

Electronic Supplementary Information

Enhanced mechanofluorochromic properties of 1,4-dihydropyridine-based fluorescence molecules caused by the introduction of halogen atoms

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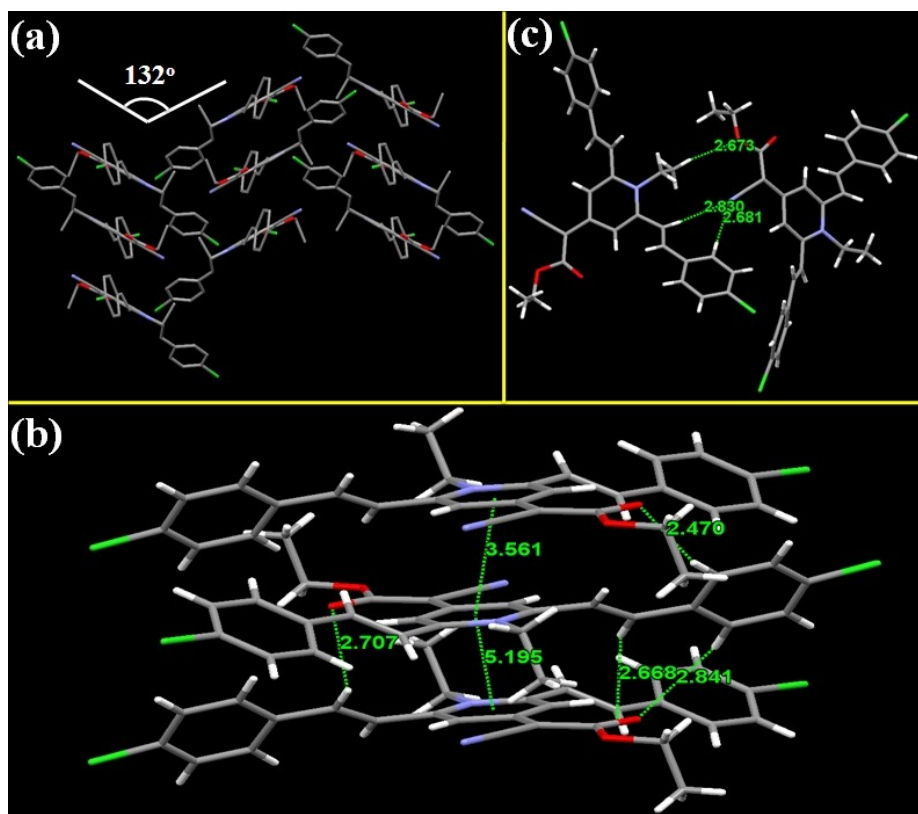


Fig. S1 Crystal **CMD-Cl**: (a) Molecular packing mode. (b) The C-H...O bond and C-H... π bond in the same column. (c) The C-H...O bond and C-H...N bond between different columns.

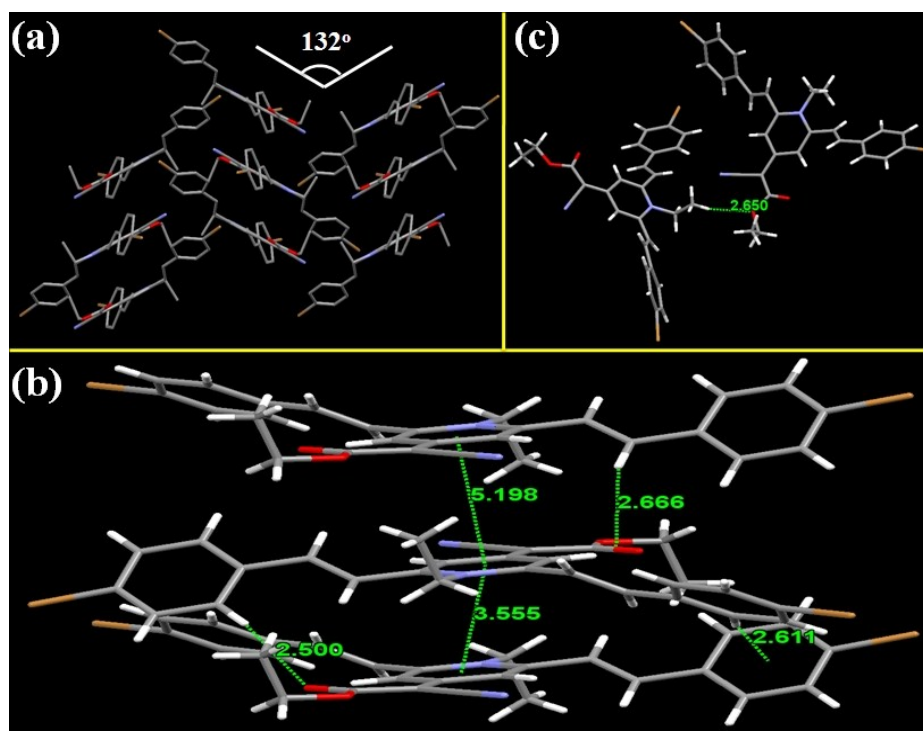


Fig. S2 Crystal **CMD-Br**: (a) Molecular packing mode. (b) The C-H...O bond and C-H... π bond in the same column. (c) The C-H...O bond between different columns.

