Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Novel D-π-A Type Near-infrared Fluorescent Probes for the Detection of $A\beta_{40}$ Aggregates

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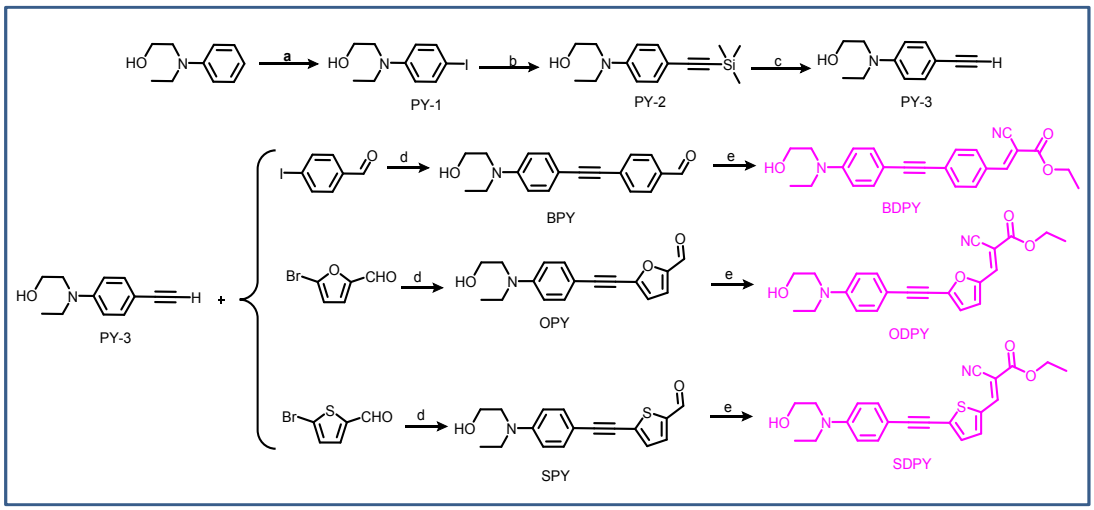
Contents

1. Synthesis details of probes



Scheme S1 a: iodine, dioxane, pyridine; b: CuI, $Pd(PPh_3)_2Cl_2$, N,N-diisopropylethylamine, tetrahydrofuran; c: tetra-n-butylammonium fluoride, H_2O; d: CuI, $Pd(PPh_3)_4$, triethanolamine, tetrahydrofuran, e: dichloromethane, piperidine, cyanoacetic acid ethyl ester.

2. Additional images and Figures

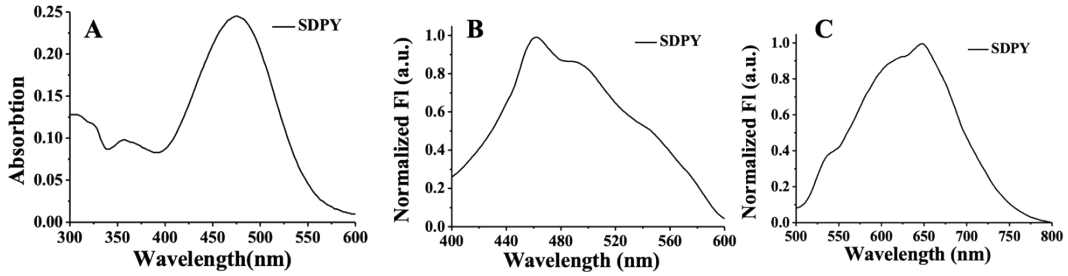


Fig. S1 The photophysical spectra of **SDPY** in organic solvent EtOH. (A): Uv-Vis absorption of **SDPY**; (B) and (C): excitation and emission spectra of **SDPY,** respectively.

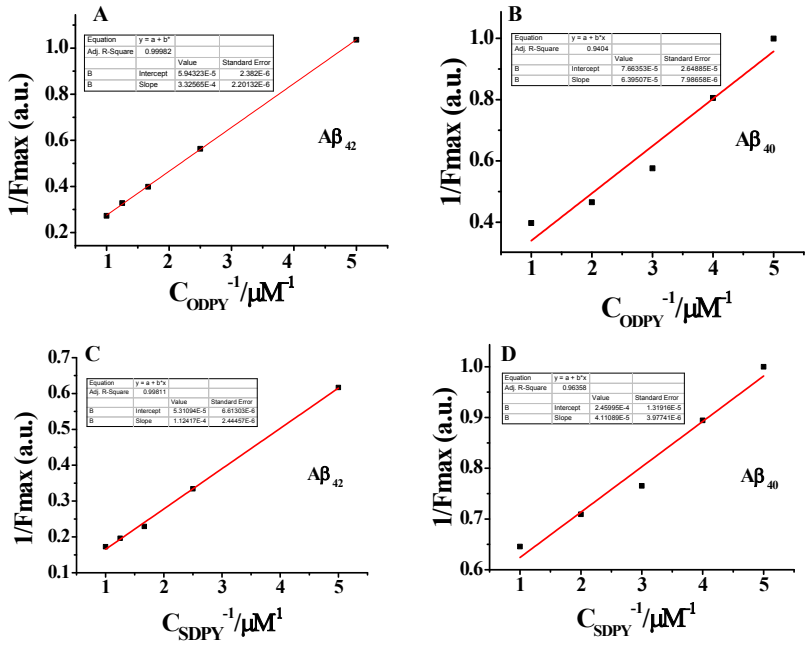


Fig. S2 Determination of the apparent binding constant (K_d) of probes to $A\beta_{40}$ aggregates and $A\beta_{42}$ aggregates. (A) and (B) were the binding constant (K_d) of **ODPY** to $A\beta_{40}$ aggregates and $A\beta_{42}$ aggregates, respectively. (C) and (D) were the binding constant (K_d) of **SDPY** to $A\beta_{40}$ aggregates and $A\beta_{42}$ aggregates, respectively.

