation efficiency of **Zinc-CP** over the course of five cycles.

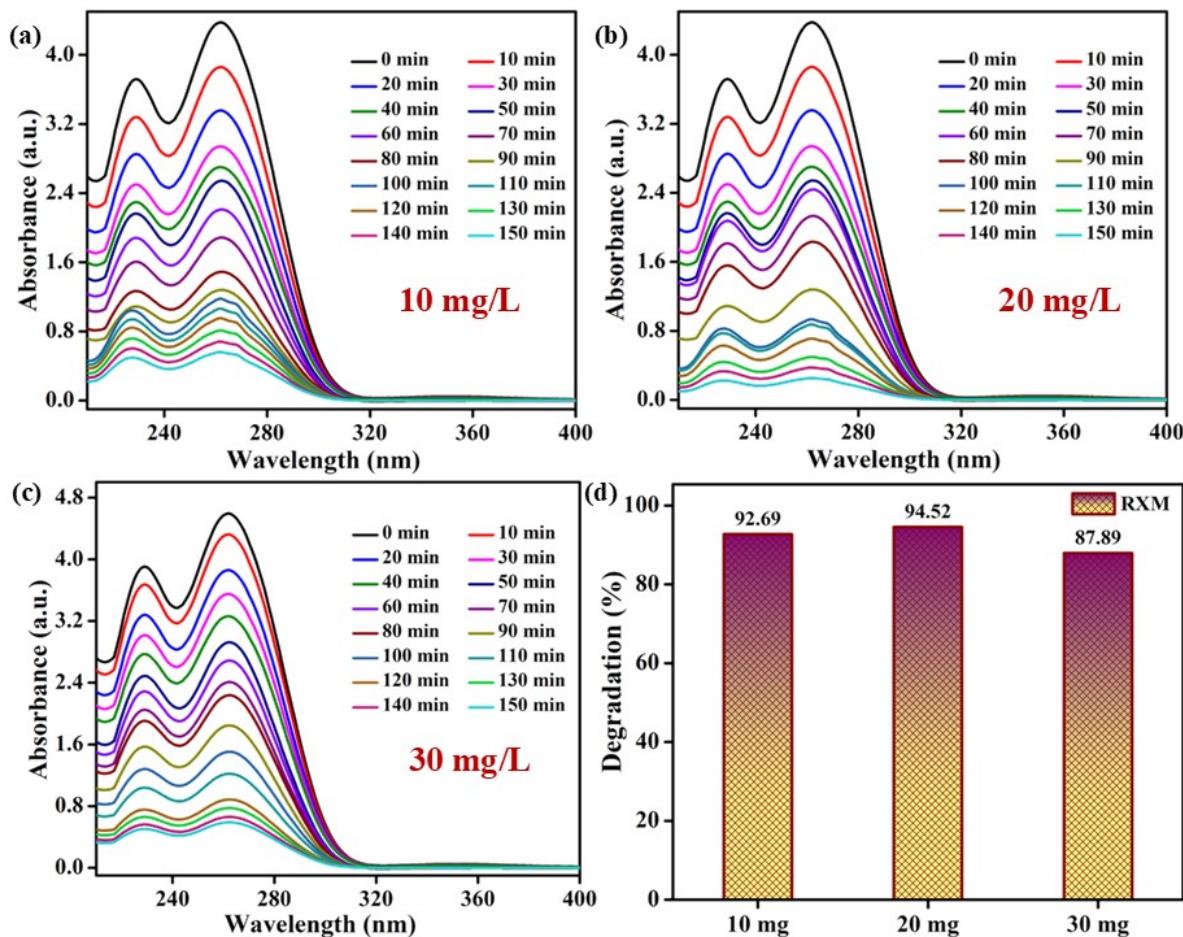


Fig. S7. Periodic UV-Vis spectra for RXM in presence of (a) 10 mg photocatalyst **Zinc-CP**; (b) 20 mg photocatalyst **Zinc-CP**; (c) 30 mg photocatalyst **Zinc-CP**; (d) bar plot indicating effect of variable photocatalyst **Zinc-CP** on percentage photodegradation of RXM.

