Electronic supplementary information

Benzothiadiazole-ethynylthiophenezoic acid as an acceptor of photosensitizer for efficient organic dye-sensitized solar cells

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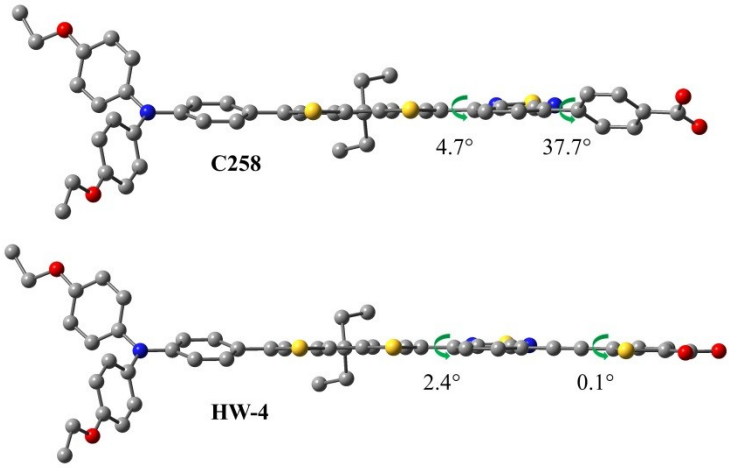

Fig. S1 Optimized geometries of **C258** and **HW-4** in THF. Carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). The hydrogen atoms are not shown.

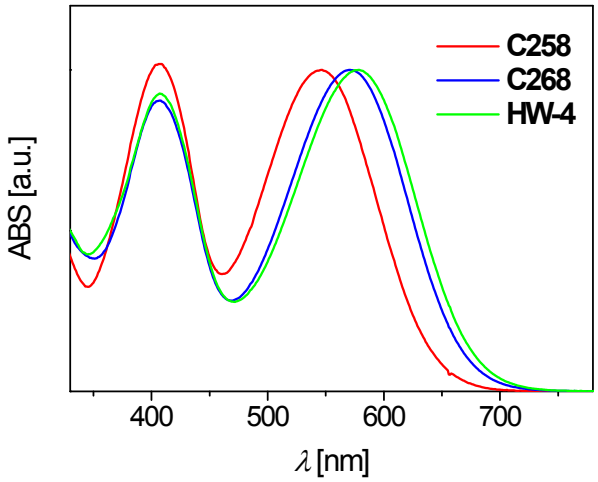

Fig. S2 Normalized electronic absorption spectra of **C258**, **C268** and **HW-4** dissolved in THF (10 μM). The datum of **C268** is derived from the ref. 24.

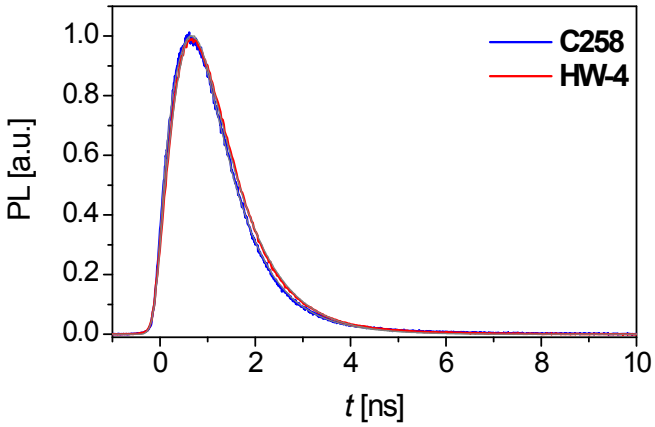

Fig. S3 Time-correlated photoluminescences (PL) of dye dissolved in THF solvent.

Excitation wavelength: 482 nm; Detection wavelength: 750 nm.

