**Supplementary Information**

**Synthesis and characterization of Single Bond Fullerene Dimer derivatives**

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**Detailed synthesis process and the 1H spectra**

Precursor 1 and the alcohols needed for reaction were purchased from Energy Chemical. Precursor 2a and 2c were prepared using literature methods1.

**Synthesis of** **Precursor 2c**

Compound 1(1.0 equiv.) and n-hexanol (3.0 equiv.) were dissolved in a dry toluene (40 mL) and p-toluenesulfonic acid (0.2 equiv.) was added under nitrogen. The resulting solution was heated to reflux and stirred for 12 hours. Subsequently, the reaction mixture was quenched by the addition of 20 mL distilled water, and then the mixture was extracted by EA. Finally, the combined organic phase was dried by anhydrous MgSO4 and concentrated to obtain a colorless viscous crude product. The residue was purified by column chromatography on silica gel hexane/ethyl acetate (20: 1) to afford yield 84.62%. 1H NMR (600 MHz, CDCl3) δ 8.02 (s, 1H), 8.00 (s, 1H), 7.46 (s, 1H), 7.44 (s, 1H), 4.49 (s, 2H), 4.31 (t, *J* = 6.7 Hz, 2H), 1.75 (dd, *J* = 14.7, 7.0 Hz, 2H), 1.46 – 1.41 (m, 2H), 1.34 (d, *J* = 3.2 Hz, 5H), 0.97 – 0.86 (m, 4H).

**Synthesis of Precursor 3**

A suspension of CoCl2 dppe (16 mg, 0.03 mmol) and Mn (50mg, 0.9 mmol) in 1, 2-dichlorobenzene (40 ml) was stirred for 1 h under Ar atmosphere at 25 ℃. C60 (216 mg, 0.3 mmol), Precursor 2 (2a, 2b or 2c)(110 μL, 0.9 mmol), and H2O (54 uL,3 mmol) were added to the suspension subsequently in glove box. The reaction mixture was stirred at 25 ℃ for 50 h and monitored by TLC. The mixture was filtered through a short florisil pad using 1, 2-dichlorobenzene as an eluent. After concentration, the residue was purified with silica gel chromatography (toluene/hexane = 1/4) to afford 3(3a, 3b or 3c) in good yields.

3a 1H NMR (600 MHz, CDCl3) δ 8.13 (s, 1H), 8.12 (s, 1H), 7.83 (s, 1H), 7.81 (s, 1H), 6.55 (s, 1H), 4.77 (s, 2H), 4.29 - 4.27 (t, *J* = 6.6 Hz, 2H), 1.75 - 1.71 (m, 2H), 1.48 – 1.44 (m, 2H), 0.97 - 0.94 (t, *J* = 7.4 Hz, 3H).

3c 1H NMR (600 MHz, CDCl3) δ 8.13 (s, 1H), 8.12 (s, 1H), 7.83 (s, 1H), 7.82 (s, 1H), 6.55 (s, 1H), 4.76 (s, 2H), 4.29 - 4.27(t, *J* = 6.7 Hz, 2H), 1.77 - 1.70 (m, 3H), 1.76 - 1.71 (m, 2H), 1.42 - 1.40 (m, 2H), 1.31 - 1.30 (m, 4H), 0.87 - 0.88 (t, *J* = 6.8 Hz, 4H).

**Synthesis of fullerene dimers**

Cu(OAc)2 (1.8 mg, 0.01 mmol) catalyst was added to a DMF and 1, 2-dichlorobenzene (1:10, 11 mL) solution of mono-functionalized hydrofullerene 3(3a,3b or 3c) (87mg, 0.1 mmol) at room temperature under air atmosphere. The reaction mixture was stirred at room temperature for 4 hours. The reaction was monitored by TLC. The mixture was subjected directly with silica gel chromatography (toluene/hexane = 1/1). Toluene and hexane containing 4(4a, 4b or 4c) were evaporated under water bath lower than 60℃, and the residue was washed with acetone to afford 4 above 90% yield (80-90 mg).

4b 1H NMR (600 MHz, CDCl3) δ 8.10 - 7.97 (m, 2H), 7.68 - 7.66 (m, 2H), 7.27 - 7.23 (m, 2H), 7.18 - 7.16 (m, 2H), 4.75 - 4.66 (m, 2H), 4.53 -4.47 (m, 2H), 4.33 - 4.29 (t, *J* = 6.7 Hz, 4H), 2.40 - 2.38 (s, 3H), 1.81 - 1.75 (m, 3H), 1.50 - 1.45 (m, 6H), 0.95 - 0.90 (t, *J* = 7.0 Hz, 3H).

4c 1H NMR (600 MHz, CDCl3) δ 8.10 - 7.97 (m, 2H), 7.68 - 7.66 (m, 2H), 7.27 - 7.23 (m, 2H), 7.18 - 7.16 (m, 2H), 4.75 - 4.66 (m, 2H), 4.53 -4.47 (m, 2H), 4.33 - 4.29 (t, *J* = 6.7 Hz, 4H), 2.40 - 2.38 (s, 3H), 1.81 - 1.75 (m, 3H), 1.50 - 1.45 (m, 4H), 1.40 - 1.32 (m, 6H), 0.95 - 0.90 (t, *J* = 7.0 Hz, 3H).

**References:**

1. Chai, X., Zhang, J., Hu, H., Yu, S., Sun, Q., Dan, Z., Jiang, Y., and Wu, Q.: Design, synthesis, and biological evaluation of novel triazole derivatives as inhibitors of cytochrome P450 14alpha-demethylase. Eur. J. Med. Chem. **44**, 1913-1920 (2009).