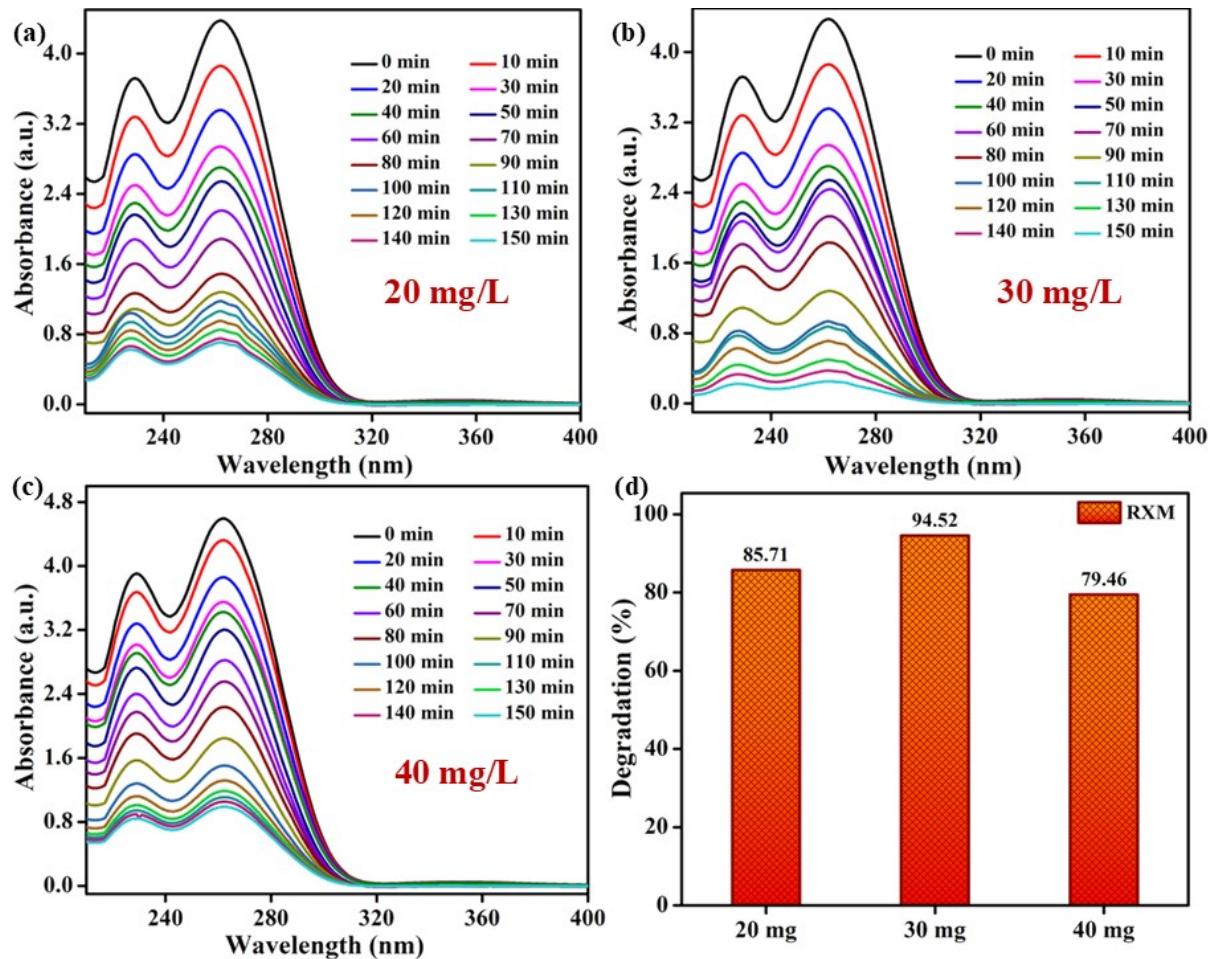


Fig. S8. Periodic UV-Vis spectra for **RXM** in presence of (a) 20 mg/L of **RXM**; (b) 30 mg/L of **RXM**; (c) 40 mg/L of **RXM**; (d) bar plot indicating effect of variable **RXM** concentration on percentage photodegradation of **RXM** (photocatalyst dosages was fixed at 20 mg/L).