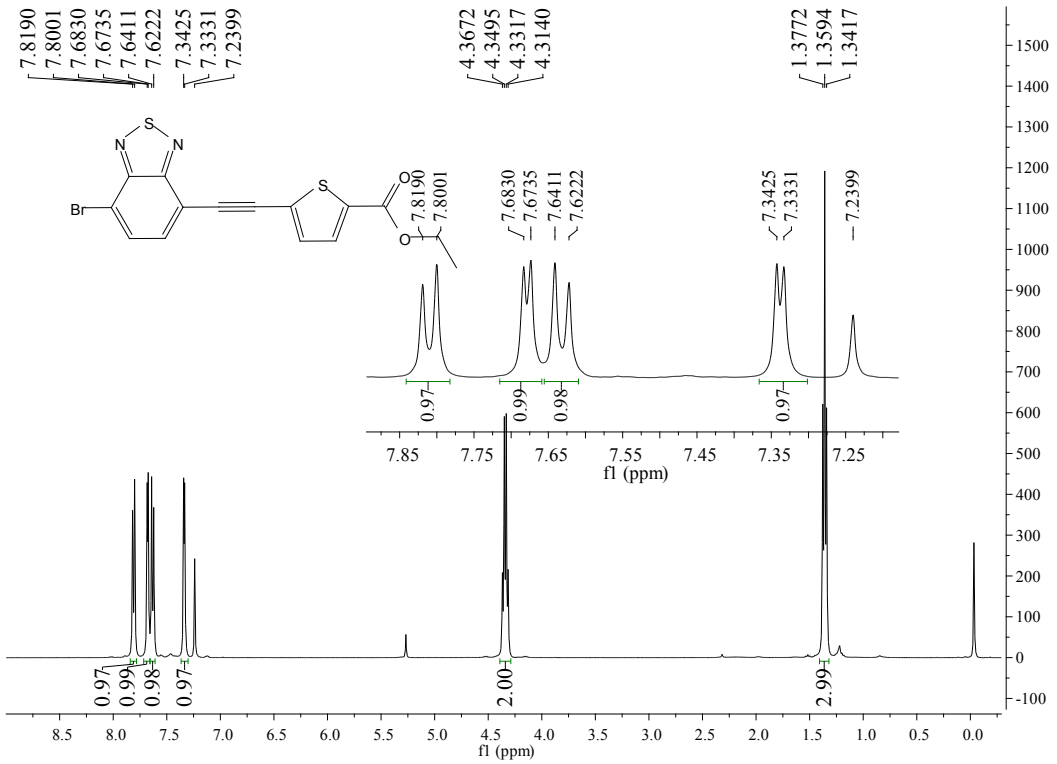

Fig. S4 The ^{1}H NMR (400 MHz) of **2** in $CDCl_3$.