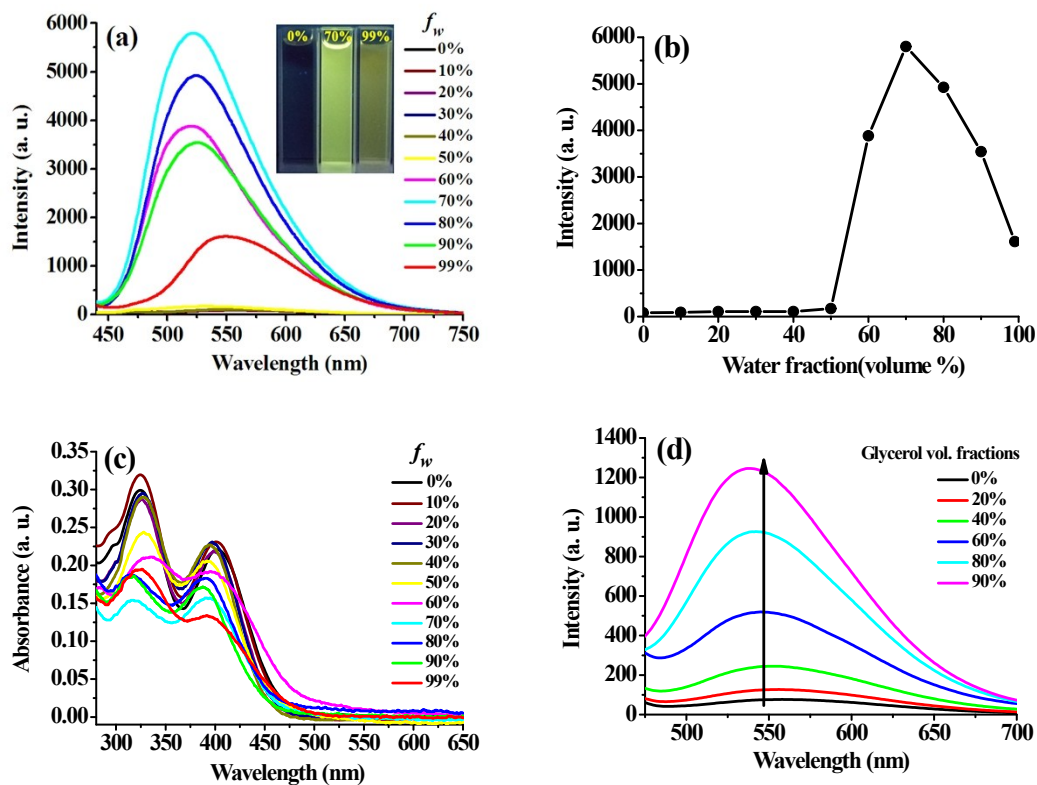


Fig. S3 CMD-F: Fluorescence spectra (a), changes in the fluorescence intensity (b), and UV-vis absorption spectra (c) in DMSO-water mixtures (10.0 $\mu\text{mol/L}$) with f_w values from 0 to 99%. Fluorescence spectra (d) in DMSO-glycerol mixtures (10.0 $\mu\text{mol/L}$) with the glycerol volume fraction from 0 to 90%. The insets in (a) show digital photographs of the fluorescence of mixtures with $f_w = 0$, 70, and 99%.

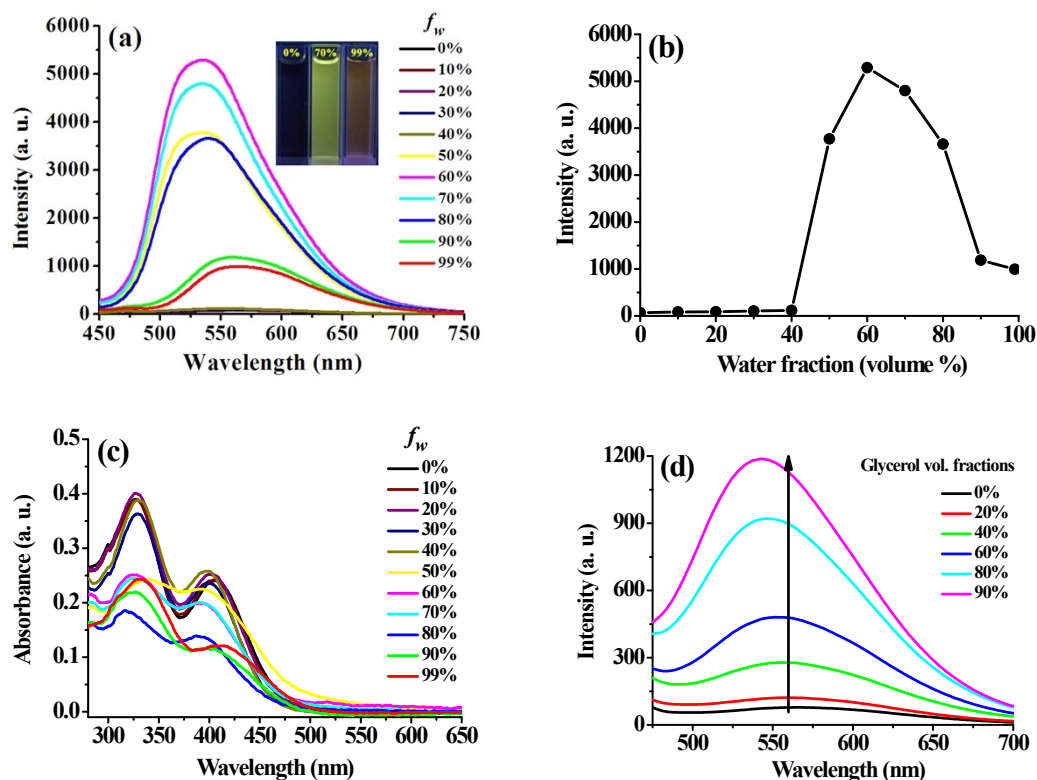


Fig. S4 CMD-CI: Fluorescence spectra (a), changes in the fluorescence intensity (b), and UV-vis absorption spectra (c) in DMSO-water mixtures (10.0 $\mu\text{mol/L}$) with f_w values from 0 to 99%. Fluorescence spectra (d) in DMSO-glycerol mixtures (10.0 $\mu\text{mol/L}$) with the glycerol volume fraction from 0 to 90%. The insets in (a) show digital photographs of the fluorescence of mixtures with $f_w = 0, 70$, and 99%.

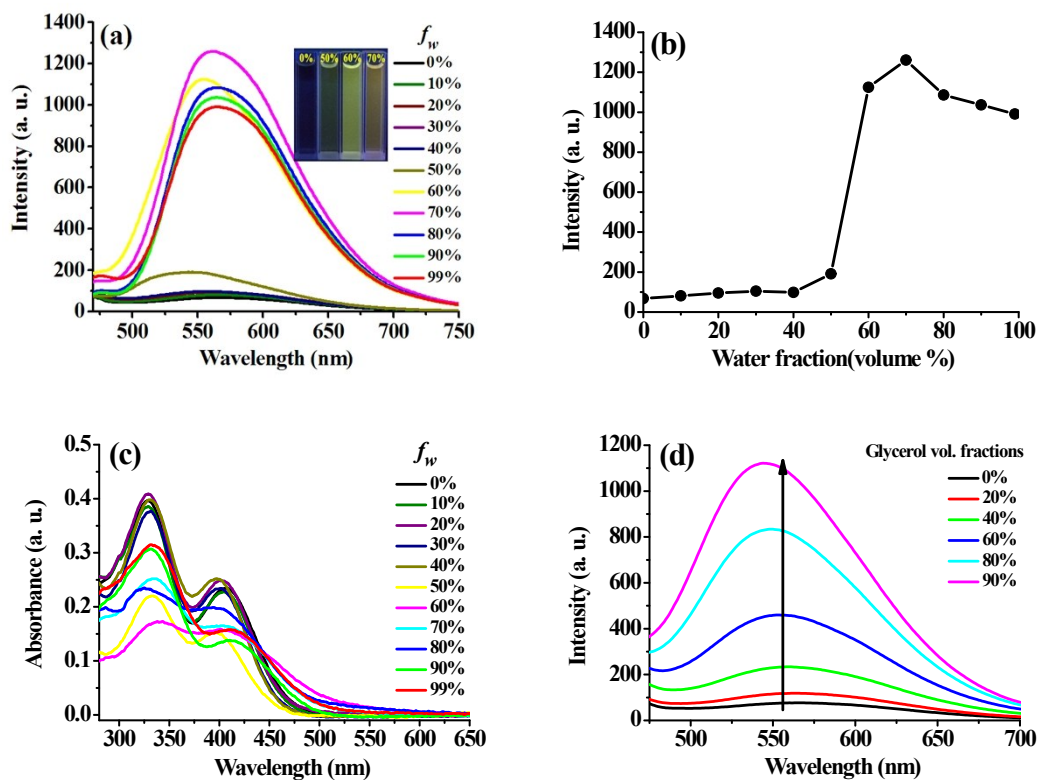


Fig. S5 CMD-Br: Fluorescence spectra (a), changes in the fluorescence intensity (b), and UV-vis absorption spectra (c) in DMSO-water mixtures (10.0 $\mu\text{mol/L}$) with f_w values from 0 to 99%. Fluorescence spectra (d) in DMSO-glycerol mixtures (10.0 $\mu\text{mol/L}$) with the glycerol volume fraction from 0 to 90%. The insets in (a) show digital photographs of the fluorescence of mixtures with $f_w = 0, 50, 60,$ and 70% .