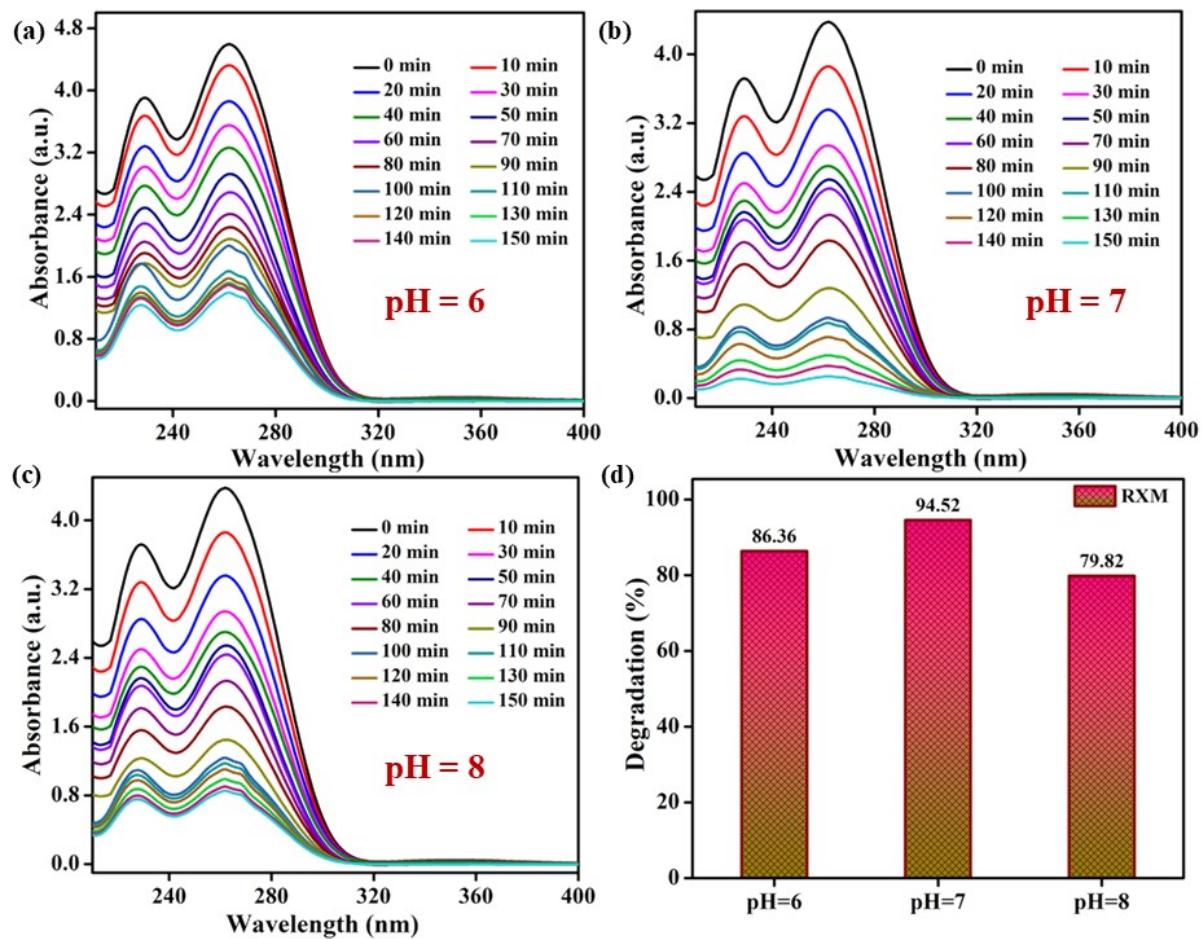


Fig. S9. Periodic UV-Vis spectra for **RXM** in presence of (a) pH = 6; (b) pH = 7; (c) pH = 8; (d) bar plot indicating effect of variable **pH** on percentage photodegradation of **RXM** with **Zinc-CP**.