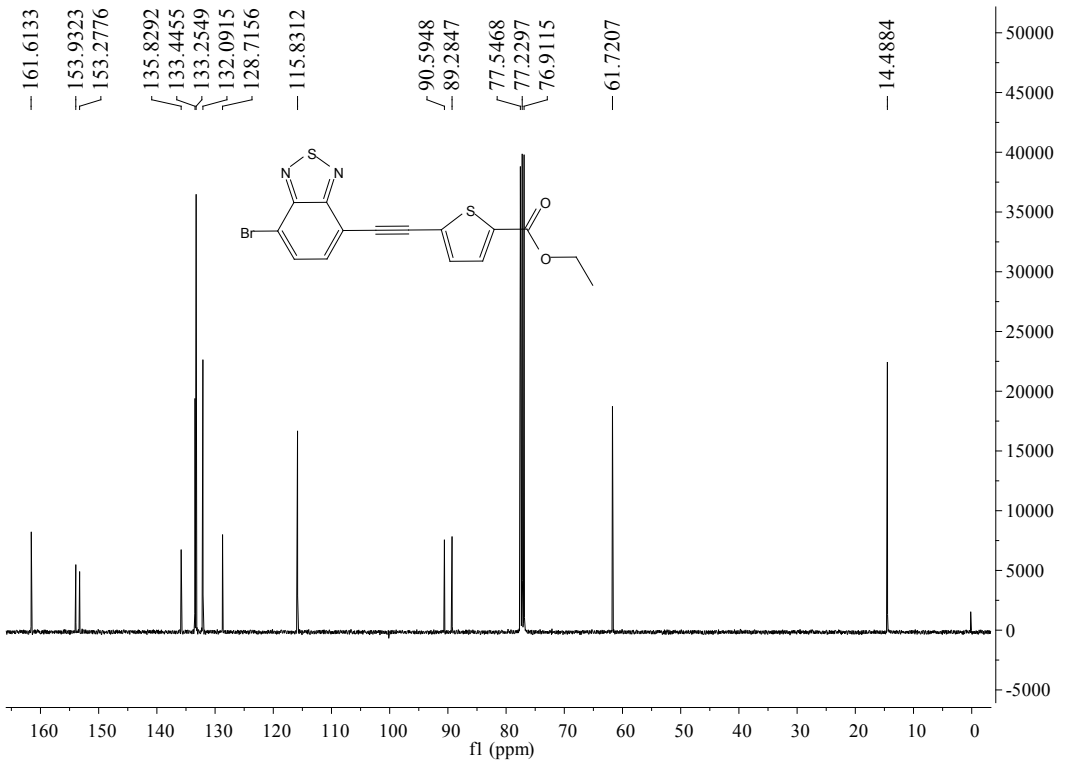

Fig. S5 The ^{13}C NMR (100 MHz) of **2** in $CDCl_3$.

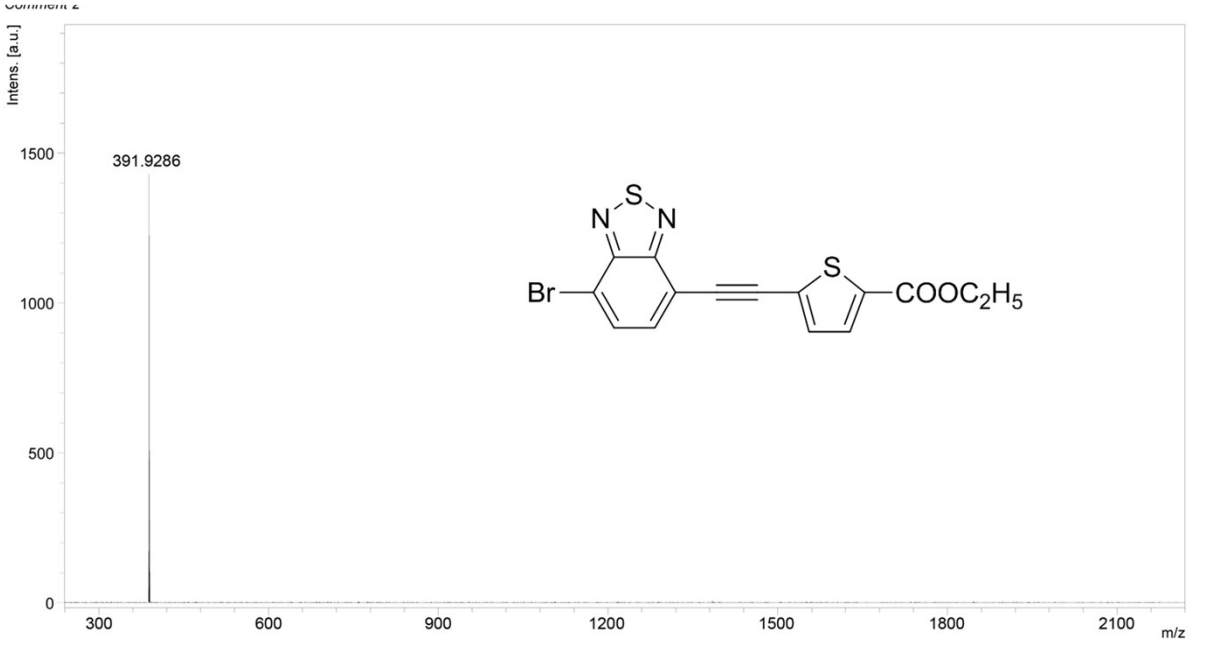

Fig. S6 The high-resolution mass spectrum of **2**.

