

## Aqueous Stable Pd Nanoparticles/Covalent Organic Framework Nanocomposite for Colorimetric Detection and Multicolor Imaging of Cancer Cells

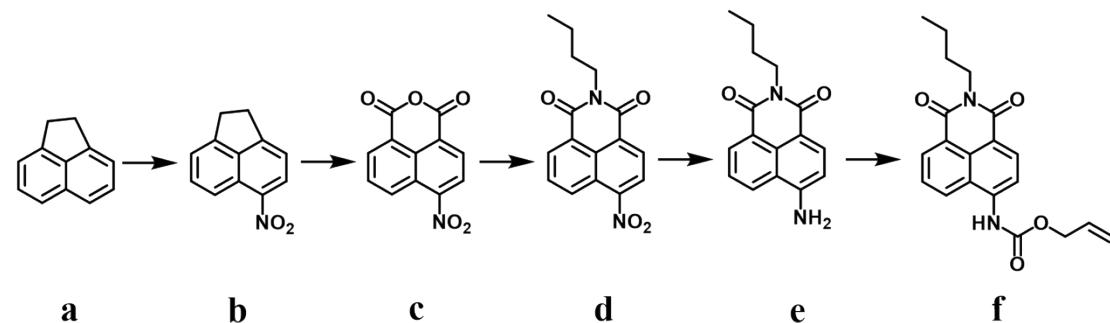
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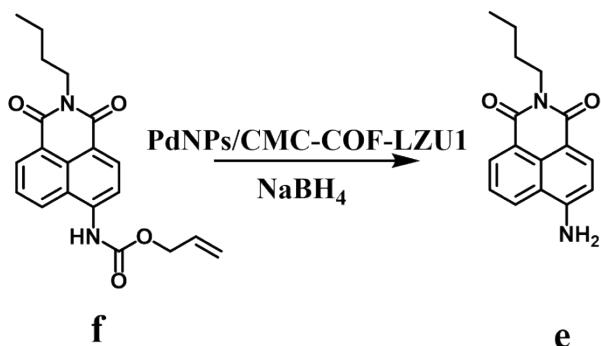
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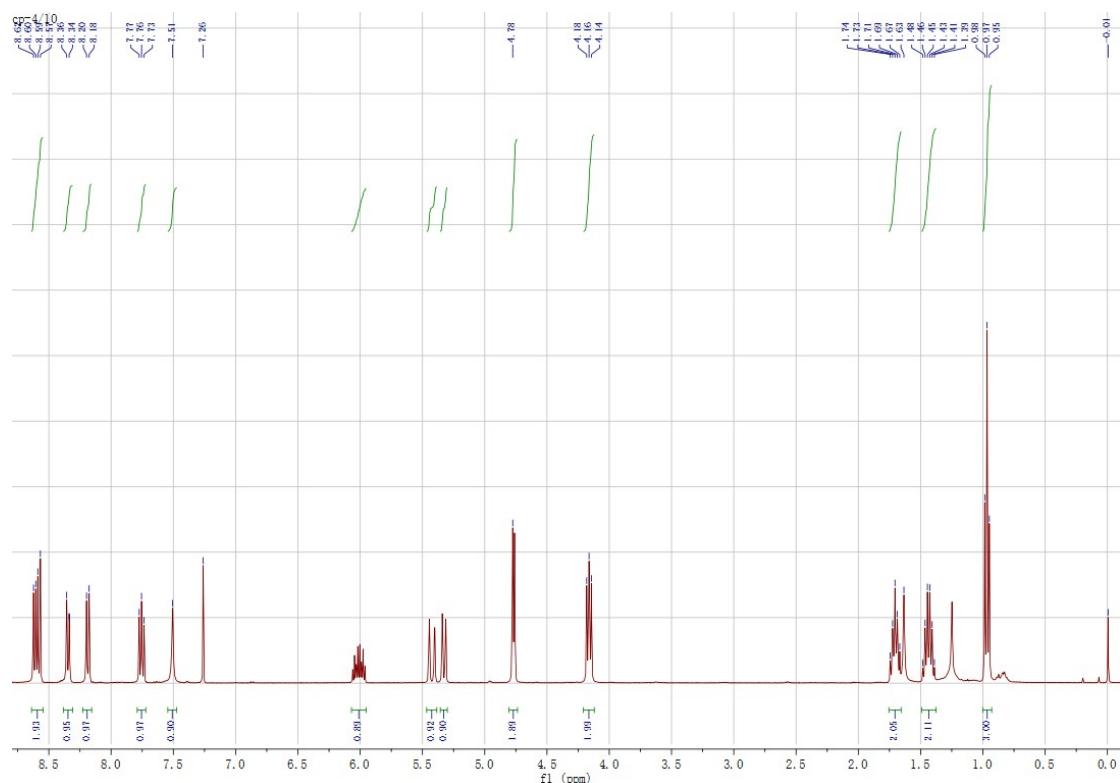


**Figure S1.** The synthesis of compound **f** was according to our previous work. ESI-MS:  $m/z = 353.0112$   $[M + H^+]$ .  $^1\text{H}$  NMR (400 MHz, Chloroform-d)  $\delta$  8.60 (dd,  $J = 14.3, 7.7$  Hz, 2H), 8.36 (d, 1H), 8.19 (d,  $J = 8.4$  Hz, 1H), 7.75 (dd, 1H), 7.51 (s, 1H), 6.01 (dd,  $J = 16.5, 10.4, 5.9$  Hz, 1H), 5.42 (dd,  $J = 17.2, 1.5$  Hz, 1H), 5.33 (dd,  $J = 10.3, 1.2$  Hz, 1H), 4.78 (s, 2H), 4.21 – 4.12 (t, 2H), 1.71 (m,  $J = 7.6$  Hz, 2H), 1.44 (m,  $J = 7.4$  Hz, 2H), 0.97 (t,  $J = 7.3$  Hz, 3H).