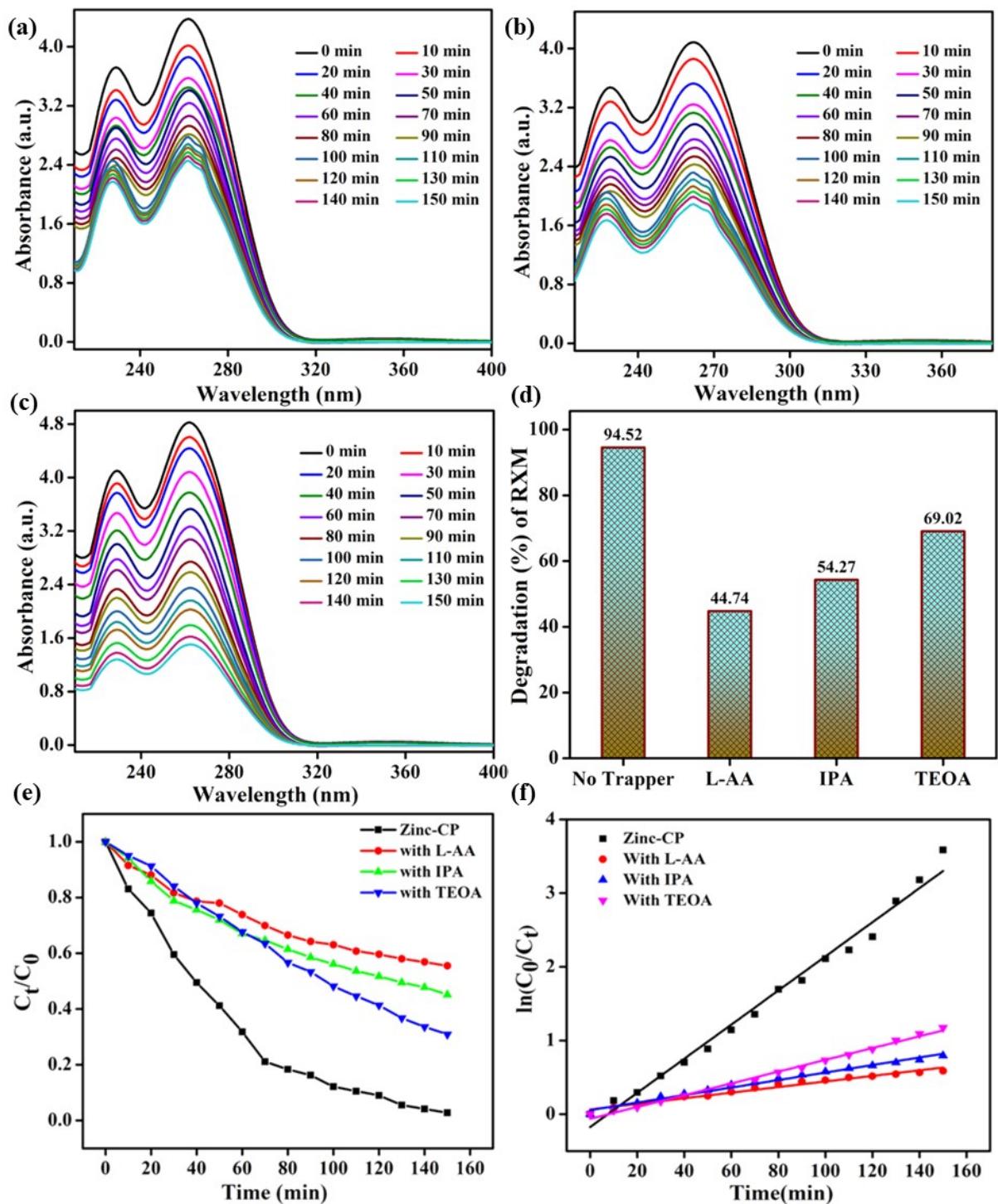


Fig. S10. The UV–Vis spectrum for RXM was analyzed in presence of the photocatalyst **Zinc-CP** and different radical trapping agents: (a) L-AA; (b) IPA; (c) TEOA; (d) the effect of trapping agents on the percentage photodegradation of RXM. (e) plot created to illustrate C_t/C_0 vs irradiation time for the photodegradation of RXM with **Zinc-CP** and various trapping agents. (f) a pseudo first-order kinetics plot ($\ln(C_0/C_t)$ Vs Time) was generated for

the degradation of RXM with **Zinc-CP** and different trapping agents. (The photocatalyst dosage was set at 20 mg/L and the RXM concentration was set at 30 mg/L).

