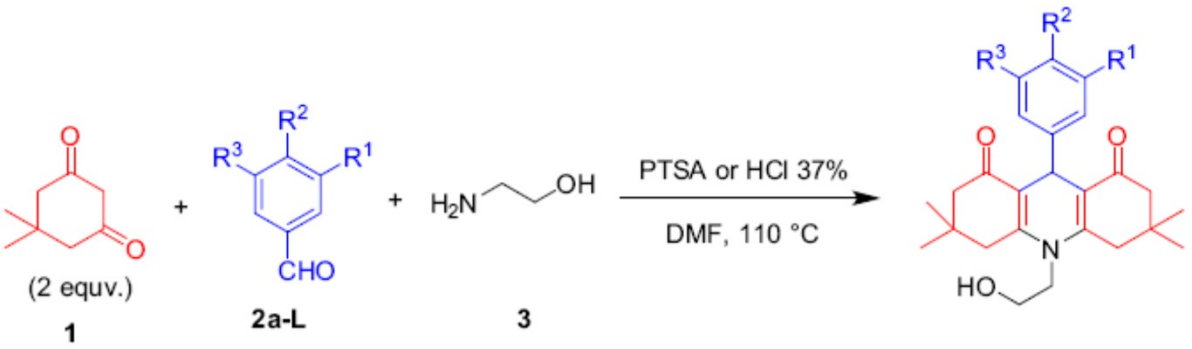
Supporting Information's

Metal-organic framework MIL-101(Fe) functionalized with folic acid as multifunctional nanocarrier for targeting chemotherapy-photodynamic therapy

Synthesis of D08

In a 50 mL round flask, a mixture of dimedone (2.8 g, 20 mmol), different aromatic aldehyde (10 mmol), 2-aminoethanol (0.72 mL, 12 mmol) was dissolved in *N*, *N*-dimethylformamide (9 mL) then *p*-toluenesulfonic acid (PTSA) (1.5 gm) or hydrochloric acid (HCl) 37% (1 mL) was added as a catalyst. The mixture was stirred at 110 °C under reflux for 24 h. The progression of the reaction was monitored by TLC. After completion, the reaction mixture was cooled to room temperature then dropped into water (120 mL) while stirring until complete precipitation. The product was filtered off, washed with water, and dried at room temperature. The crude products were recrystallized from toluene to get pure compound **D08**.

Compound **(D08)** was obtained as pale-yellow powder, (3.9 g, 86% yield); **mp.** 206-208 °C. **IR (KBr)** ν_{max} **(cm^{-1}):** 3311 (O–H); 3075 (=C–H, sp2); 2959, 2867 (C–H, sp3); 1644, 1612 (C=O, conjugated ketone); 1563, 1513, 1460 (C=C); 1341 (C–N stretching);1079 (C–O stretching). **^{1}H NMR (400 *MHz*, DMSO-d_6) δ (ppm)**: 0.86 (s, 6 H, 2 CH_3), 1.01 (s, 6 H, 2 CH_3), 2.01 (d, 2 H, CH_2), 2.15 (d, 2 H, CH_2), 2.44 (d, 2 H, CH_2), 2.71 (d, 2 H, CH_2), 3.55 (t, 2 H, CH_2–N), 3.63(s, 3 H, OCH_3), 3.64(s, 3 H, OCH_3), 3.88 (t, 2 H, CH_2–O), 4.90 (s, 1 H, acridinedione-H_9), 5.16 (br. s, 1 H, O–H), 6.70-6.75 (m, 3H, Ar-H). **^{13}C NMR (100 *MHz*, DMSO-d_6) δ (ppm):** 196.25 (2 C=O), 152.12, 148.45 (**C**-OCH_3), 147.03 (**C**-OCH_3), 139.43, 120.20, 111.50, 111.34 (Ar-C), 113.83, 61.36, 55.72, 55.53, 49.84, 46.77, 39.68 (under DMSO-d_6), 32.39, 31.26, 29.61, 26.94. **MS (ESI+) *m/z*:** Expected for $C_{27}H_{35}NO_5$ $[M+H]^{+:}$ 454.25, found 454.