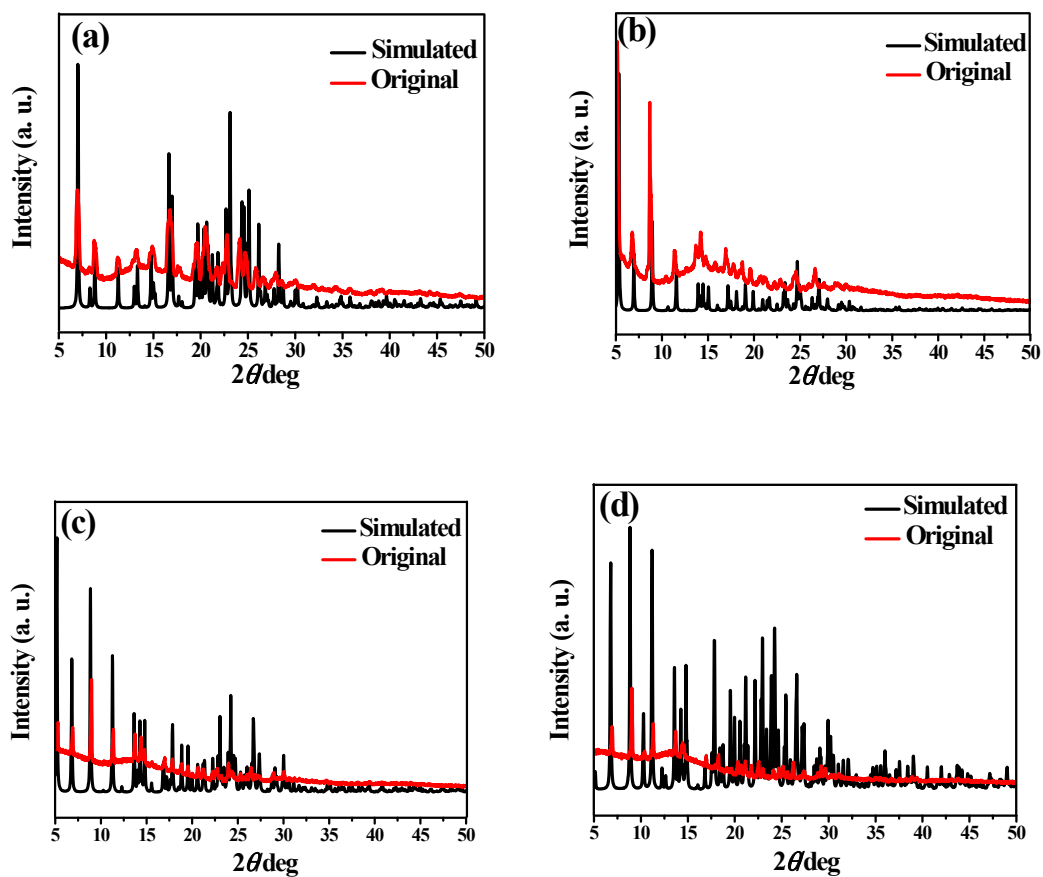


Fig. S6 Comparison of XRD curves of the original samples of the CMD derivatives and the simulated XRD curves obtained from the corresponding single crystals: **CMD-H** (a), **CMD-F** (b), **CMD-Cl** (c), and **CMD-Br** (d).

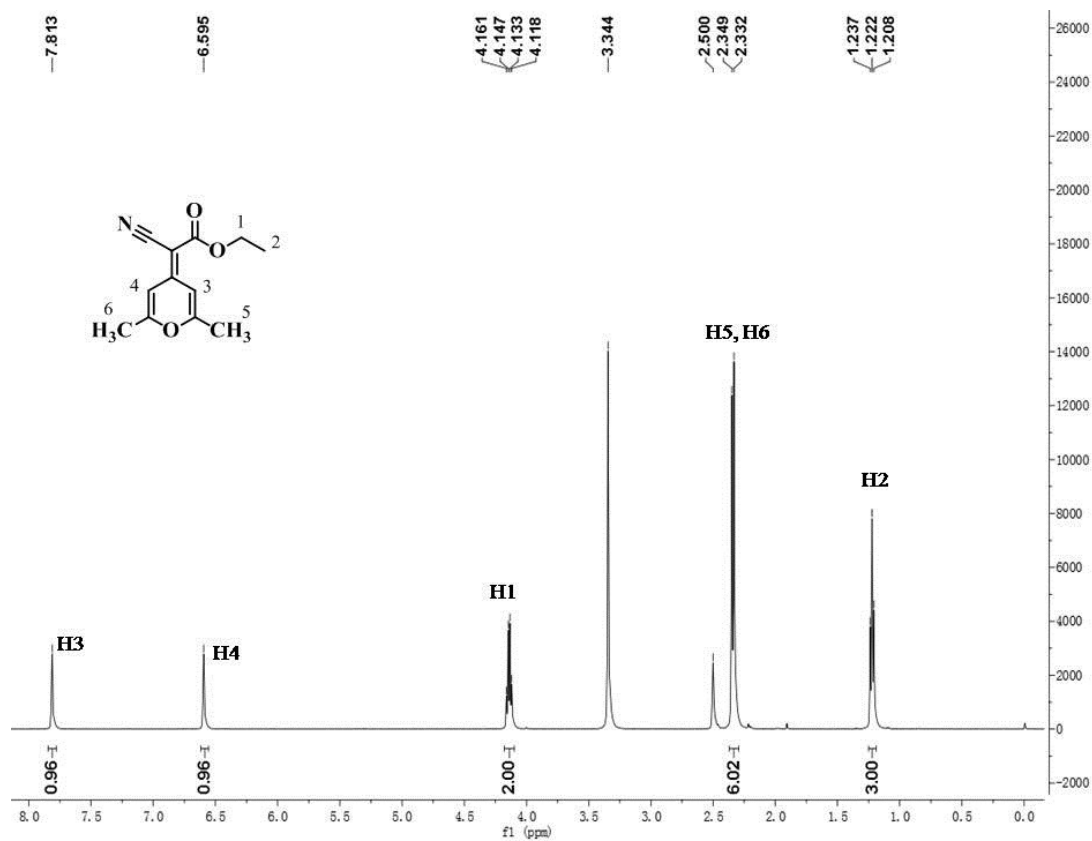


Fig. S7 ¹H NMR of compound 2 (DMSO-*d*₆, 500 MHz).