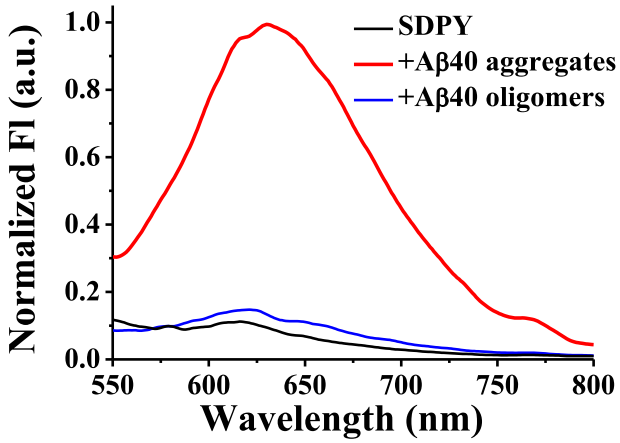


Fig. S3 The fluorescence spectrum of **SDPY** in the presence of $A\beta_{40}$ aggregates or oligomers.

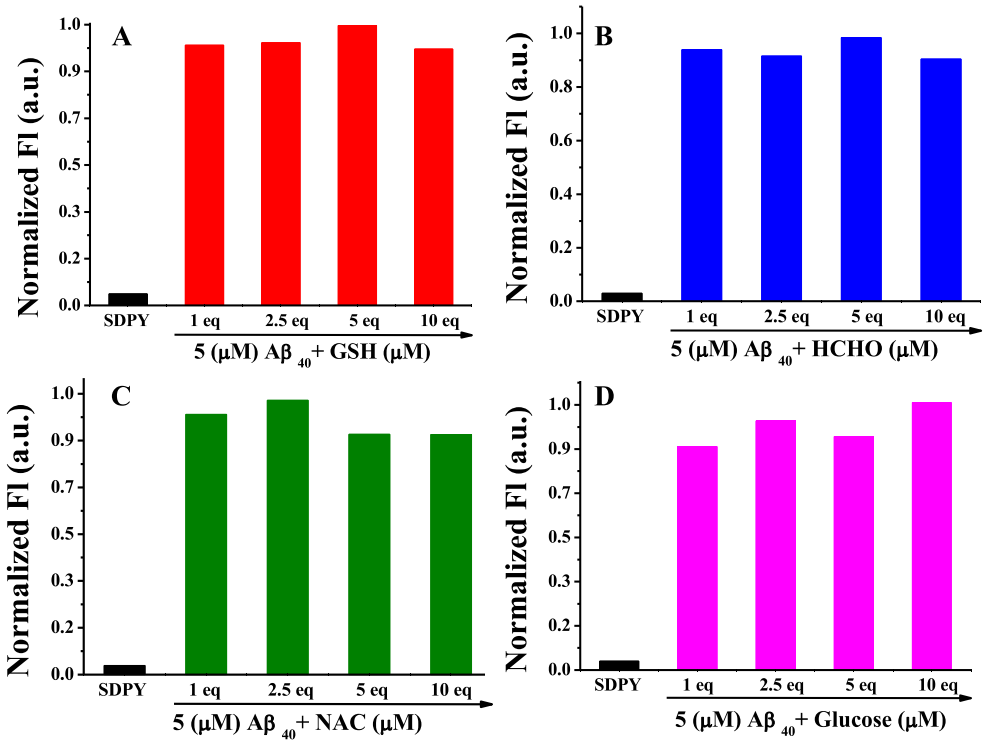


Fig. S4 Fluorescence intensity changes of **SDPY** at 620 nm with $A\beta_{40}$ aggregates in the presence of (A) GSH, (B) HCHO, (C) NAC and (D) Glucose.

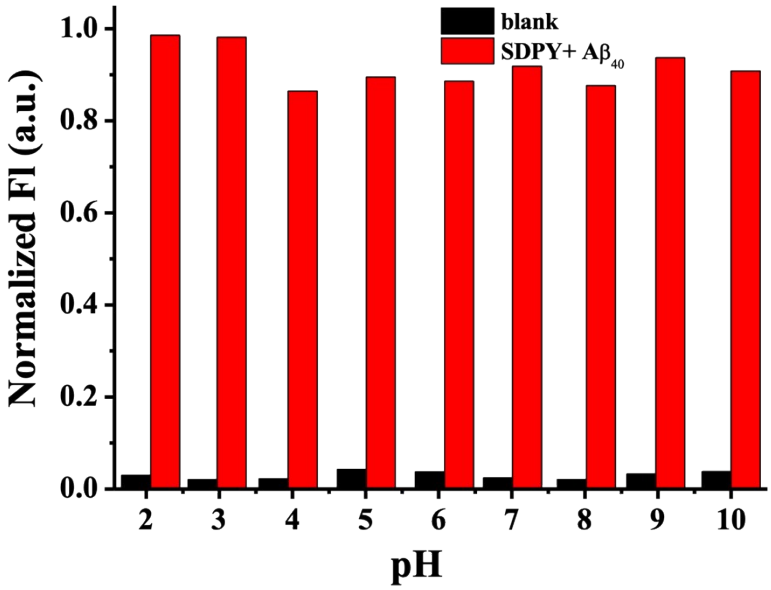


Fig. S5 Fluorescence intensity changes of **SDPY** at 620 nm under different pH values in the absence or presence of $A\beta_{40}$ aggregates.