R1=OCH3
R2=OCH3
R3=H

Scheme 1S Illustrate the synthesis of DO8.

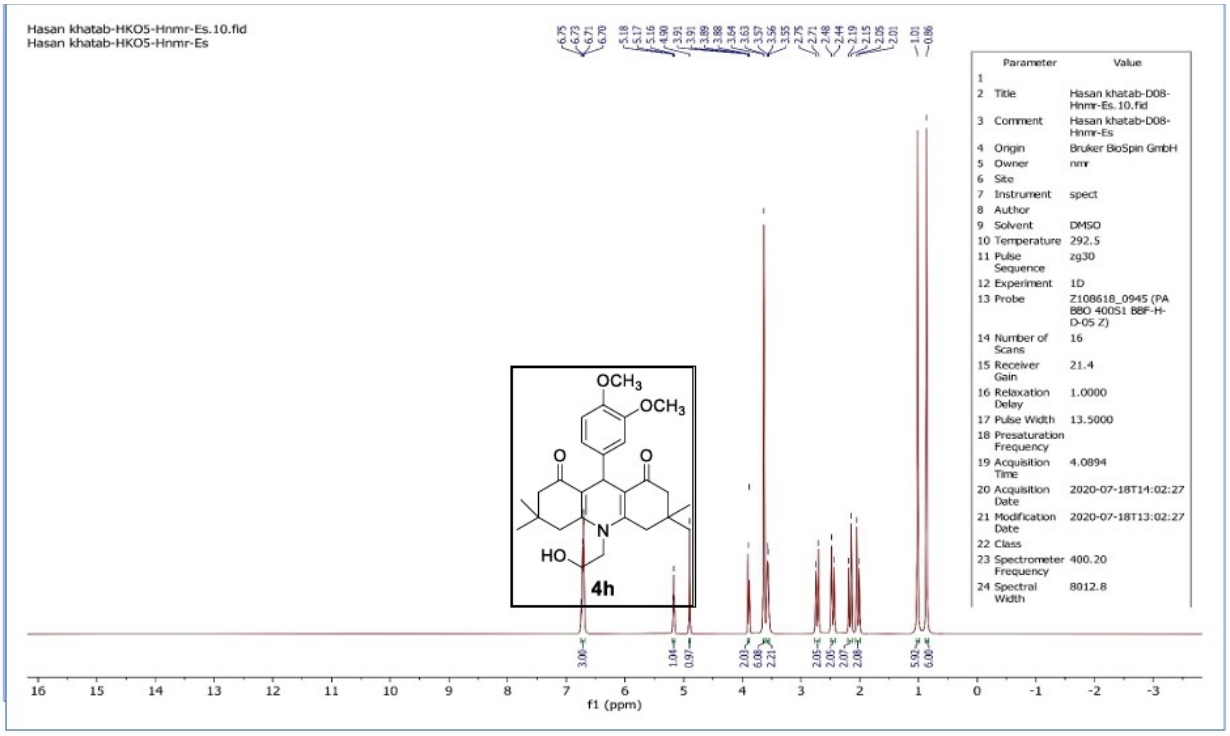
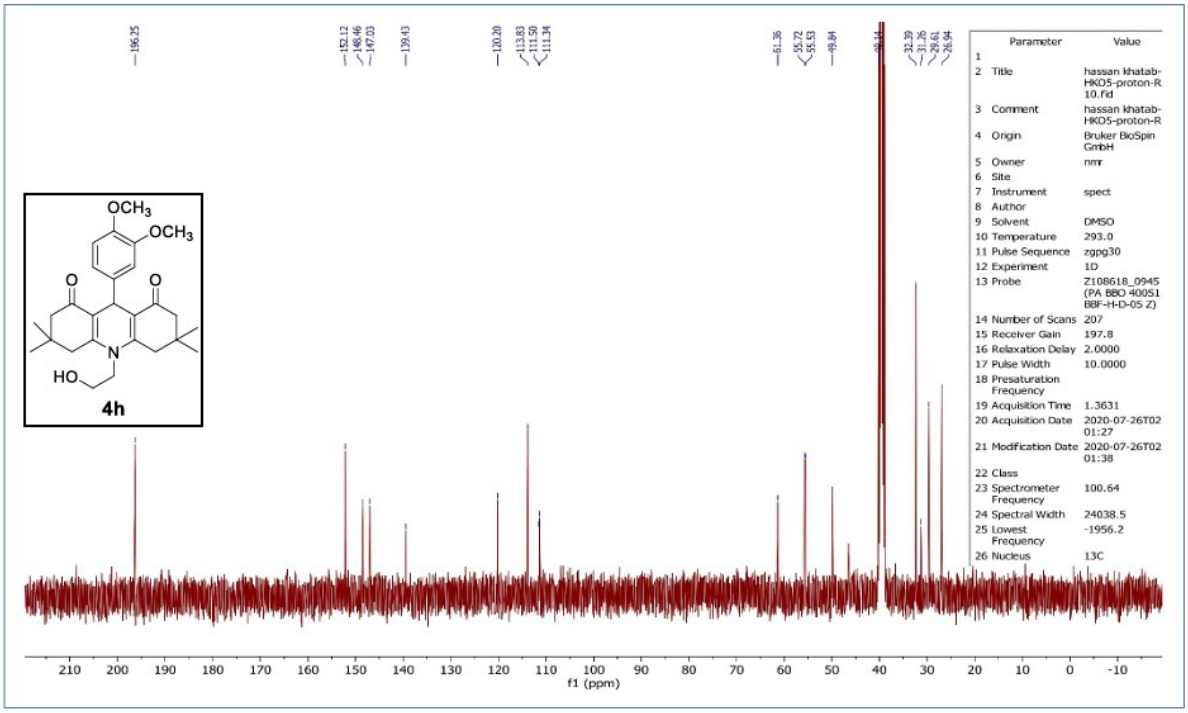