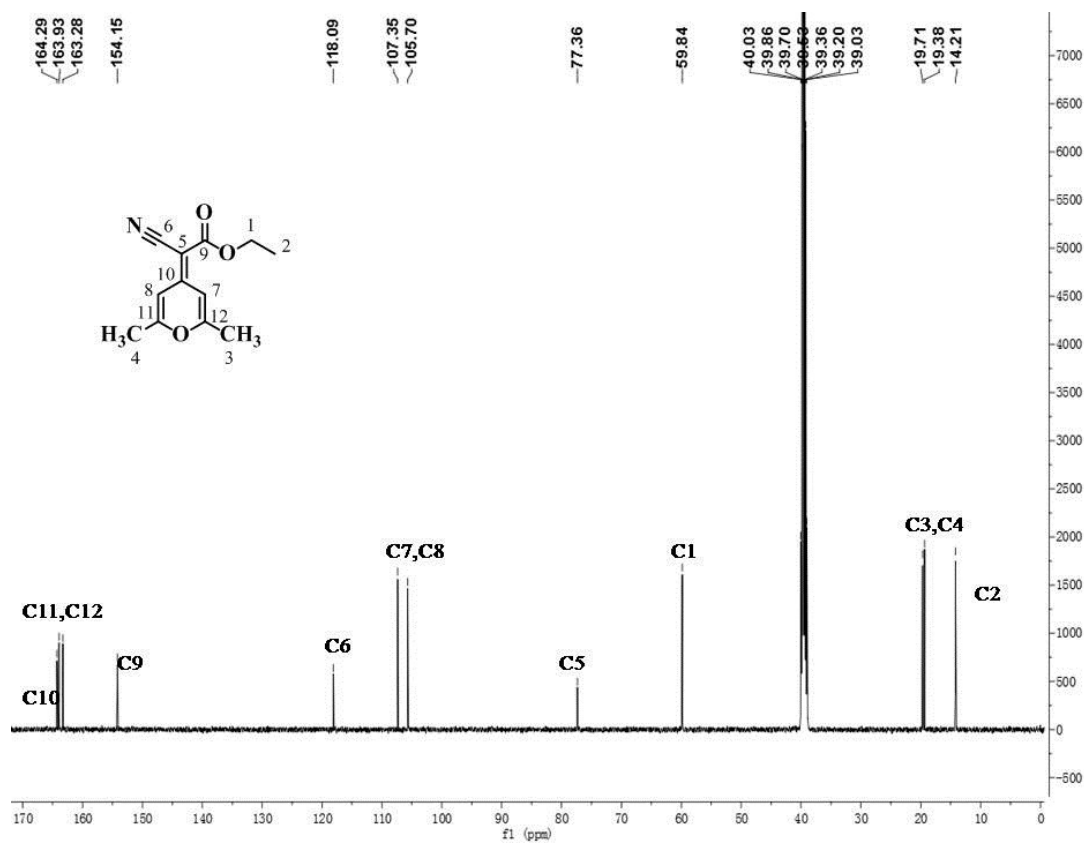


Fig. S8 ¹³C NMR of compound 2 (DMSO-*d*₆, 125 MHz).

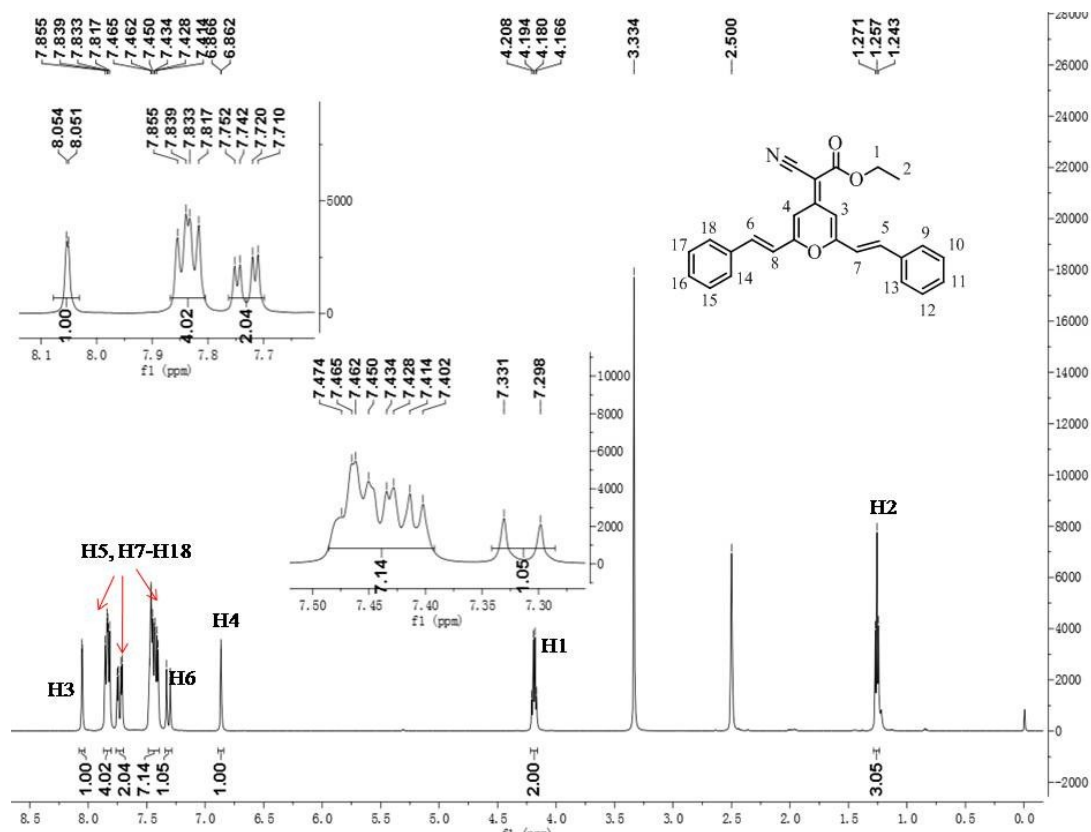


Fig. S9 ¹H NMR of compound 3a (DMSO-*d*₆, 500 MHz).