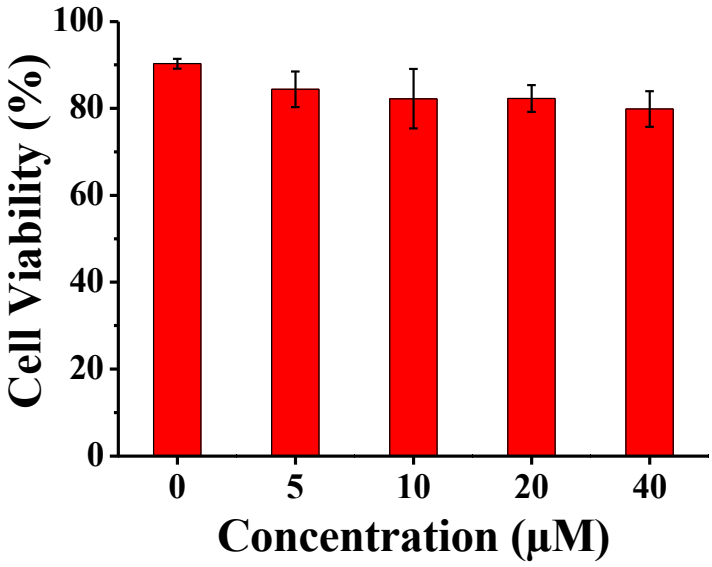


Fig. S6 Cell viability values (%) estimated by MTT assay in Hela cells in the presence of 0-40 μM **SDPY** for 6 h at 37 ^{O}C.

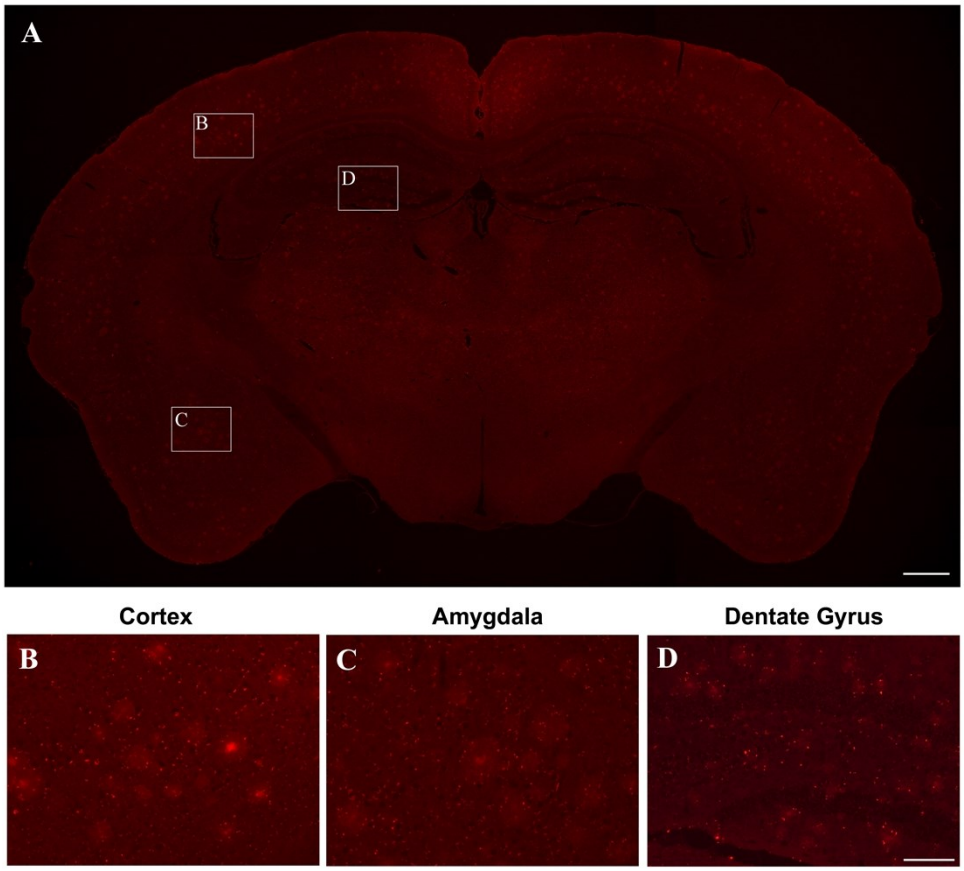


Fig. S7 Representative *in vivo* labeling of **SDPY** in AD transgenic mouse models. **SDPY** was systemically administrated in the APP/PS1 transgenic mice. (A) **SDPY** *in vivo* labeling was examined by *ex-vivo* imaging. (B, C and D) enlarged images of box frames in A. Scale bar: 500 μm in A and 100 μm in B-D.

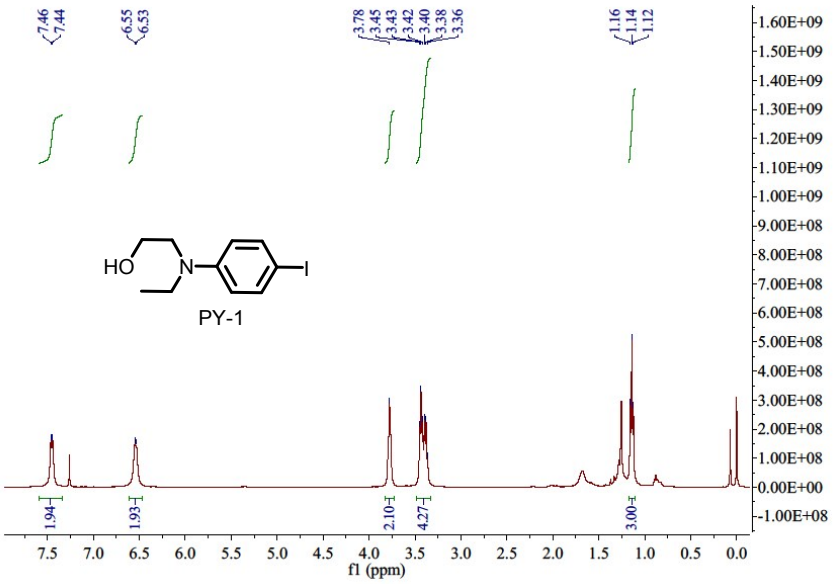


Fig. S8 The ^{1}H NMR of **PY-1**.