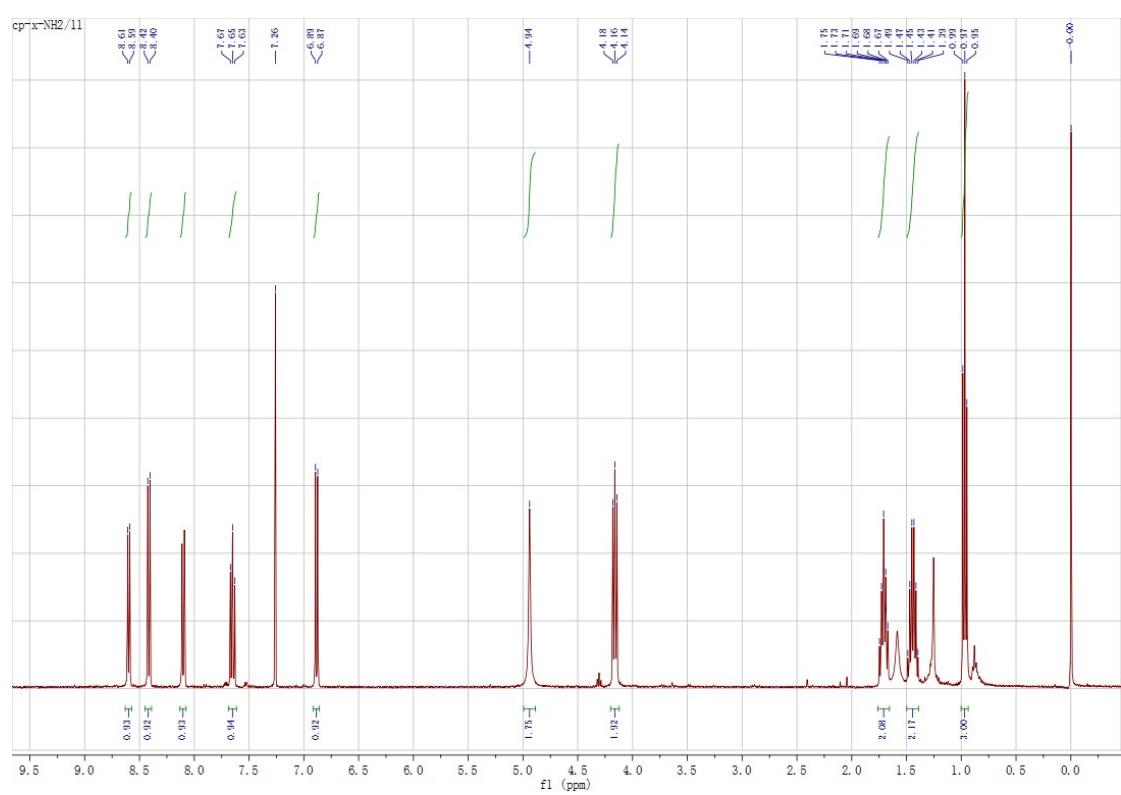


**Figure S2.** 5 mg PdNPs/CMC-COF-LZU1 was added to a mixture of compound **f** (352 mg) with NaBH<sub>4</sub> (0.2 mg) in ethanol (20 mL) and stirred at room temperature. After one minute, the solvent was removed by vacuo, and the crude product was purified by silica gel column chromatography to give 246 mg compound **e** (yield: 92%). ESI-MS: m/z = 269.1879 [M + H<sup>+</sup>].

<sup>1</sup>H NMR (400 MHz, Chloroform-d) δ 8.60 (d, J = 7.2 Hz, 1H), 8.41 (d, J = 8.1 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.66 (t, 1H), 6.88 (d, J = 8.2 Hz, 1H), 4.94 (s, 2H), 4.17 (m, 2H), 1.71 (m, J = 7.6 Hz, 2H), 1.44 (m, J = 14.8, 7.4 Hz, 2H), 0.97 (t, J = 7.4 Hz, 3H).



**Figure S3.** <sup>1</sup>H NMR Spectrum of NNPH in CDCl<sub>3</sub> (400 MHz).



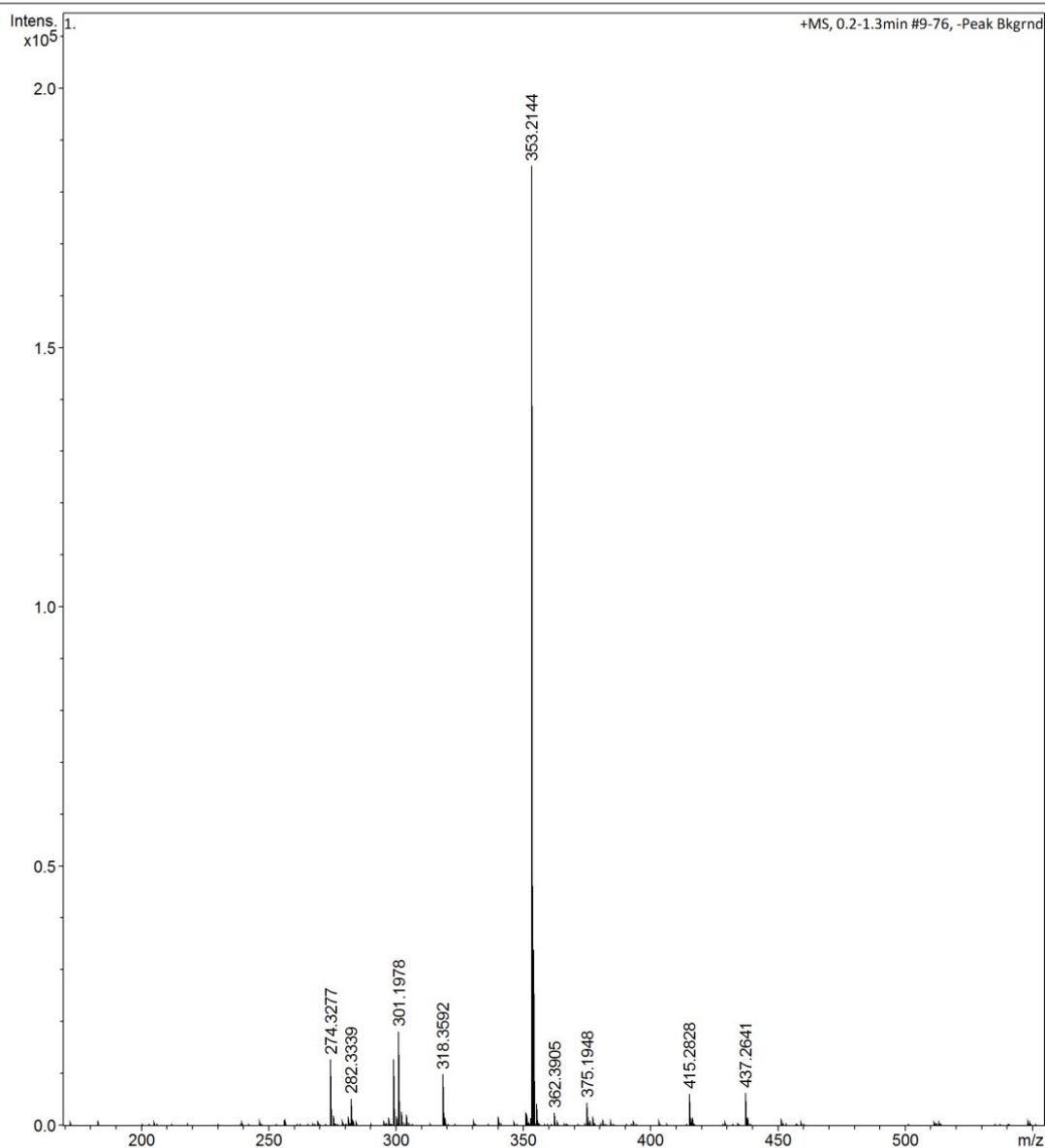
**Figure S4.**  $^1\text{H}$  NMR Spectrum of NPH in  $\text{CDCl}_3$  (400 MHz)