Fig. S1. HNMR-DO8.



^{13} C of DO8

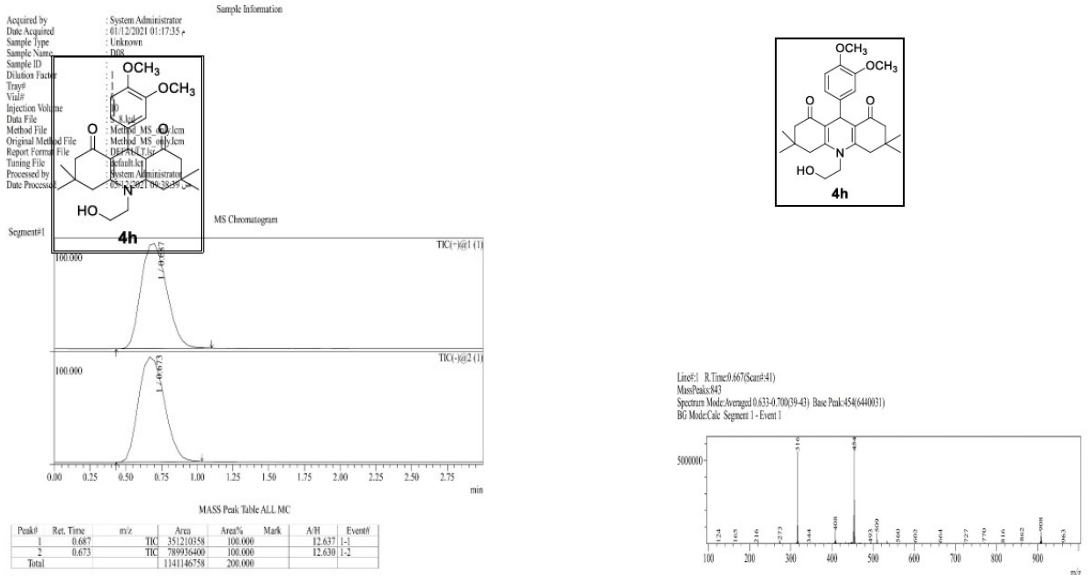


Fig. S2. LC-Mass of DO8.