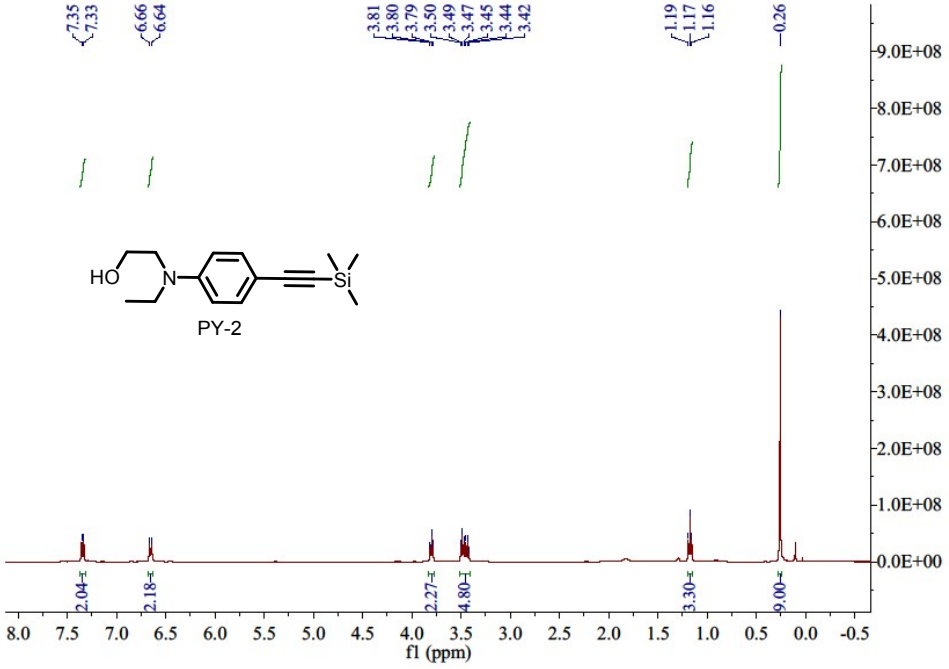


Fig. S9 The ^{1}H NMR of **PY-2**.

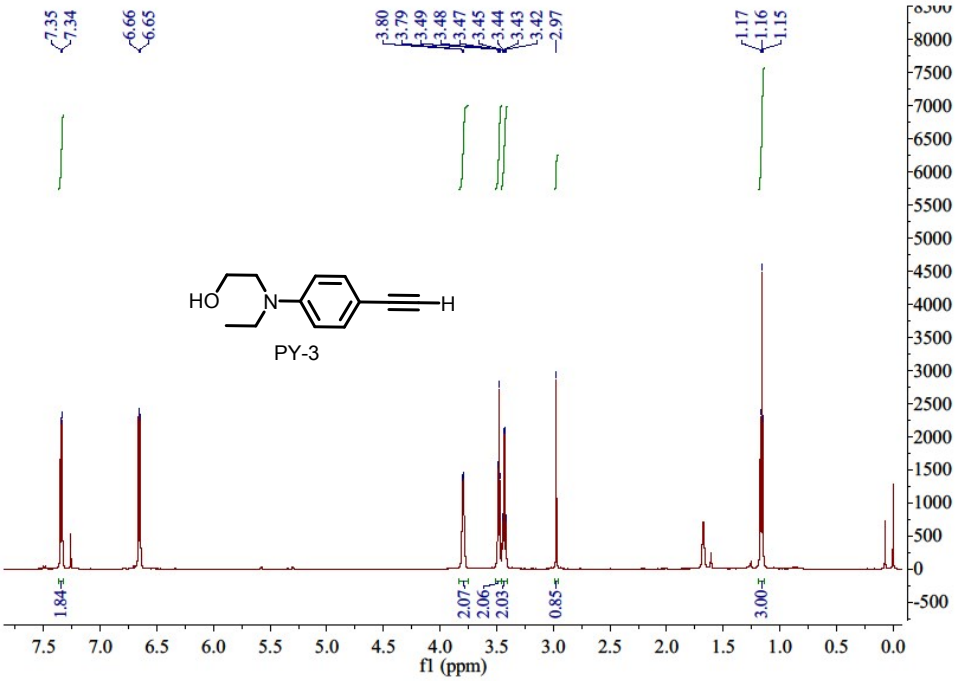


Fig. S10 The ^{1}H NMR of **PY-3**.