## Generic Display Report

### Analysis Info

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Sample Name SUNPANPAN181210  
Comment

Acquisition Date 12/12/2018 12:52:04 PM  
Operator LZU  
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Bruker Compass DataAnalysis 4.1

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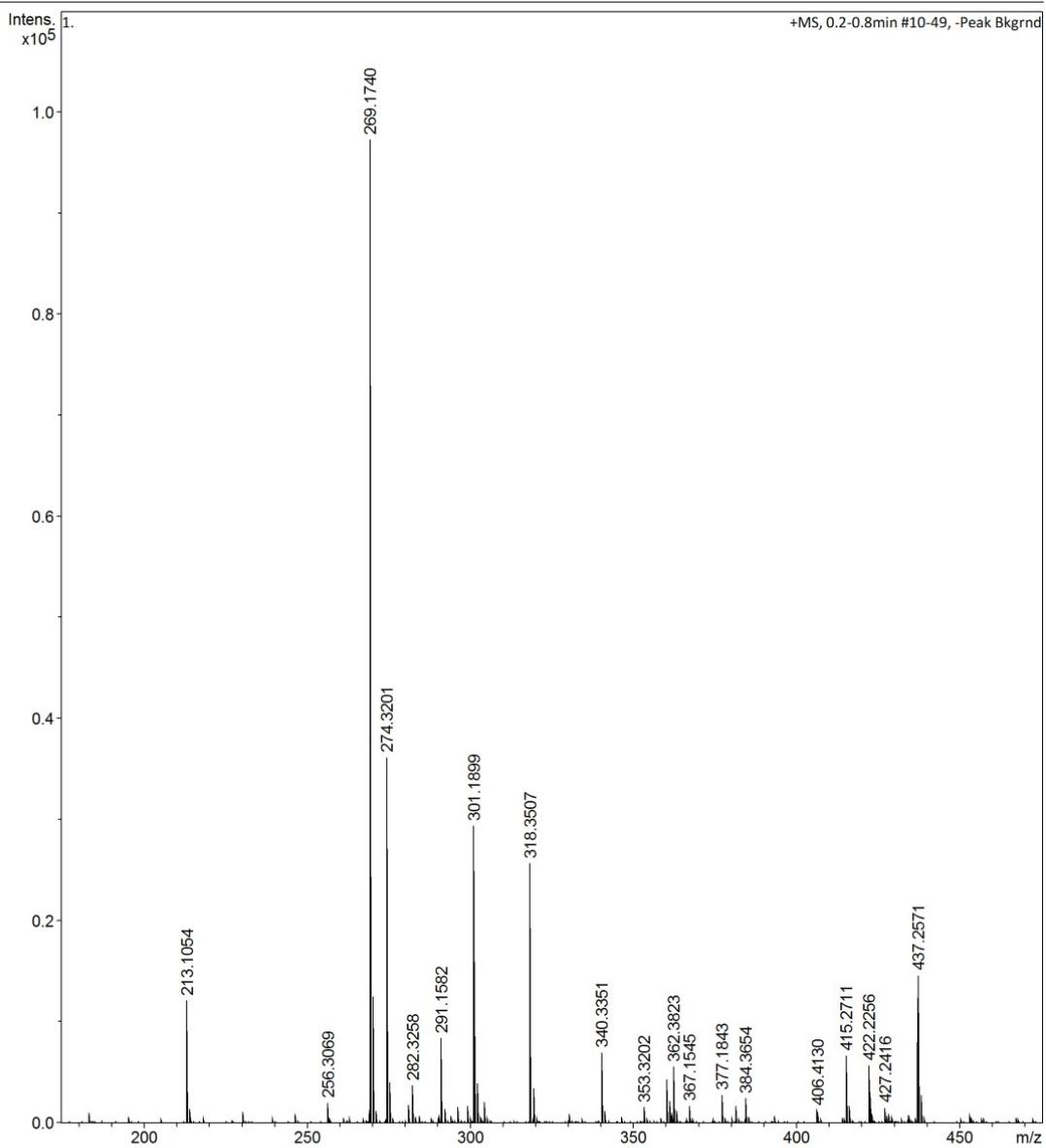
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**Figure S5.** Mass spectrum of NNPH.

## Generic Display Report

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**Figure S6.** Mass spectrum of NPH.