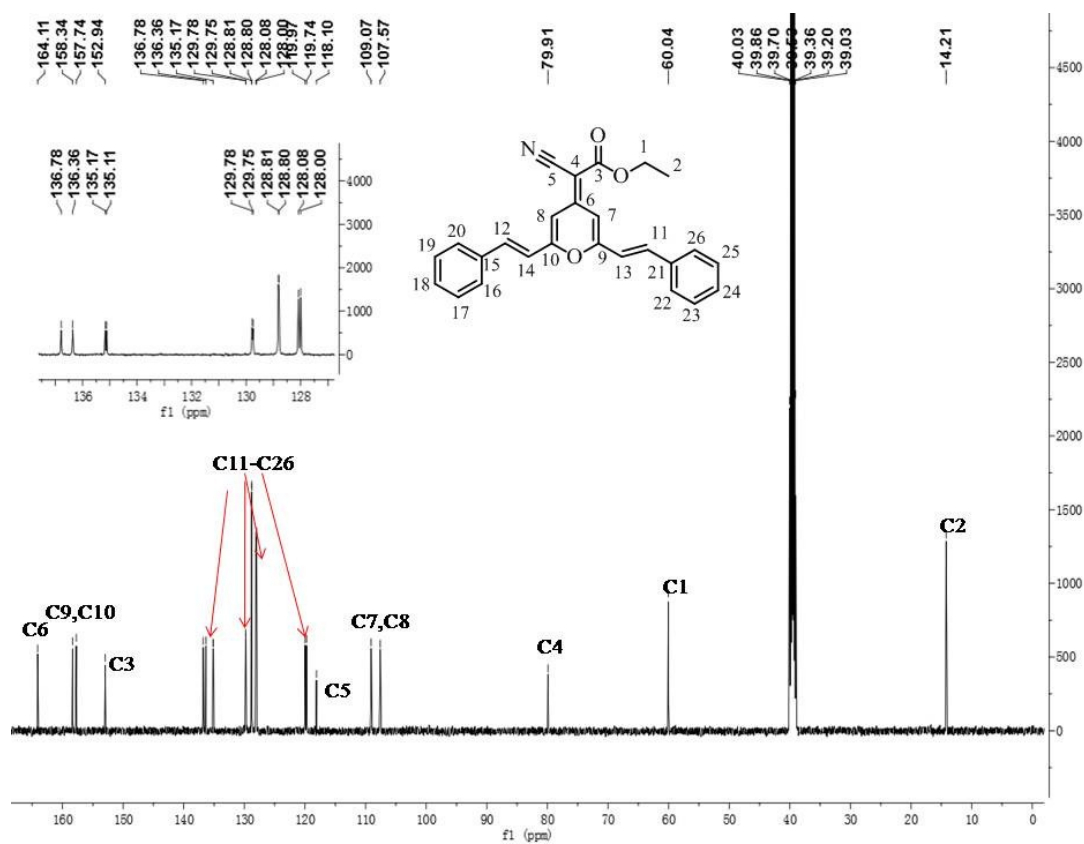


Fig. S10 ¹³C NMR of compound 3a (DMSO-*d*₆, 125 MHz).

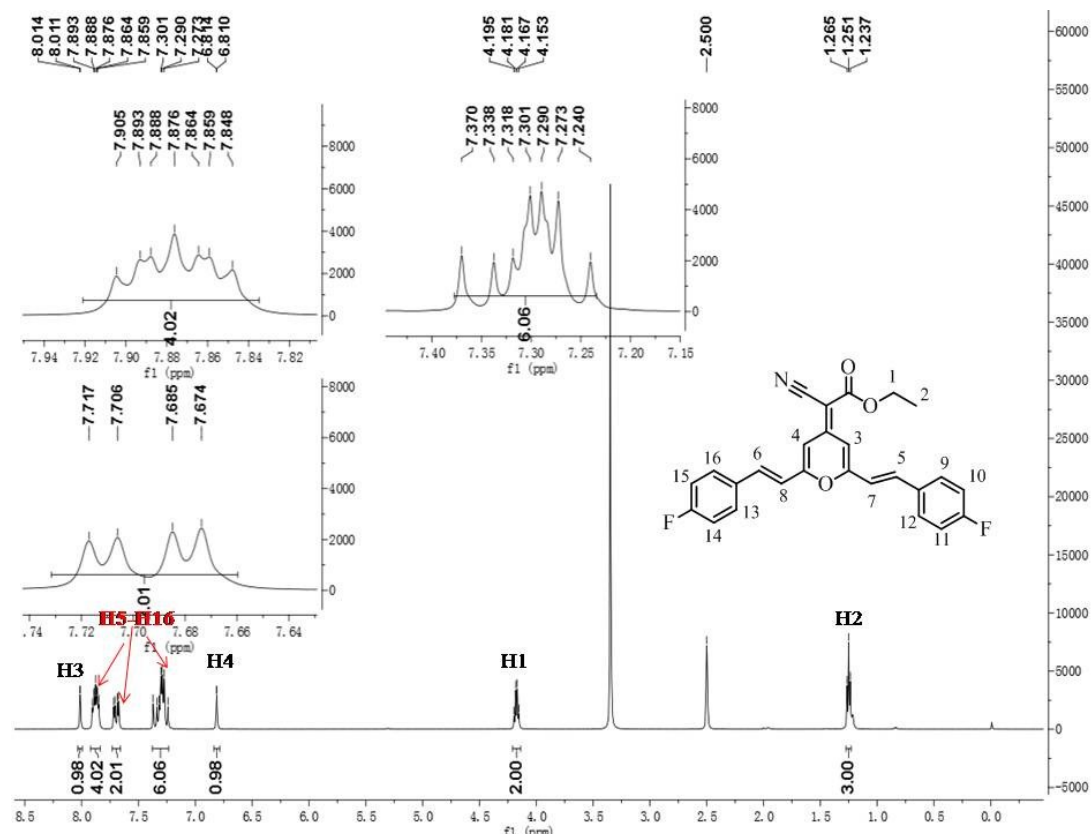


Fig. S11 ¹H NMR of compound 3b (DMSO-*d*₆, 500 MHz).

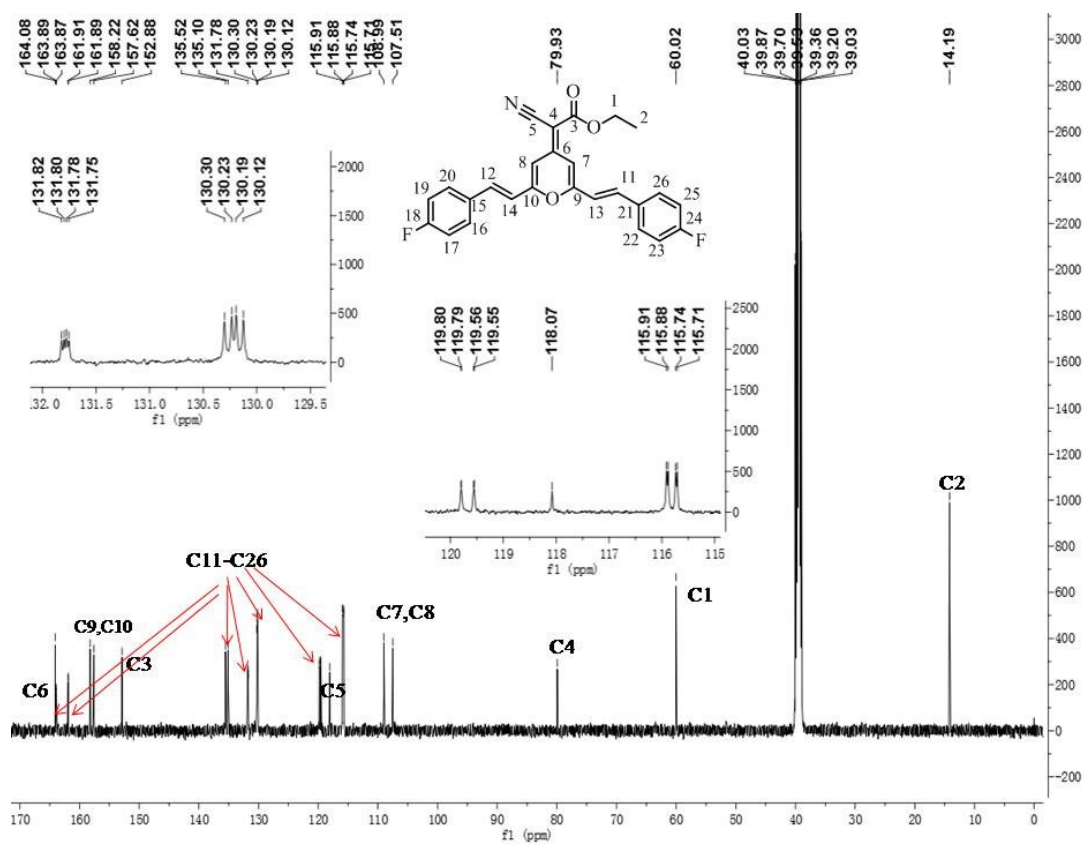


Fig. S12 ¹³C NMR of compound 3b (DMSO-*d*₆, 125 MHz).