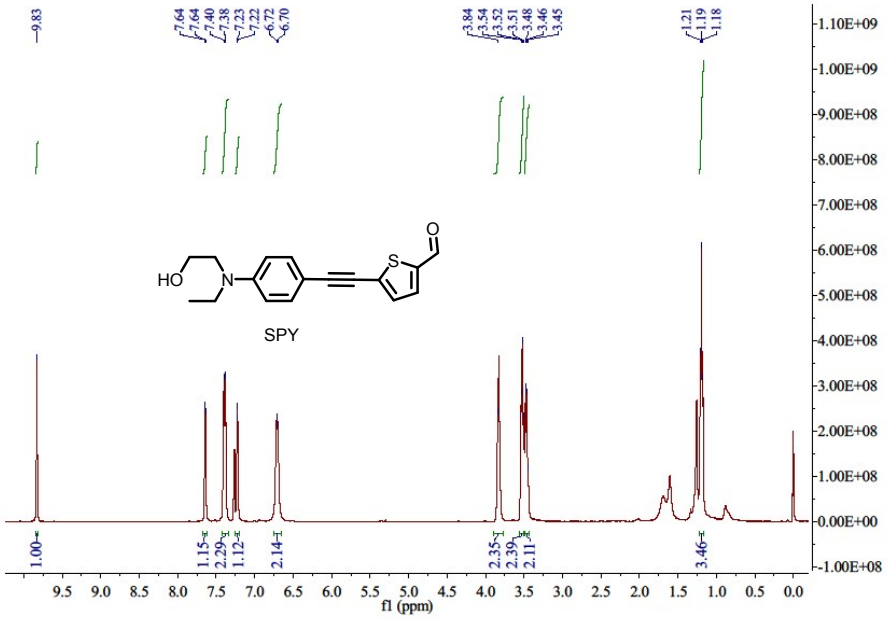


Fig. S11 The ^{1}H NMR of **SPY**.

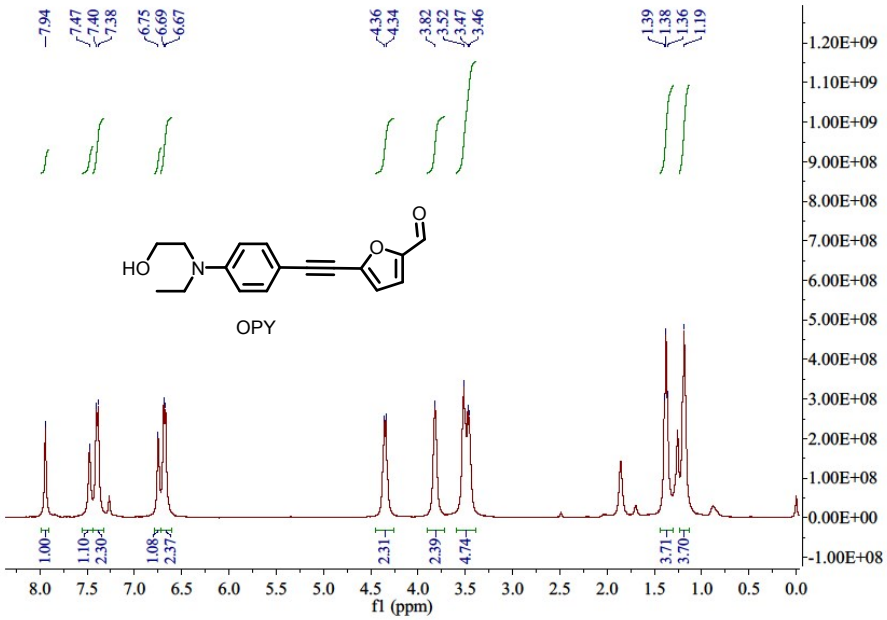


Fig. S12 The ^{1}H NMR of **OPY**.

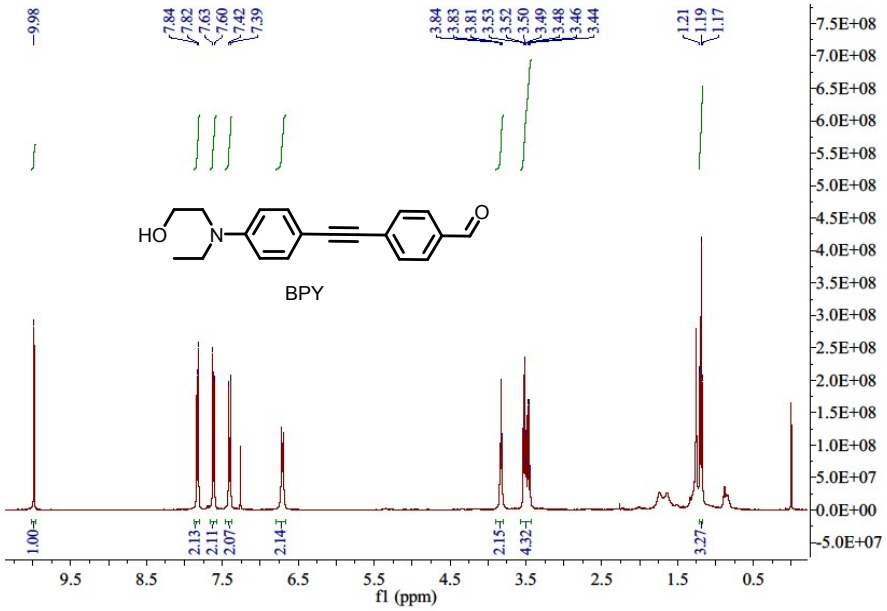


Fig. S13 The ^{1}H NMR of **BPY**.