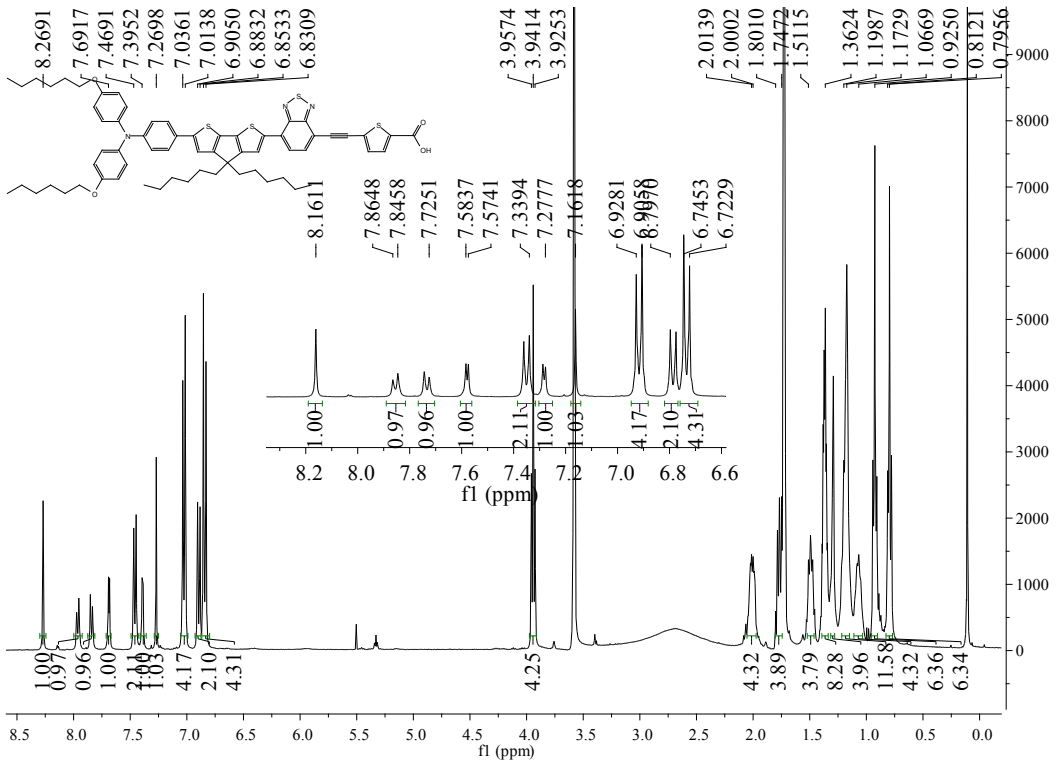

Fig. S7 ^{1}H NMR (400 MHz) of **HW-4** in THF-d_8.