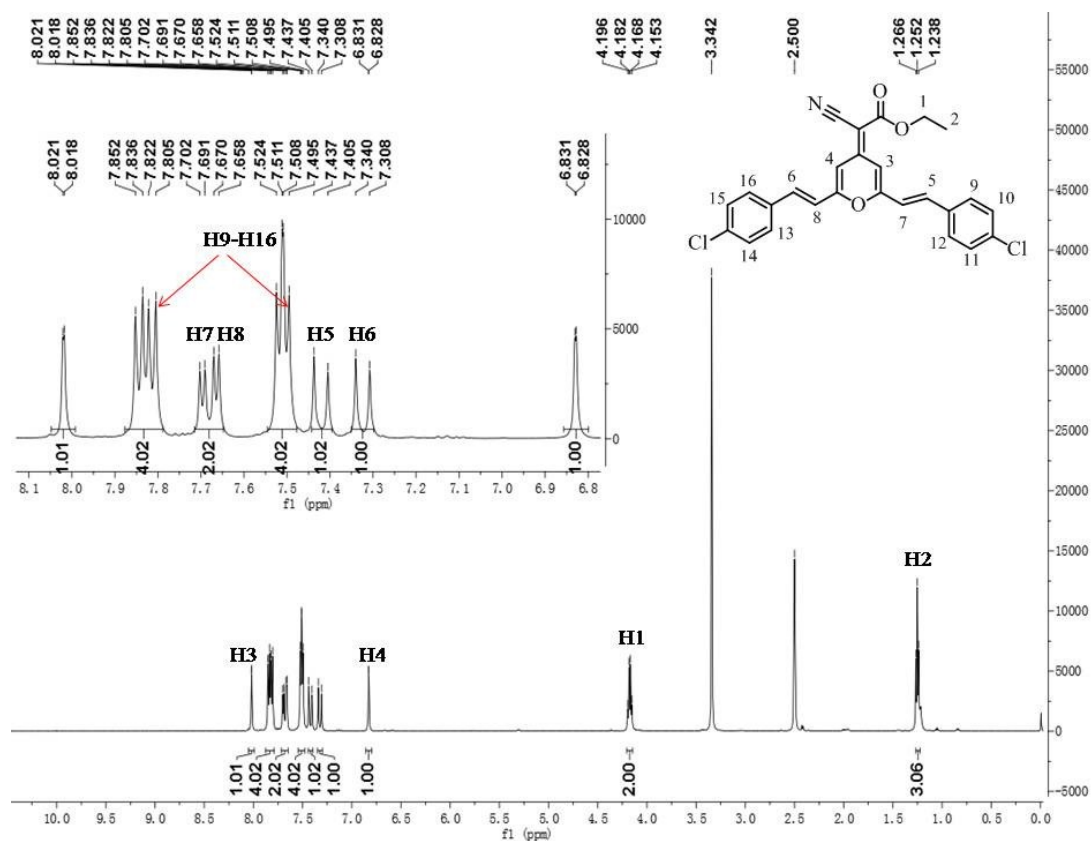


Fig. S13 ¹H NMR of compound 3c (DMSO-*d*₆, 500 MHz).

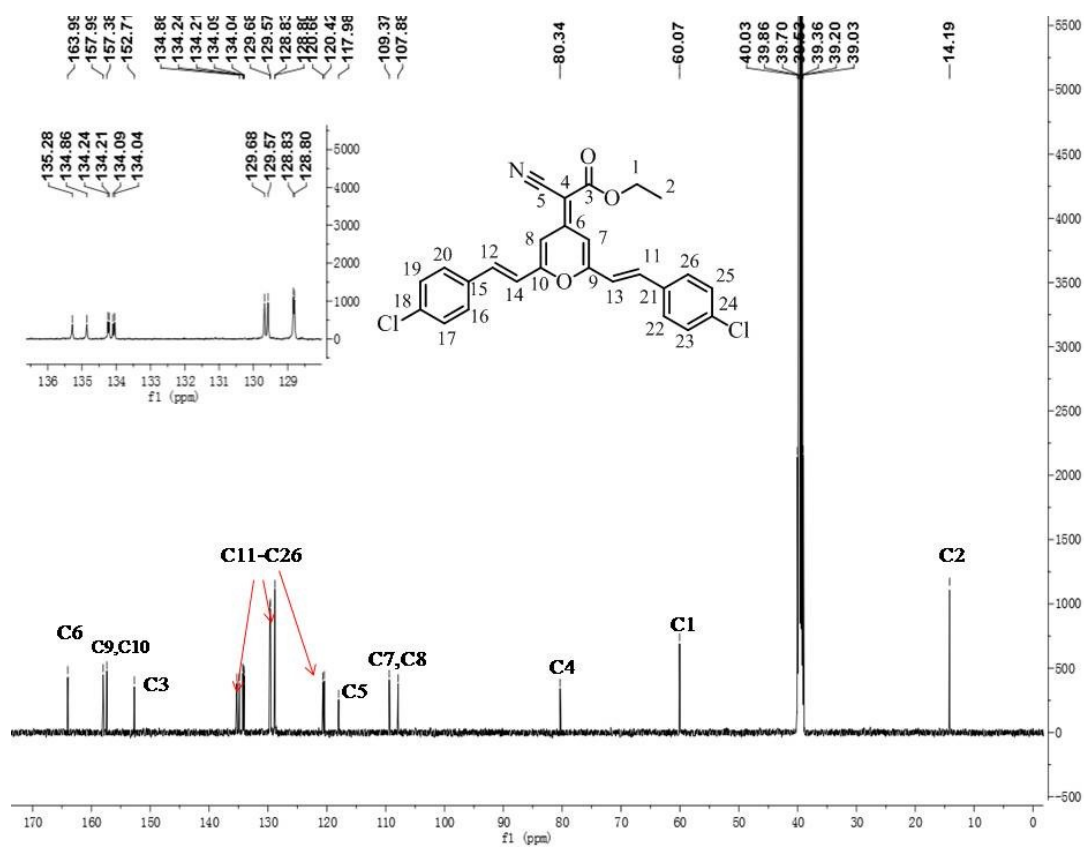


Fig. S14 ¹³C NMR of compound 3c (DMSO-*d*₆, 125 MHz).