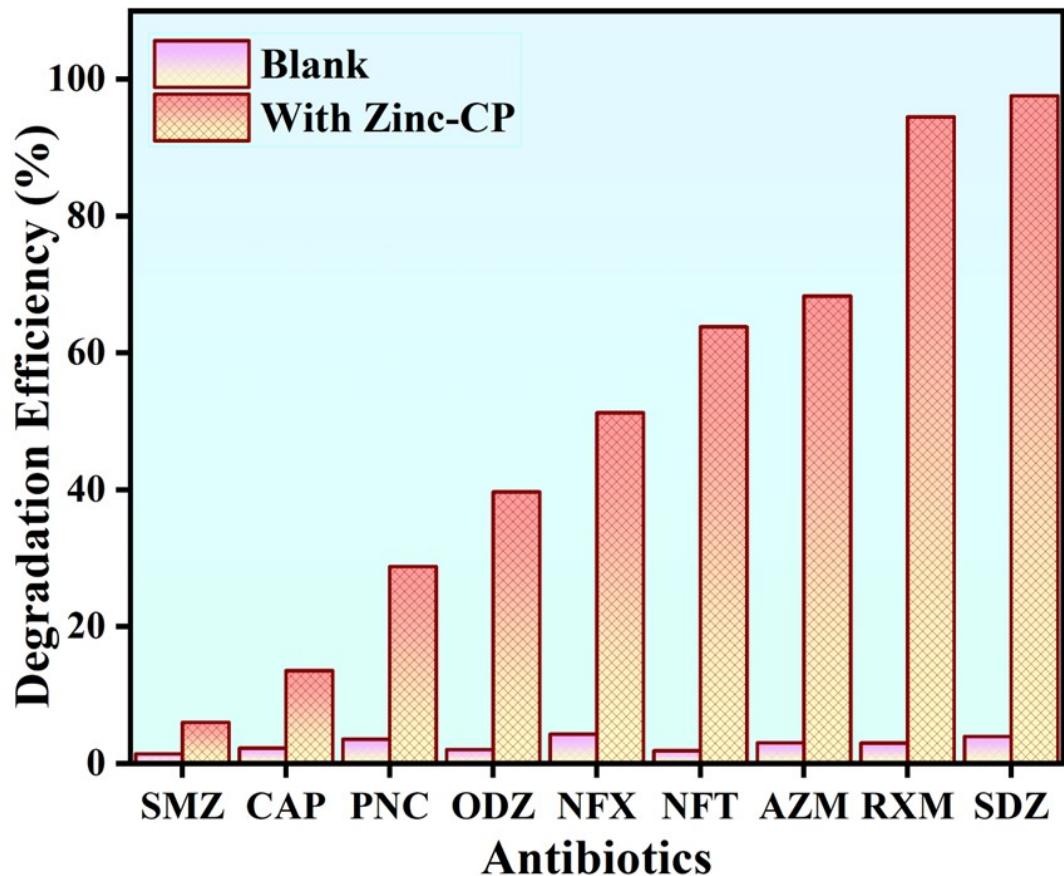


Fig. S11. The degradation efficiency percentage of antibiotics with and without Zinc-CP.

Table S1 Bond Lengths for Zinc-CP.

| Atom | Atom | Length/Å | | Atom | Atom | Length/Å |
|------|------|------------|--|------|------|------------|
| I13 | Zn17 | 2.5825(19) | | I15 | Zn19 | 2.587(2) |
| Zn17 | N13 | 2.173(11) | | Zn19 | N5 | 2.123(11) |
| Zn17 | N14 | 2.114(13) | | Zn19 | N6 | 2.103(12) |
| Zn17 | N15 | 2.206(12) | | Zn19 | N7 | 2.209(11) |
| Zn17 | N16 | 2.082(13) | | Zn19 | N8 | 2.070(10) |
| I14 | Zn18 | 2.582(2) | | I16 | Zn1A | 2.5808(19) |
| Zn18 | N9 | 2.093(13) | | Zn1A | N1 | 2.158(14) |

| | | | | | | | |
|-------------|------------|-----------|--|-------------|-----------|--|-----------|
| Zn18 | N10 | 2.166(12) | | Zn1A | N2 | | 2.115(11) |
| Zn18 | N11 | 2.110(12) | | Zn1A | N3 | | 2.186(13) |
| Zn18 | N12 | 2.145(13) | | Zn1A | N4 | | 2.067(12) |

Table S2 Bond Angles for Zinc-CP.