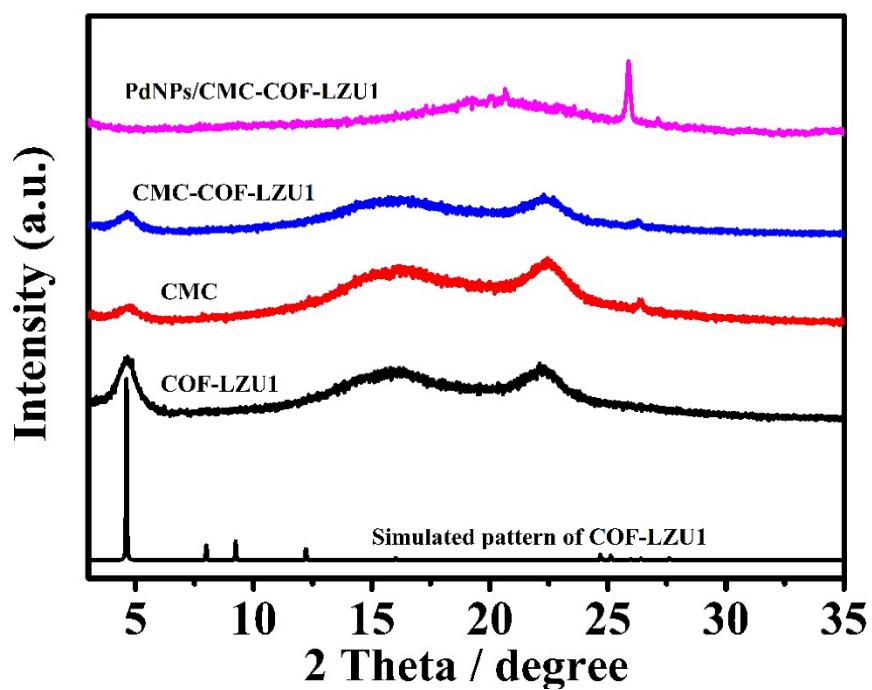
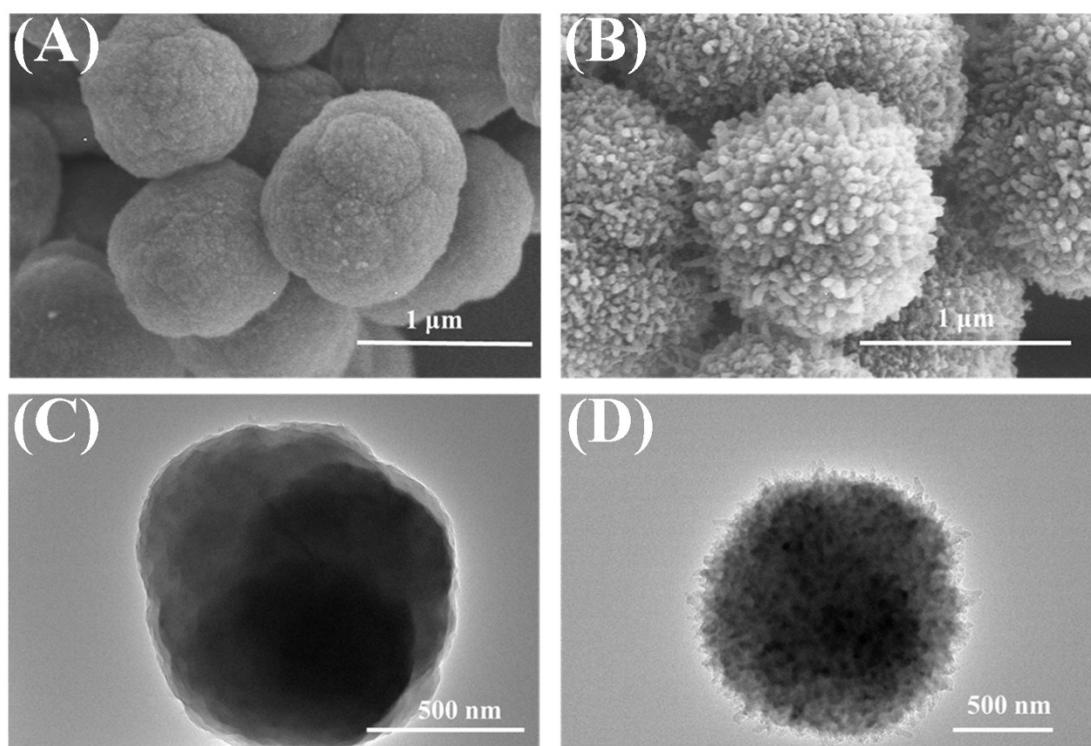
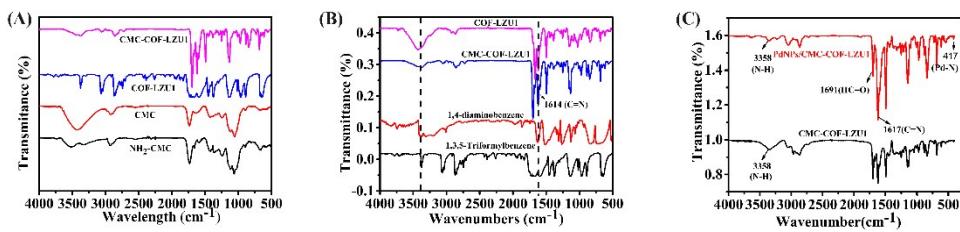
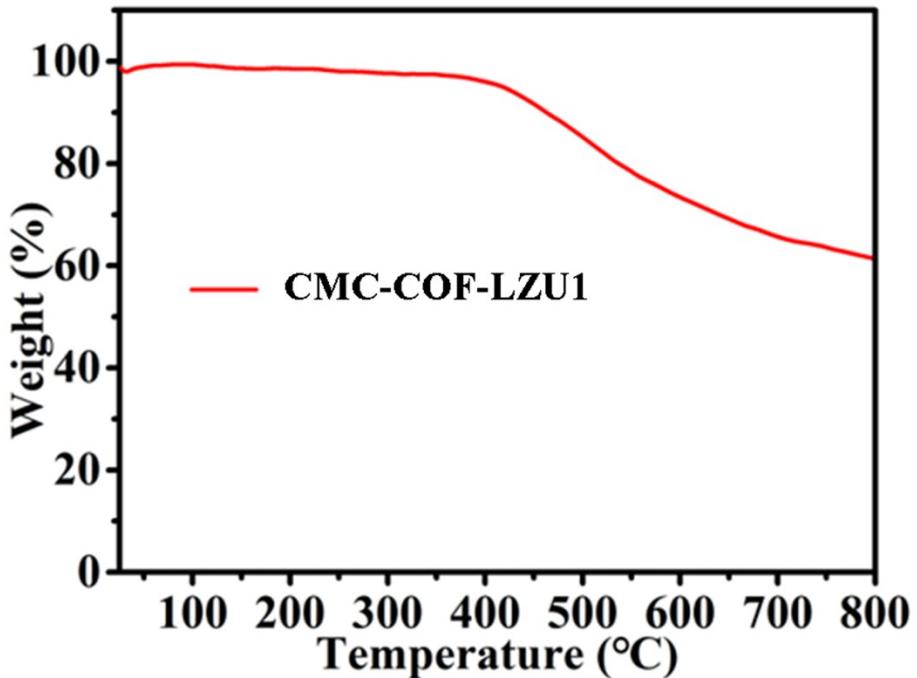