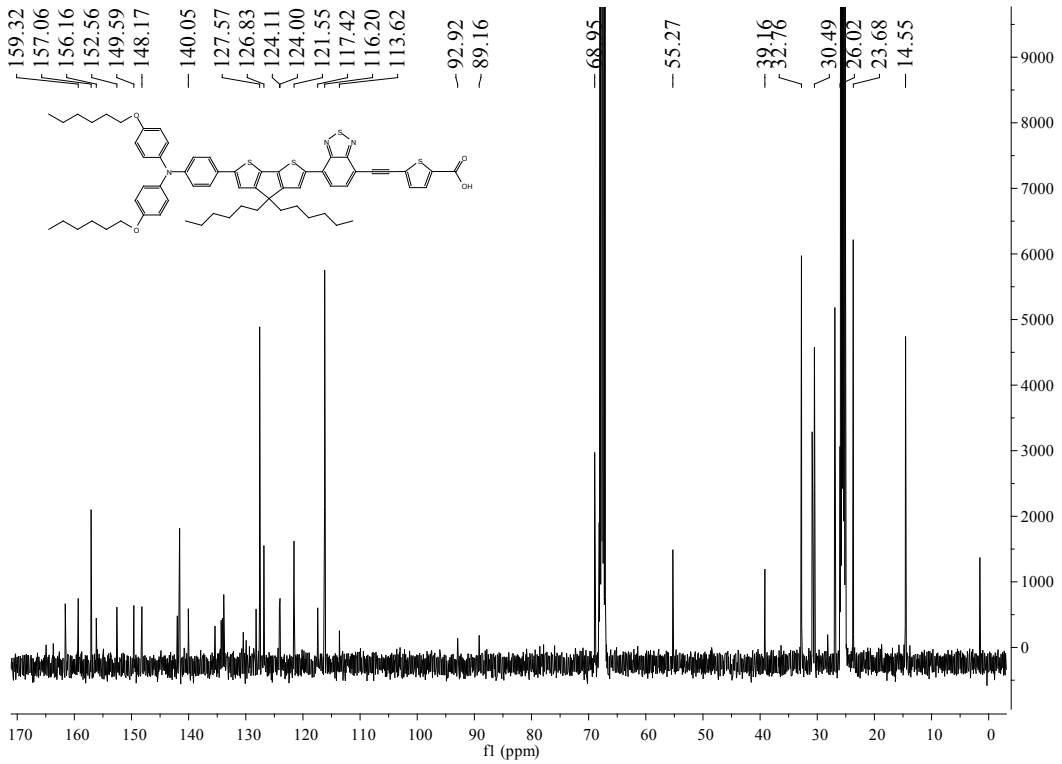

Fig. S8 ^{1}C NMR (100 MHz) of **HW-4** in THF-d_8.

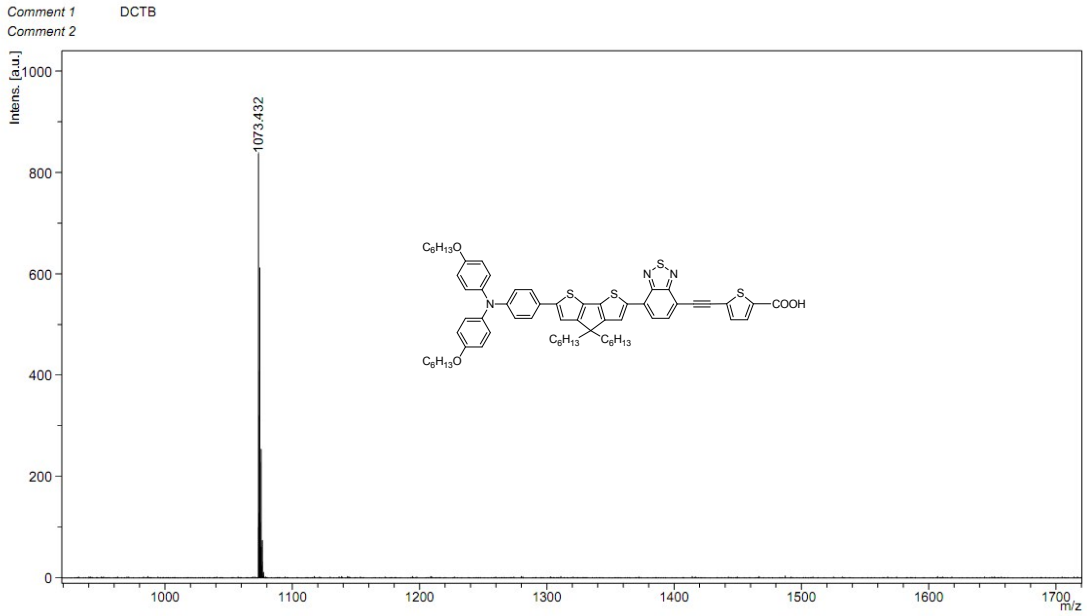

Fig.S9 The high-resolution mass spectrum of **HW-4**.

Dye Loading Measurement

A newly prepared dye solution (12 g) was divided into three equal shares, which were coded as solutions 1, 2, and 3. A 5-μm-thick translucent titania film and a sheet of FTO glass of the same size were respectively immersed into solutions 1 and 2 for overnight. Then, the TiO_2 film was taken out from solution 1 and washed with acetonitrile carefully to remove the weakly absorbed dyes. The acetonitrile solution was combined with the mother dye solution to have a total weight of 5 g. Solution 2 with the bare FTO glass was treated with the same procedure as solution 1. In addition, 1 g of acetonitrile was added into solution 3. Finally, 3 g of THF was added to each bottle of combined solutions to make sure that the dyes were completely dissolved. Furthermore, UV−Vis spectroscopies of these three solutions were recorded. The dye-loading amount (c_m) can be calculated via the following equation:

$$c_m = \frac{(A_2 - A_1) \times c \times V}{A_3 \times S \times l},$$

where A_1, A_2, and A_3 are the absorbances of final solutions 1, 2, and 3 at the same wavelength; c and V are the concentration and volume of fresh solutions 1, 2, and 3; S and l are the area and thickness of a titania film.