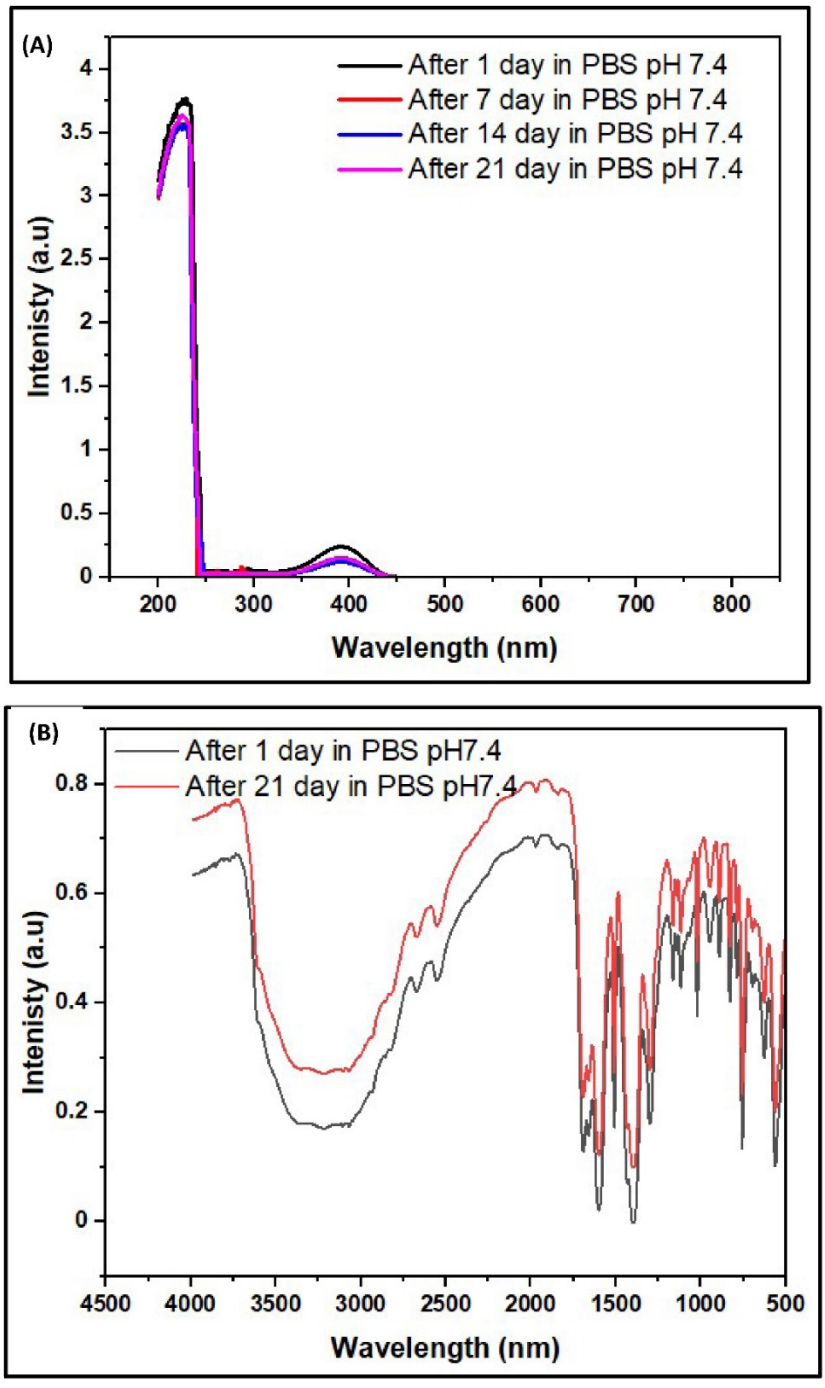


Fig. S3 (A) UV-Vis monitoring for MIL-101 (Fe) MOF –FA@DO8 at PBS pH7.4 for time interval 1-21 days, (B) FTIR of MIL-101 (Fe) MOF –FA@DO8 before and after dispersion in PBS pH 7.4.