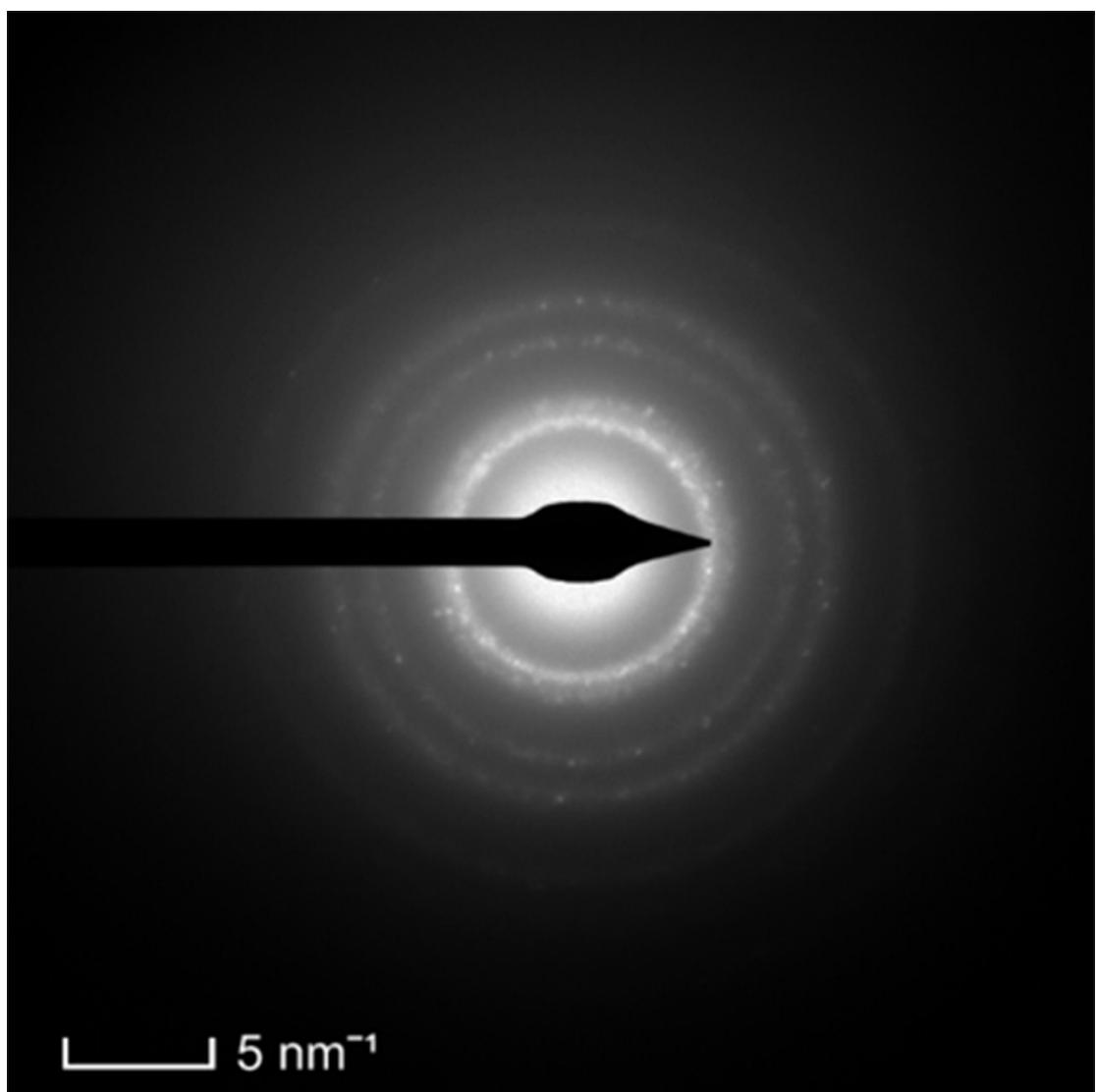
Figure S8. Simulated PXRD pattern of COF-LZU1, CMC, CMC-COF-LZU1 and Pd NPs/CMC-COF-LZU1.



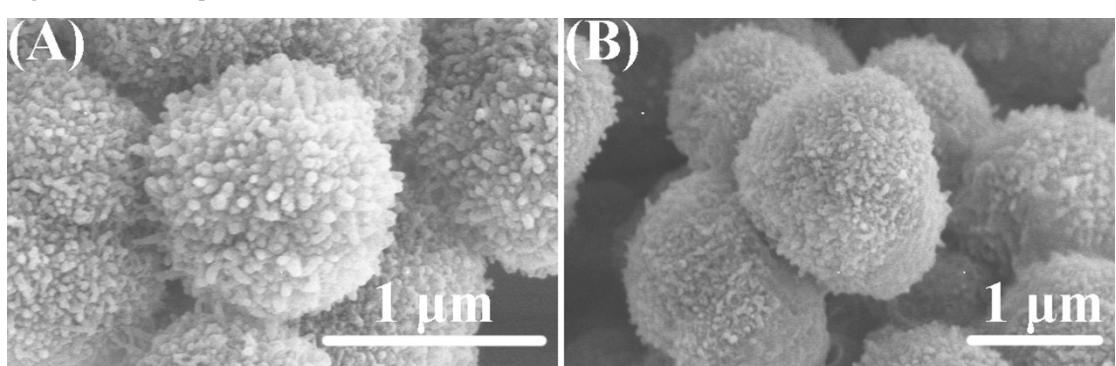
**Figure S9.** (A) FT-IR spectra of CMC(black), NH<sub>2</sub>-CMC (red), COF-LZU1(blue) and CMC-COF-LZU1 (pink). (B) FT-IR spectra of 1,3,5-triformylbenzene(black), p-phenylenediamine(red), CMC-COF-LZU1(blue) and COF-LZU1(pink). (C) FT-IR spectra of CMC-COF-LZU1 (black) and PdNPs/CMC-COF-LZU1 (red).



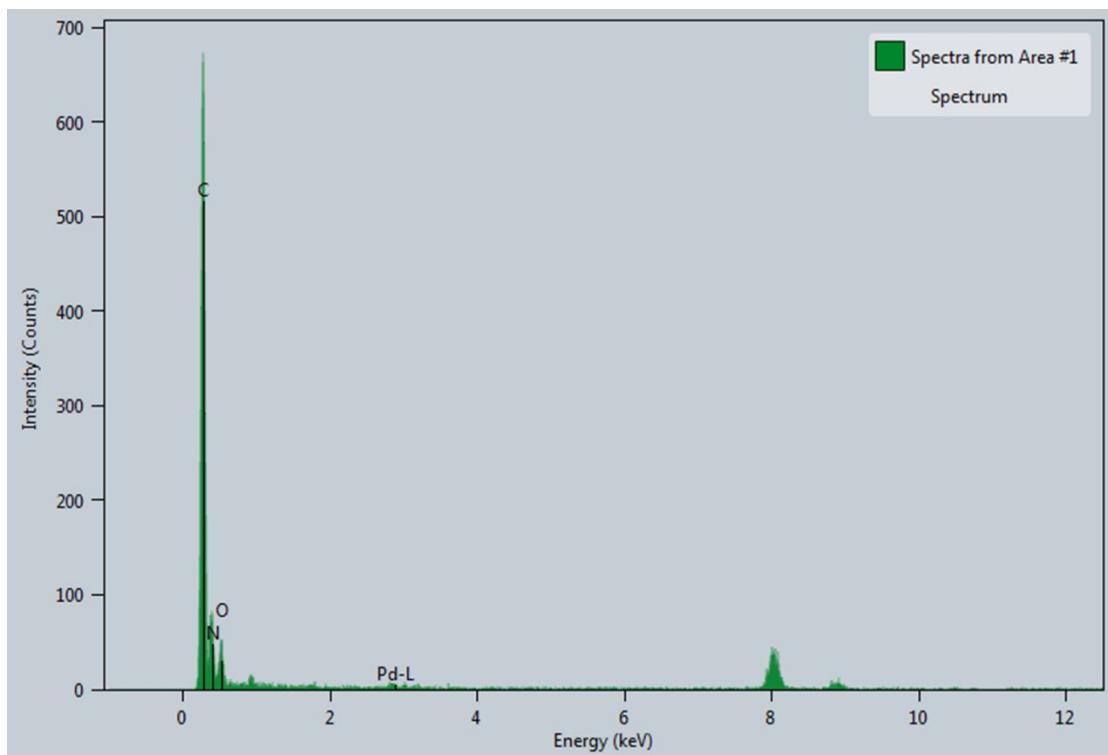
**Figure 10.** TGA curves for CMC-COF-LZU1. No obvious weight losses were observed up to 379.8°C, indicating their good thermostability.