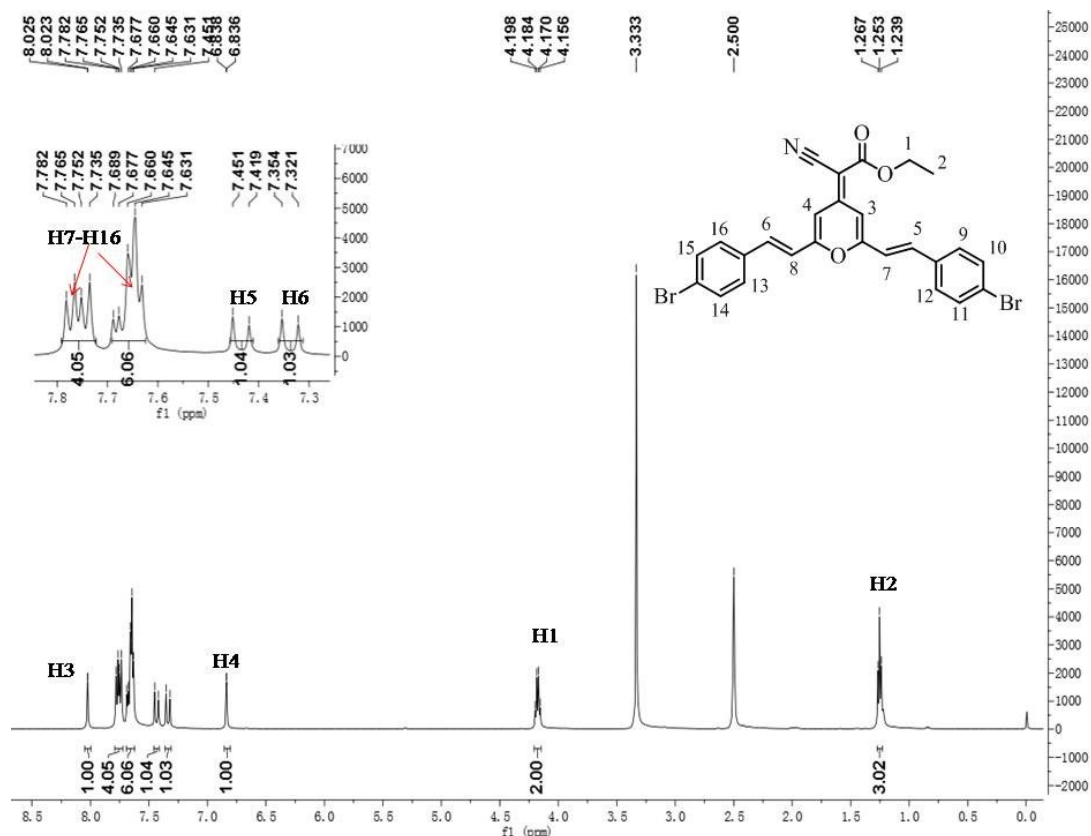


Fig. S15 ^1H NMR of compound 3d (DMSO- d_6 , 500 MHz).

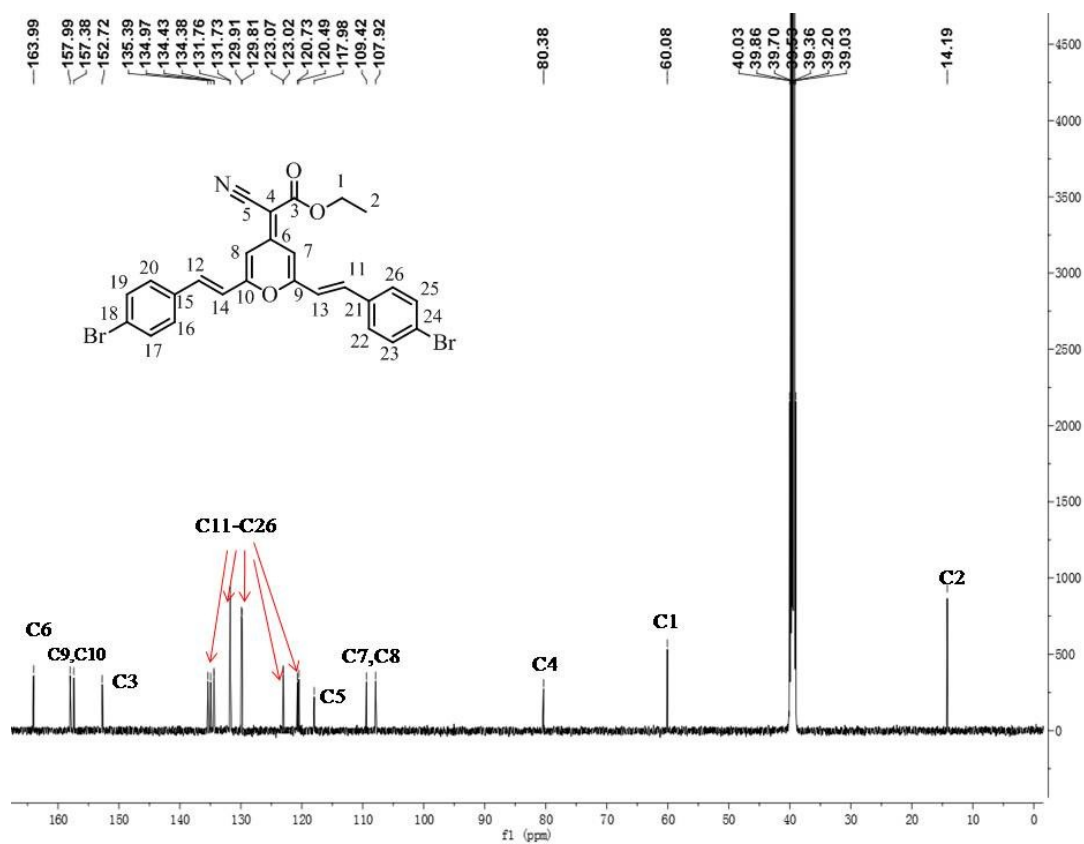


Fig. S16 ^{13}C NMR of compound 3d (DMSO- d_6 , 125 MHz).