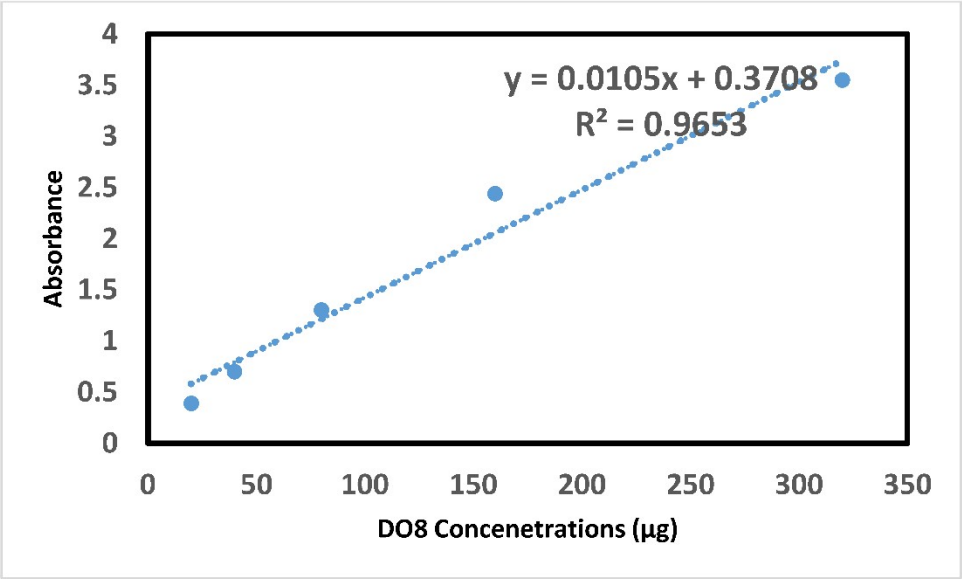


Fig. S4. Calibration curve of DO8 at 370 nm.

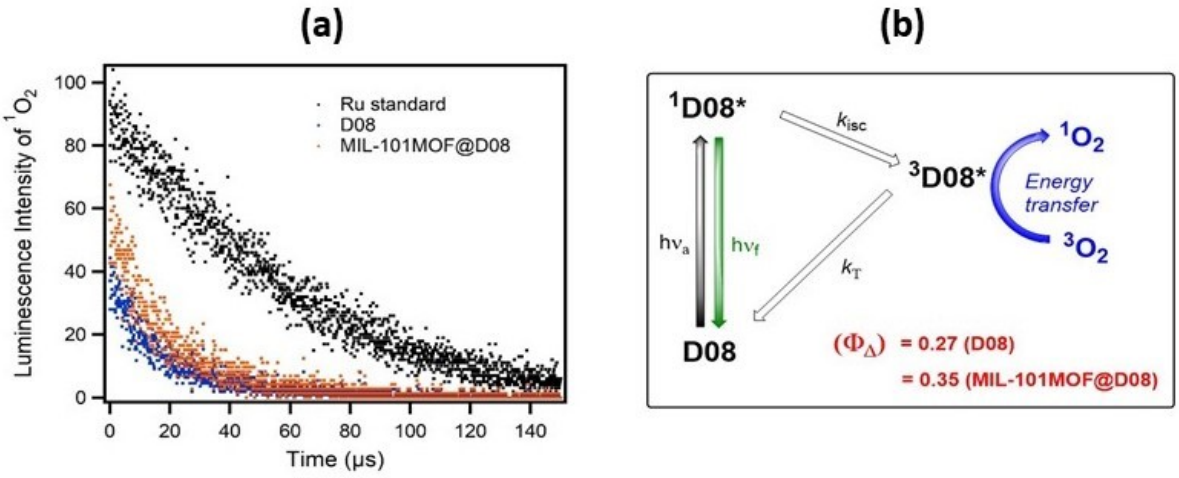


Fig. S5. (a) Decay traces of singlet oxygen phosphorescence at 1275 nm produced by the standard D08 and MIL-101MOF@D08 in acetonitrile; λ_{ex} = 355 nm. (d) Conceptual relation between the relevant energy levels of the D08 photosensitizer, oxygen, and light to generate the singlet oxygen active species.