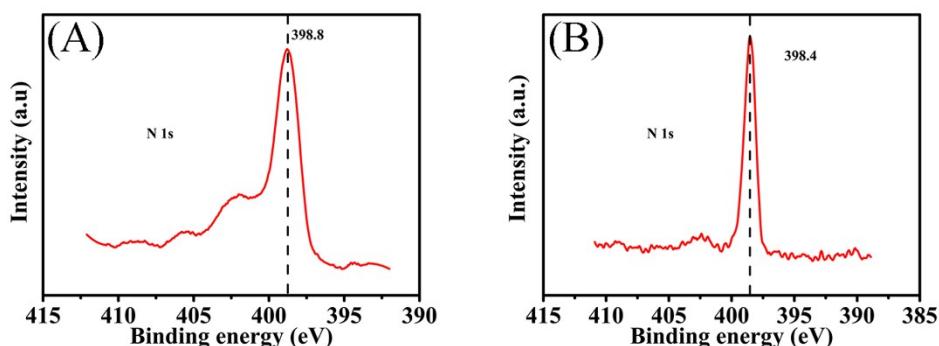
**Figure S11.** SAED pattern of Pd NPs/CMC-COF-LZU1.



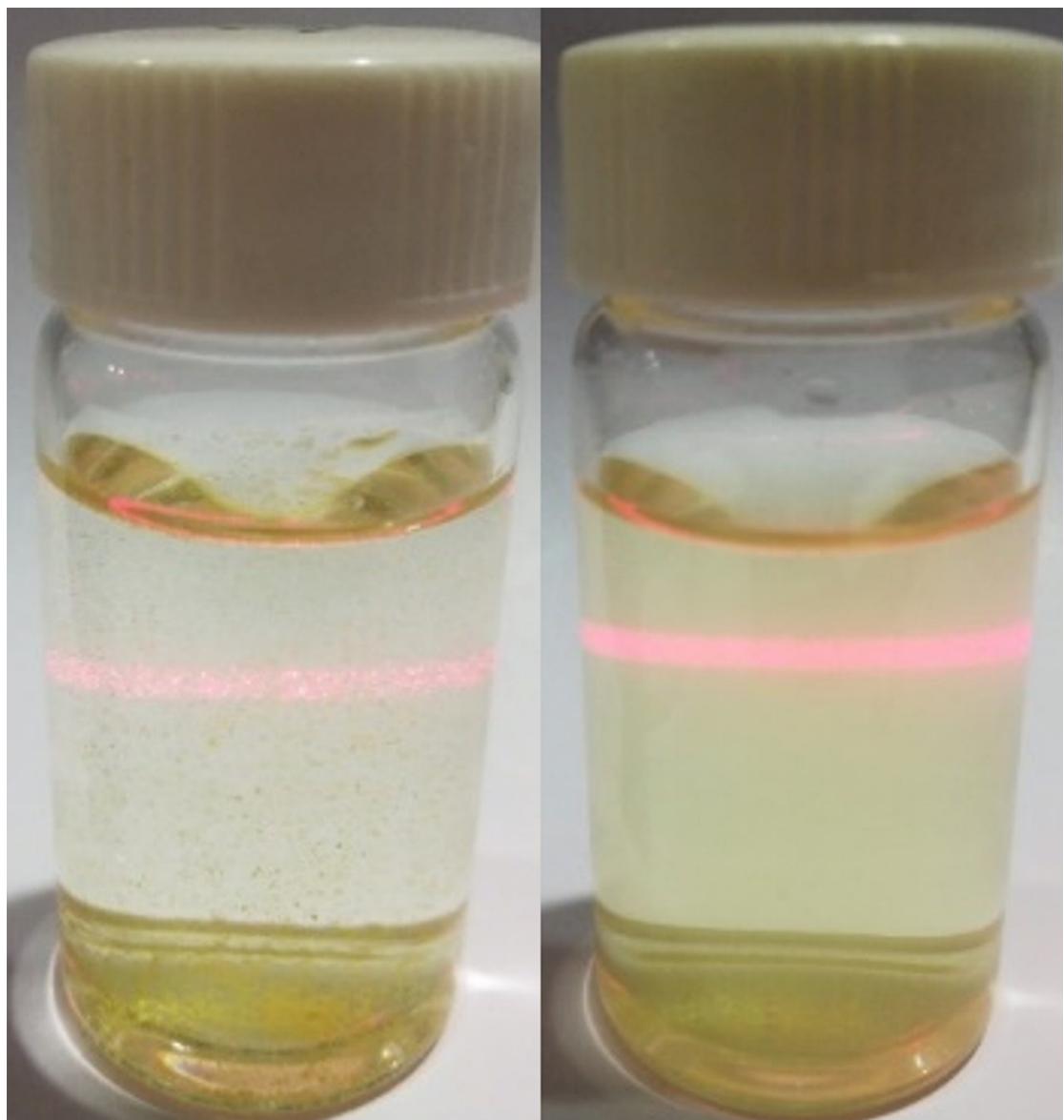
**Figure S12.** SEM image of CMC-COF-LZU1 (a) and PdNPs/CMC-COF-LZU1 (b).



**Figure S13.** EDX image of Pd NPs/CMC-COF-LZU1.



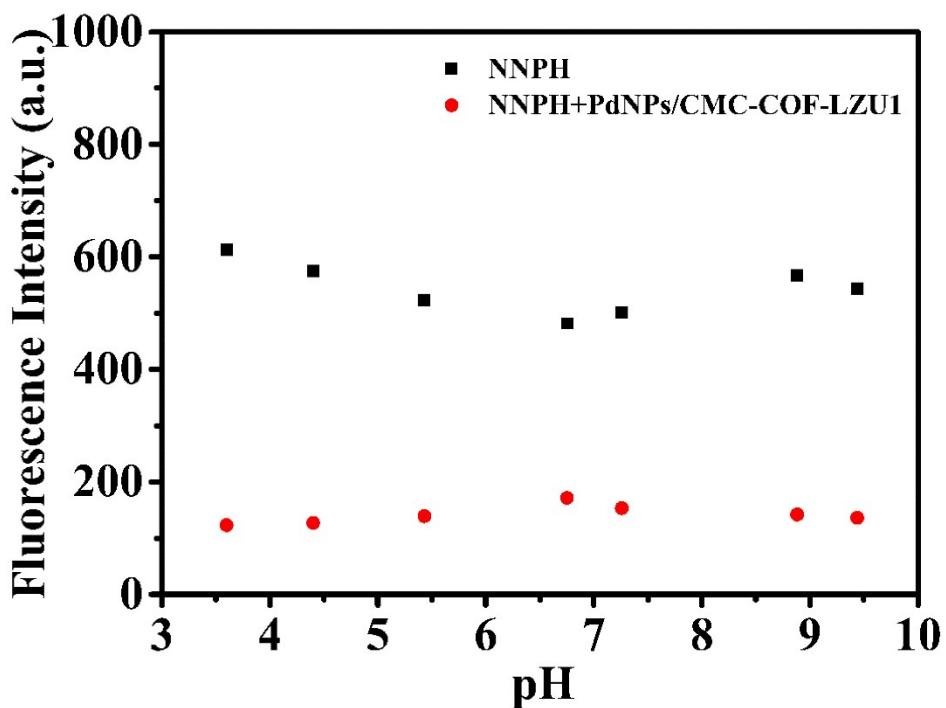
**Figure 14.** High-resolution XPS spectrum of N 1s(A) in PdNPs/CMC-COF-LZU1 and N 1s(B) in CMC-COF-LZU1.