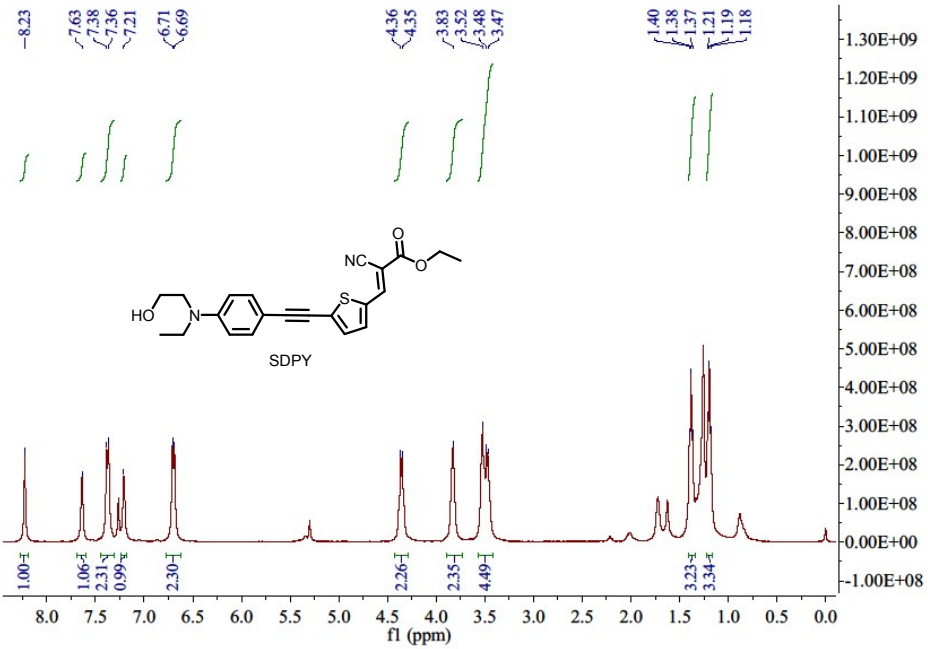


Fig. S14 The ^{1}H NMR of **SDPY**.

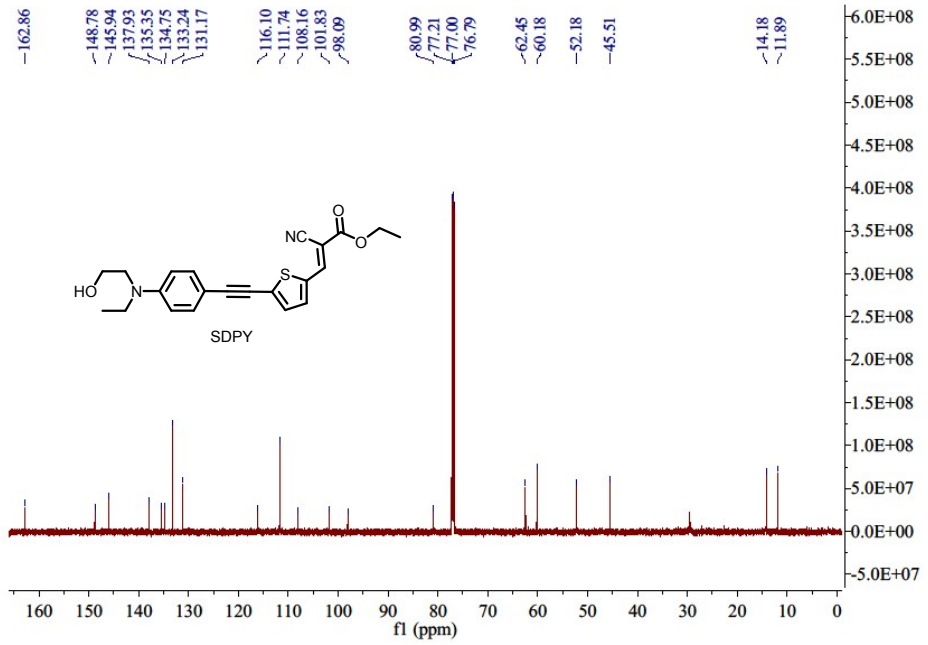


Fig. S15 The ^{13}C NMR of **SDPY**.

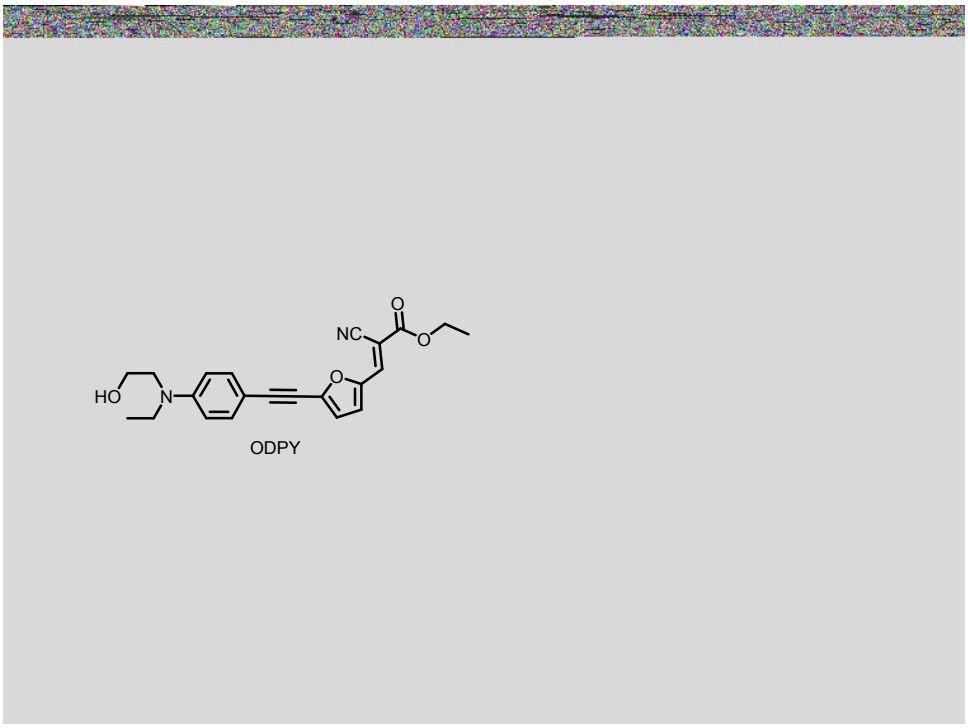


Fig. S16 The ^{1}H NMR of **ODPY**.