| Atom | Atom | Atom | Angle/ [°] | Atom | Atom | Atom | Angle/ [°] | |
|------------|-------------|-------------|---------------------|------|------------|-------------|---------------------|-----------|
| N13 | Zn17 | I13 | 102.8(3) | | N5 | Zn19 | I15 | 102.6(3) |
| N14 | Zn17 | I13 | 119.3(4) | | N6 | Zn19 | I15 | 117.9(3) |
| N14 | Zn17 | N13 | 78.8(5) | | N6 | Zn19 | N5 | 79.2(5) |
| N15 | Zn17 | I13 | 99.7(3) | | N7 | Zn19 | I15 | 100.4(3) |
| N15 | Zn17 | N13 | 155.2(5) | | N7 | Zn19 | N5 | 154.8(5) |
| N15 | Zn17 | N14 | 81.1(4) | | N7 | Zn19 | N6 | 80.9(5) |
| N16 | Zn17 | I13 | 112.6(3) | | N8 | Zn19 | I15 | 112.9(3) |
| N16 | Zn17 | N13 | 102.2(5) | | N8 | Zn19 | N5 | 101.8(5) |
| N16 | Zn17 | N14 | 126.5(5) | | N8 | Zn19 | N6 | 127.6(5) |
| N16 | Zn17 | N15 | 78.5(5) | | N8 | Zn19 | N7 | 78.5(5) |
| C52 | N13 | Zn17 | 113.8(10) | | C24 | N5 | Zn19 | 114.5(10) |
| C56 | N13 | Zn17 | 125.4(11) | | C28 | N5 | Zn19 | 128.0(10) |
| C50 | N14 | Zn17 | 111.7(10) | | C22 | N6 | Zn19 | 110.1(9) |
| C51 | N14 | Zn17 | 109.1(9) | | C23 | N6 | Zn19 | 110.7(9) |
| C48 | N15 | Zn17 | 108.0(10) | | C20 | N7 | Zn19 | 107.7(10) |
| C49 | N15 | Zn17 | 106.3(9) | | C21 | N7 | Zn19 | 107.6(9) |
| C43 | N16 | Zn17 | 124.6(11) | | C15 | N8 | Zn19 | 124.4(10) |
| C47 | N16 | Zn17 | 117.2(12) | | C19 | N8 | Zn19 | 116.4(12) |
| N9 | Zn18 | I14 | 113.1(3) | | N1 | Zn1A | I16 | 102.0(3) |
| N10 | Zn18 | I14 | 100.0(4) | | N2 | Zn1A | I16 | 119.8(3) |
| N10 | Zn18 | N9 | 81.2(5) | | N2 | Zn1A | N1 | 78.9(5) |
| N11 | Zn18 | I14 | 118.5(4) | | N3 | Zn1A | I16 | 100.4(3) |

| | | | | | | | | |
|------------|-------------|-------------|-----------|--|------------|-------------|-------------|-----------|
| N11 | Zn18 | N9 | 127.3(5) | | N3 | Zn1A | N1 | 155.0(5) |
| N11 | Zn18 | N10 | 80.0(5) | | N3 | Zn1A | N2 | 80.5(5) |
| N12 | Zn18 | I14 | 102.7(4) | | N4 | Zn1A | I16 | 112.6(3) |
| N12 | Zn18 | N9 | 101.2(5) | | N4 | Zn1A | N1 | 101.5(5) |
| N12 | Zn18 | N10 | 153.9(5) | | N4 | Zn1A | N2 | 126.4(4) |
| N12 | Zn18 | N11 | 78.0(5) | | N4 | Zn1A | N3 | 79.9(5) |
| C38 | N9 | Zn18 | 114.7(10) | | C1 | N1 | Zn1A | 127.1(13) |
| C42 | N9 | Zn18 | 127.7(12) | | C5 | N1 | Zn1A | 113.2(11) |
| C36 | N10 | Zn18 | 110.0(9) | | C7 | N2 | Zn1A | 109.5(9) |
| C37 | N10 | Zn18 | 107.6(9) | | C8 | N3 | Zn1A | 108.6(10) |
| C34 | N11 | Zn18 | 111.9(9) | | C9 | N3 | Zn1A | 107.8(9) |
| C35 | N11 | Zn18 | 111.5(9) | | C10 | N4 | Zn1A | 117.3(11) |
| C29 | N12 | Zn18 | 126.5(13) | | C14 | N4 | Zn1A | 125.2(12) |
| C33 | N12 | Zn18 | 116.1(11) | | | | | |

Table S3: Influence of SDZ and RXM Concentration, Zinc-CP Dosage, and pH Variations on the Photocatalytic Degradation Process.

| S.No. | Effect of Reaction Parameters | Degradation (%) | |
|--------------|--------------------------------------|------------------------|------------|
| | | SDZ | RXM |
| 1. | Effect of Dosages of Zinc-CP | | |
| a. | 10 mg/L | 91.69 | 92.69 |
| b. | 20 mg/L | 97.59 | 94.52 |

| | | | |
|-----------|---|-------|-------|
| c. | 30 mg/L | 83.59 | 87.89 |
| 2. | Effect of Concentration of Antibiotics (SDZ & RXM) | | |
| a. | 20 mg/L | 88.58 | 85.71 |
| b. | 30 mg/L | 97.59 | 94.52 |
| c. | 40 mg/L | 83.59 | 79.46 |
| 3. | Effect of pH level | | |
| a. | pH = 6 | 87.93 | 86.36 |
| b. | pH = 7 | 97.59 | 94.52 |
| c. | pH = 8 | 76.17 | 79.82 |