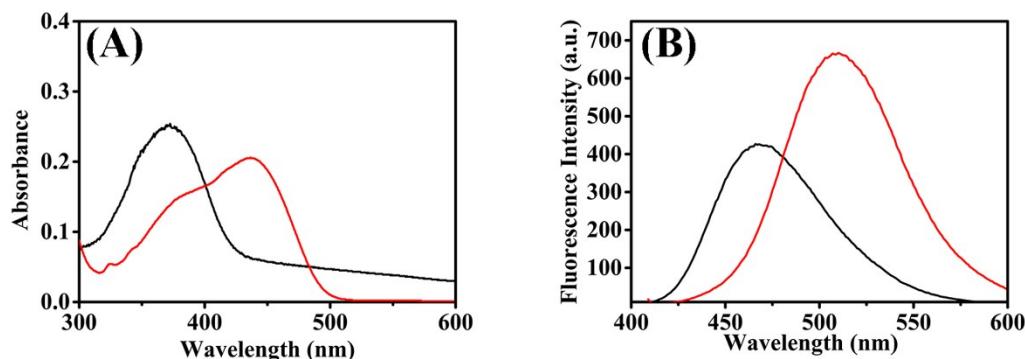
(E)

(F)

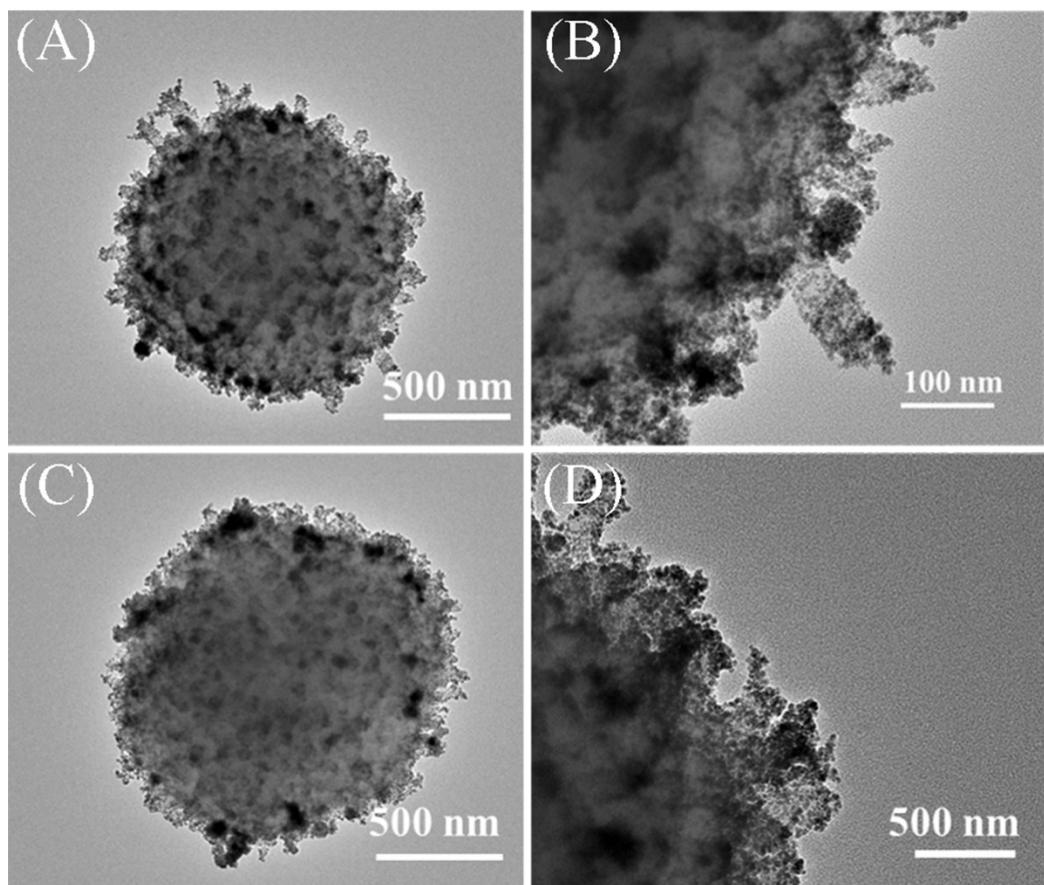
**Figure S15.** Tyndall effect of COF-LZU1(e) and COF-CMC-LZU1(f) in water.



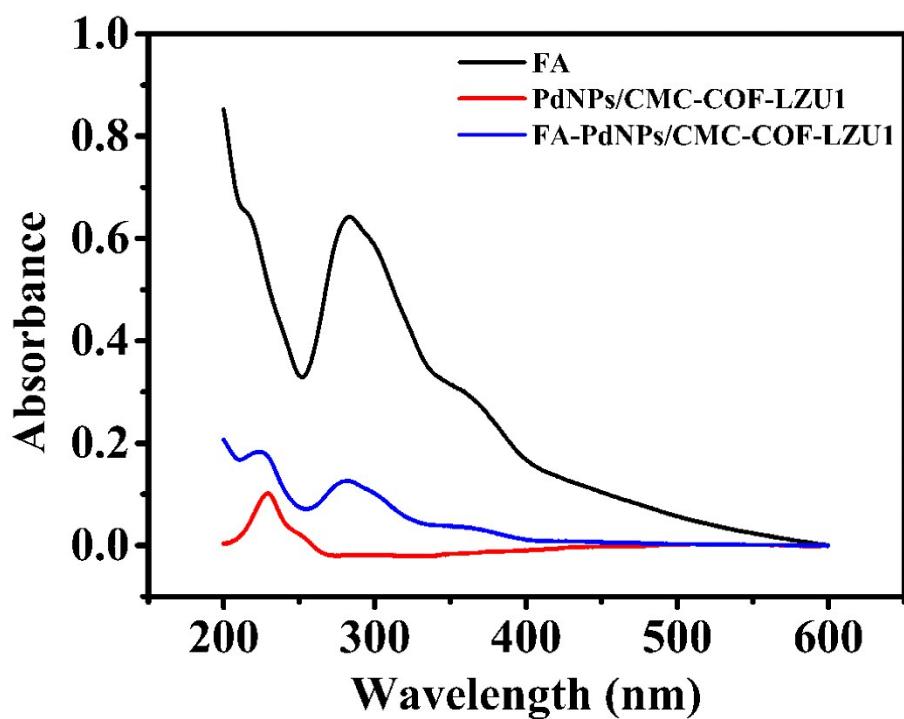
**Figure S16.** Fluorescence intensity of NNPH (40  $\mu$ M) at 460 nm in the solution with different pH values (black). The fluorescence intensity of Pd NPs/CMC-COF-LZU1 at 524 nm (red) as a function of pH under a series of buffer solution incubated with various pH values for 15 minutes. Ex = 403 nm, Slit: 3.0 nm/1.5 nm.