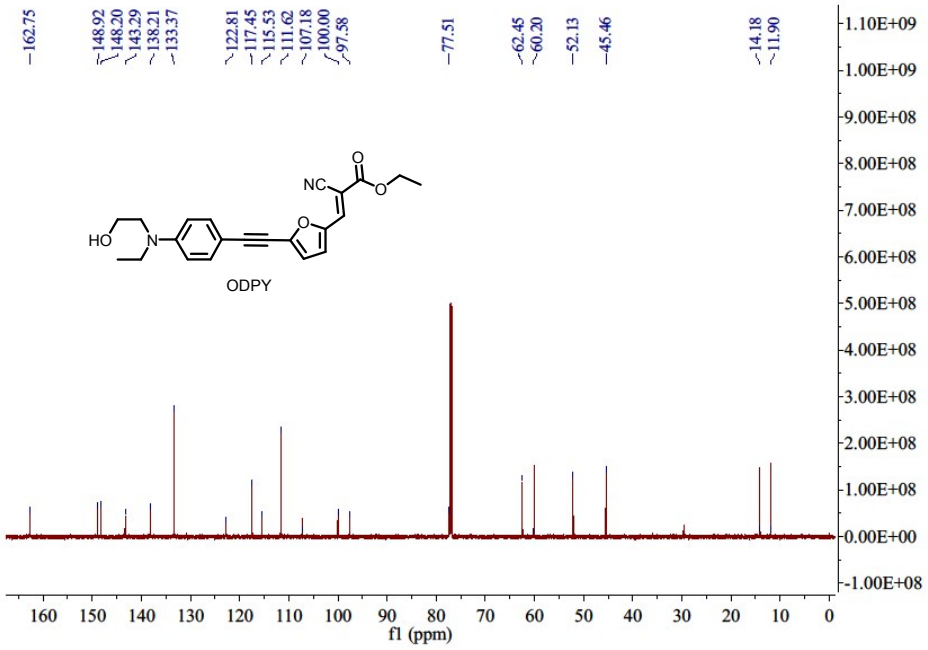


Fig. S17 The ^{13}C NMR of **ODPY**.

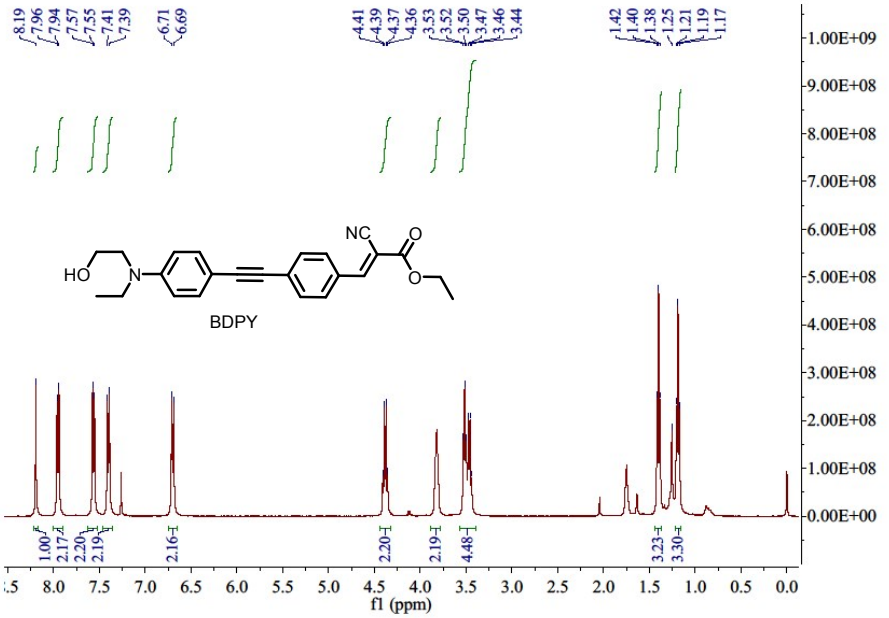


Fig. S18 The ^{1}H NMR of **BDPY**.