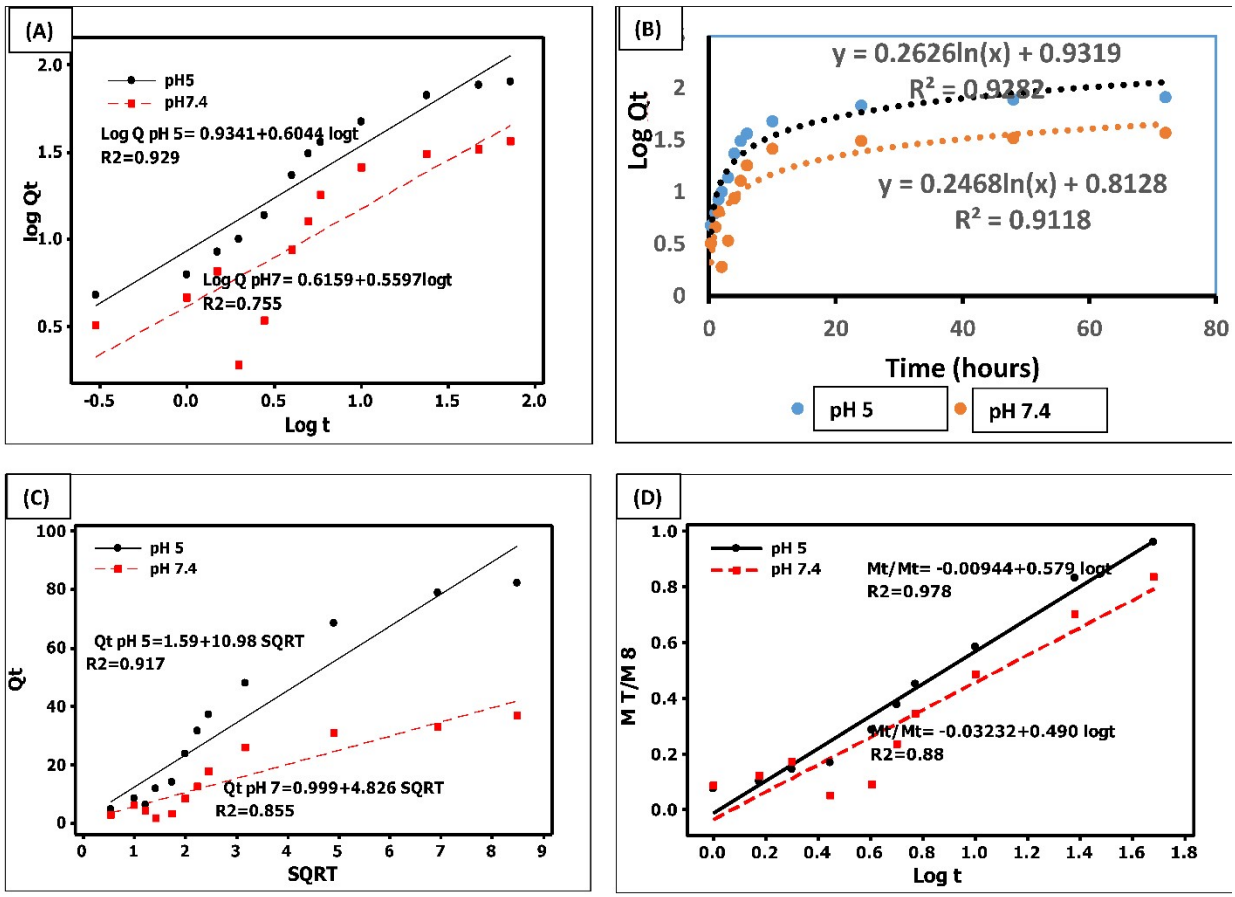


Fig. S6. Kinetic drug release models. (A) zero order, (B) first order, (C) Higuchi's diffusion control model, and (D) Korsmeyer and Peppas model.