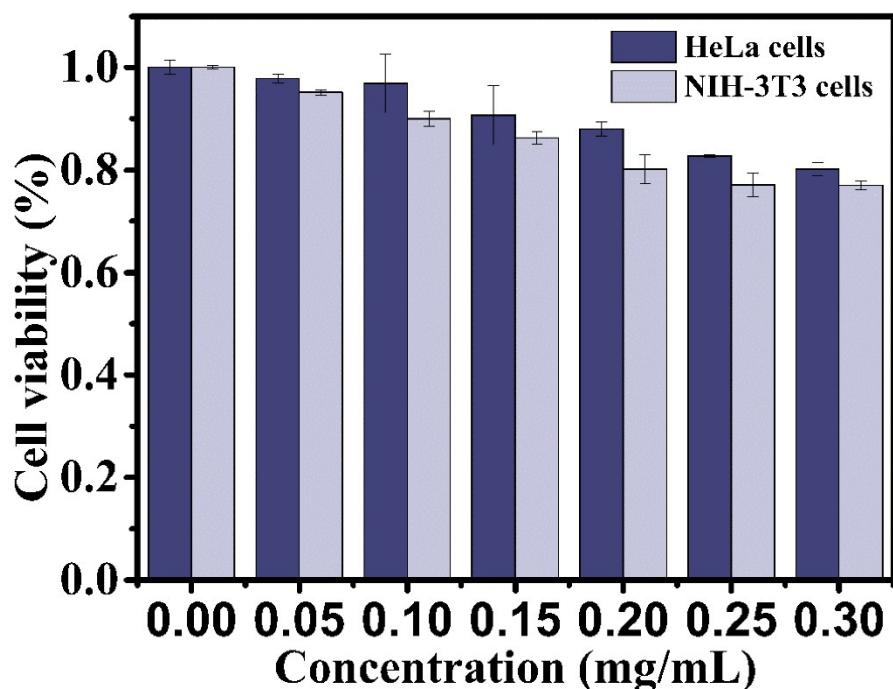
**Figure S17.** (A) Absorbance and (B) Emission spectra of NNPH in EtOH/H<sub>2</sub>O (v/v = 2/7) solution upon addition of PdNPs/CMC-COF-LZU1 in the presence of serum.



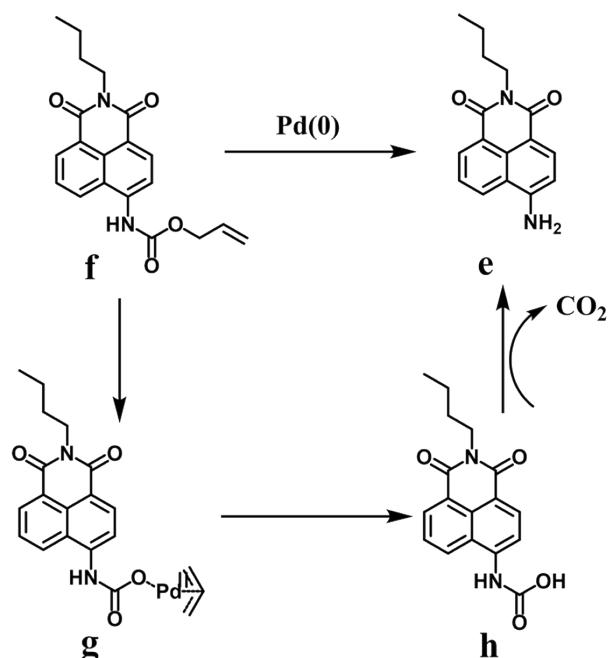
**Figure S18.** (a) TEM and (b) magnified TEM images of Pd NPs/CMC-COF-LZU1; (c) TEM and (d) magnified TEM images of Pd NPs/CMC-COF-LZU1 after catalytic reaction.



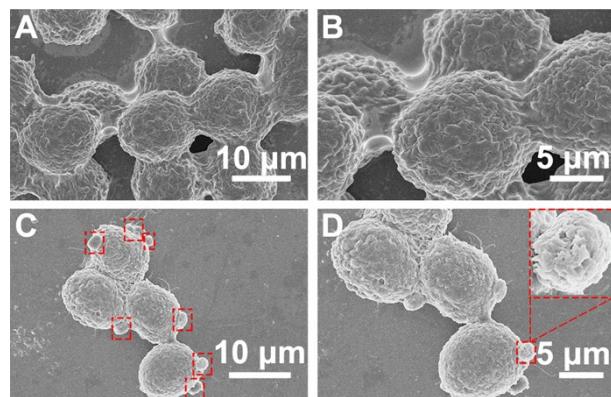
**Figure S19.** UV-vis spectrum of PdNPs/CMC-COF-LZU1 (black), folic acid (red) and FA-PdNPs/CMC-COF-LZU1 (blue).



**Figure S20.** *In vitro* cell viability tests by CCK-8 assay for HeLa cells (black) and NIH-3T3 cells (red) incubated with different concentrations of FA-PdNPs/CMC-COF-LZU1 for 48 h.



**Figure S21.** The mechanism of palladium-catalyzed cleavage of the allyl carbamates group of NNPH(f).



**Figure S22.** (A) The SEM image of HeLa cells. (B) Higher resolution SEM image of HeLa cells. (C) The SEM image FA-Pd NPs/CMC-COFLZU1 nanocomposites interacted with HeLa cells. (D) Higher resolution SEM image of FA-Pd NPs/CMC-COFLZU1 nanocomposites interacted with HeLa cells. The inserted figure is an enlarged view of FA-Pd NPs/CMC-COFLZU1. The red box indicated the FA-Pd NPs/CMC-COFLZU1.