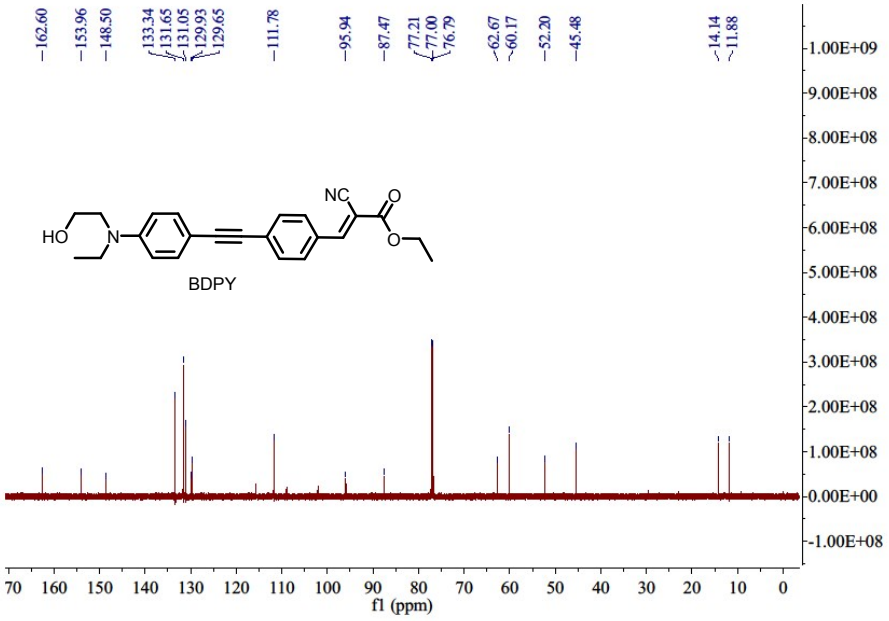


Fig. S19 The ^{13}C NMR of **BDPY**

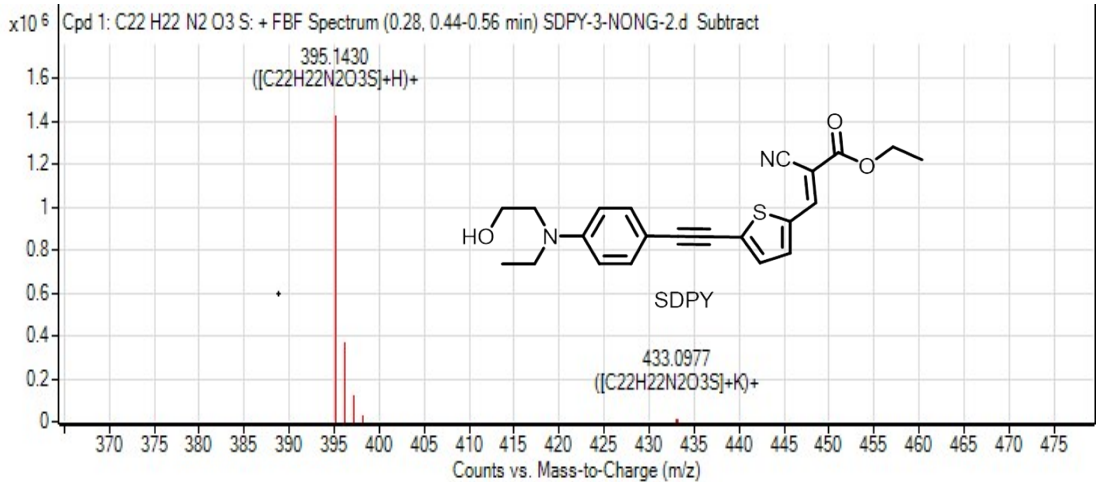


Fig. S20 The HRMS of **SDPY**.

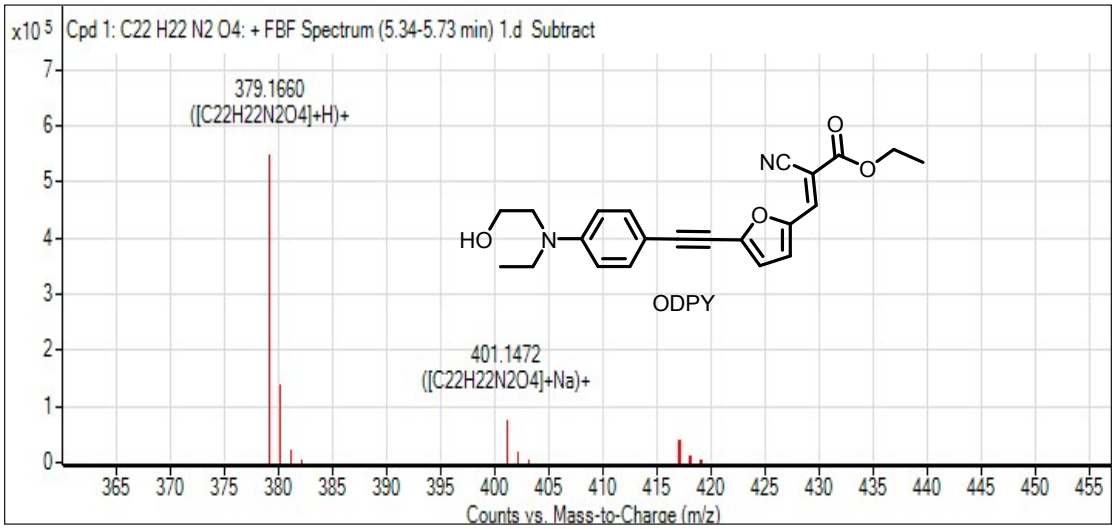


Fig. S21 The HRMS of **ODPY.**

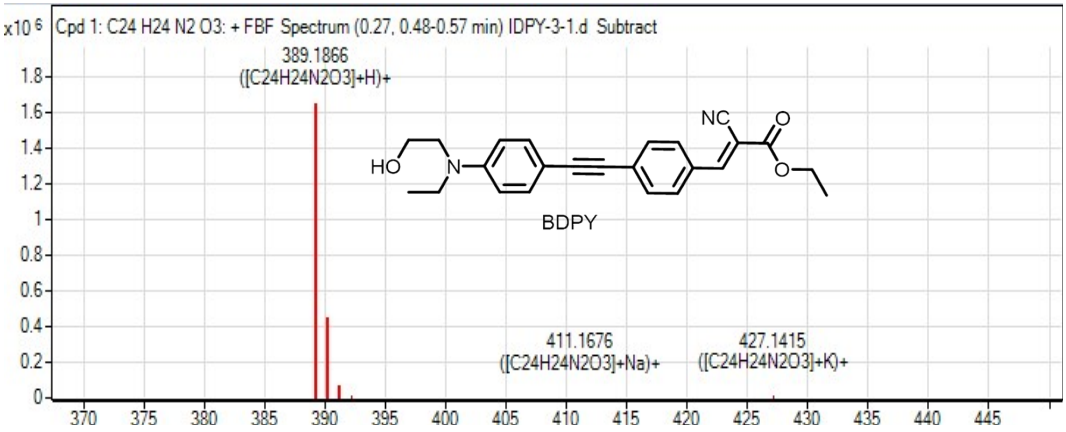


Fig. S22 The HRMS of **BDPY**.