

Supplementary Information for

A water-soluble poly(diphenylacetylene)-based photoredox system for visible-light-driven DNA fragmentation

Authors

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Author Affiliation

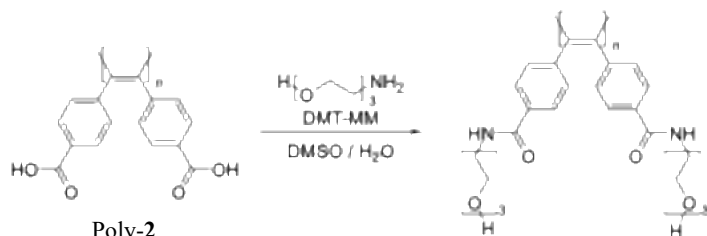
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S1. Experimental Section

S1-1. Synthesis of photoredox polymer catalysts (poly-1)

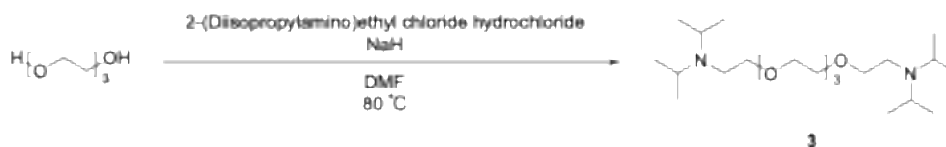


Poly-2
 $M_n = 15 \times 10^4$
 $M_w/M_n = 2.88$

Under a nitrogen atmosphere, poly-2 (106 mg, 0.398 mmol, 1.0 equiv) was placed in a 9 mL screw-cap vial and dissolved completely in a mixed solvent of DMSO/H₂O (5:1, v/v, 4.80 mL). To the resulting solution were added Amino-PEG3 (221 μ L, 1.60 mmol, 4.0 equiv) and DMT-MM (443 mg, 1.60 mmol, 4.0 equiv), and the reaction mixture was stirred at room temperature for 6 h. After completion of the reaction, the solution was diluted with methanol and then reprecipitated into acetonitrile. The resulting precipitate was collected, washed with acetonitrile, and dried under vacuum to afford poly-1 as a yellow fibrous solid. To confirm the introduction of amine groups, a small portion of the polymer was subjected to methyl esterification using TMSD. IR spectroscopic analysis indicated complete conversion of all carboxylic acid groups to the corresponding amide functionalities.

Yield: 183 mg (87%).

S1-2. Synthesis of water-soluble dopant compound 3.



Under a nitrogen atmosphere, triethylene glycol (885 μL , 6.66 mmol, 1.0 equiv), sodium hydride (798 mg, 33.3 mmol, 5.0 equiv), DMF (50.0 mL), and 2-(diisopropylamino)ethyl chloride hydrochloride (2.94 g, 14.7 mmol, 2.2 equiv) were placed in a 300 mL two-necked round-bottom flask. The reaction mixture was stirred at 80 $^\circ\text{C}$ for 3 h. After cooling to room temperature, the reaction mixture was subjected to extraction with toluene/brine. The organic layer was dried over Na_2SO_4 , filtered through cotton, and concentrated under reduced pressure. The residue was further dried under vacuum to afford compound 3 as a pale-yellow viscous liquid. Yield: 2.31 g (86%).

^1H NMR (500 MHz, CDCl_3): δ 3.66–3.61 (m, 8H), 3.43–3.39 (t, 4H), 3.01–2.95 (m, 4H), 2.62–2.60 (t, 4H), 1.01–0.99 (d, 24H).

S2. Supporting Data

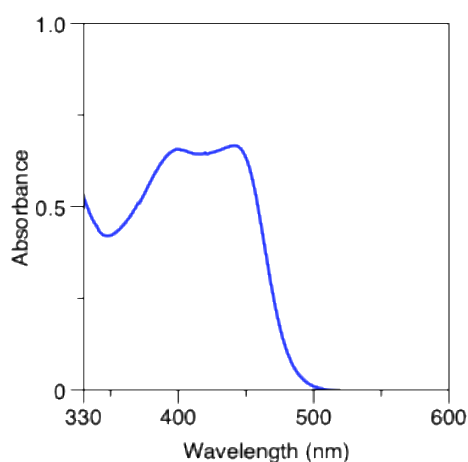


Figure S1. Absorption spectrum of poly-1 in H_2O at 25 $^\circ\text{C}$ ([polymer] = 1.0 mM).

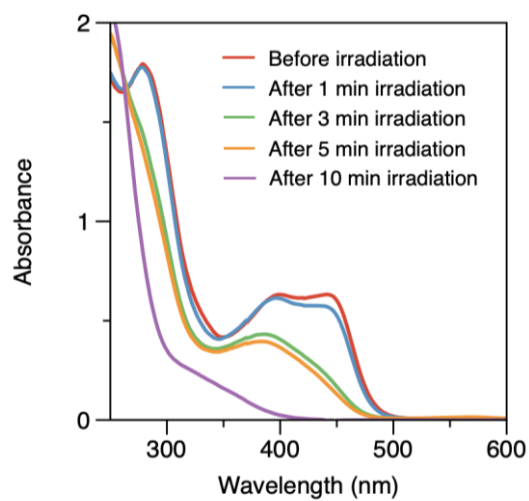


Figure S2. Absorption spectra of poly-**1** with 1.0 vol% dopant **2** in H₂O at 25 °C before and after irradiation ([poly-**1**] = 1 mM).

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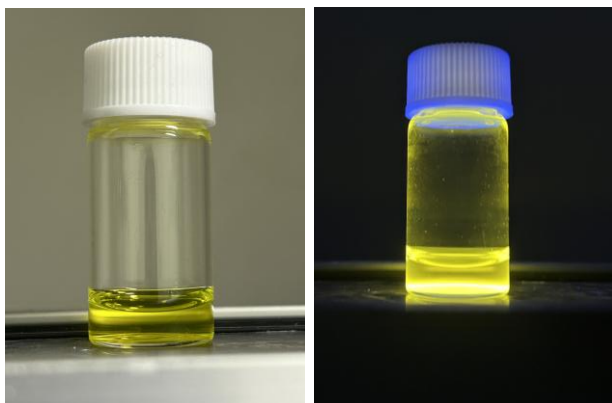


Figure S3. Pictures of fluorescence under illumination with a TLC UV lamp.

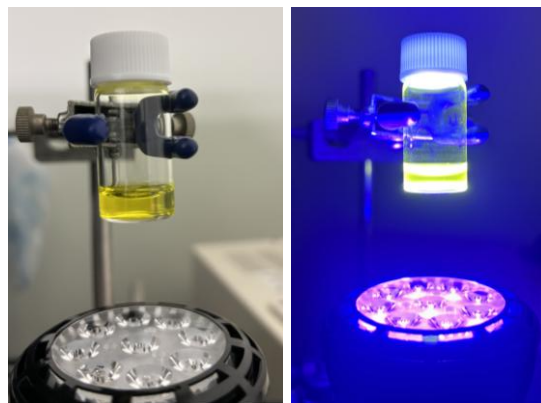


Figure S4. Pictures of fluorescence under illumination with a 425 nm LED.