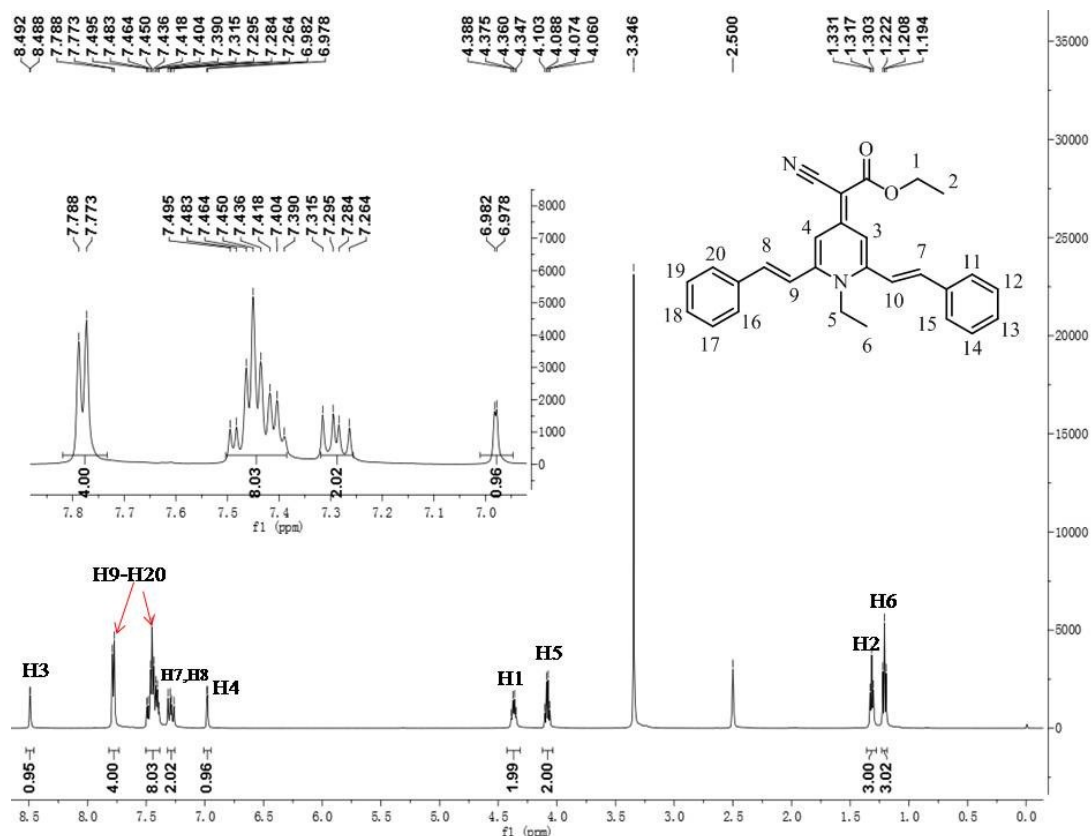


Fig. S17 ^1H NMR of CMD-H (DMSO- d_6 , 500 MHz).

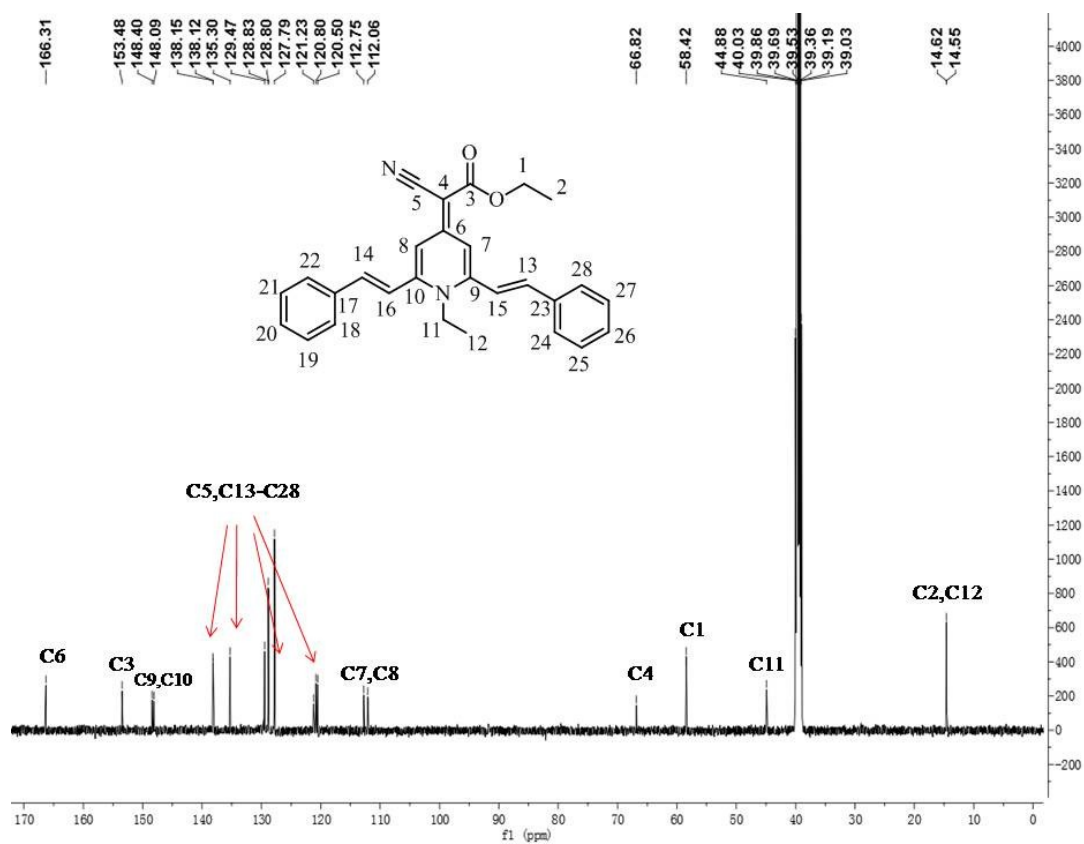


Fig. S18 ^{13}C NMR of CMD-H (DMSO- d_6 , 125 MHz).

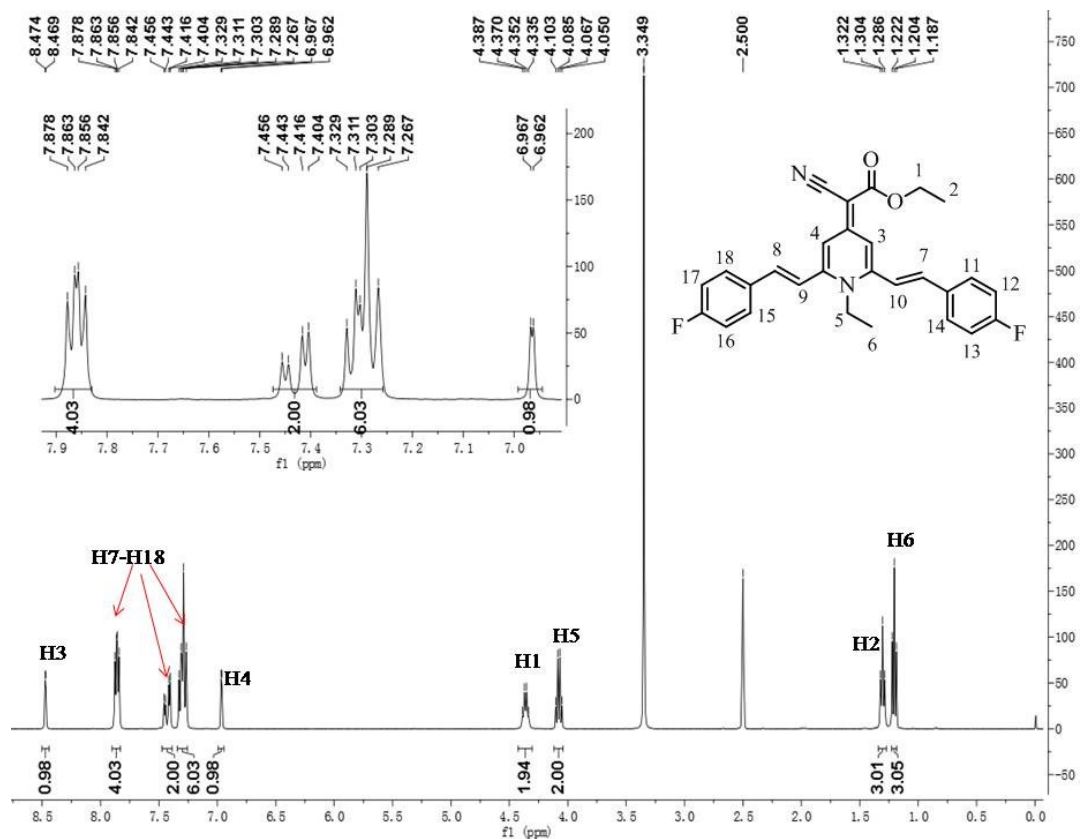


Fig. S19 ¹H NMR of CMD-F (DMSO-*d*₆, 400 MHz).

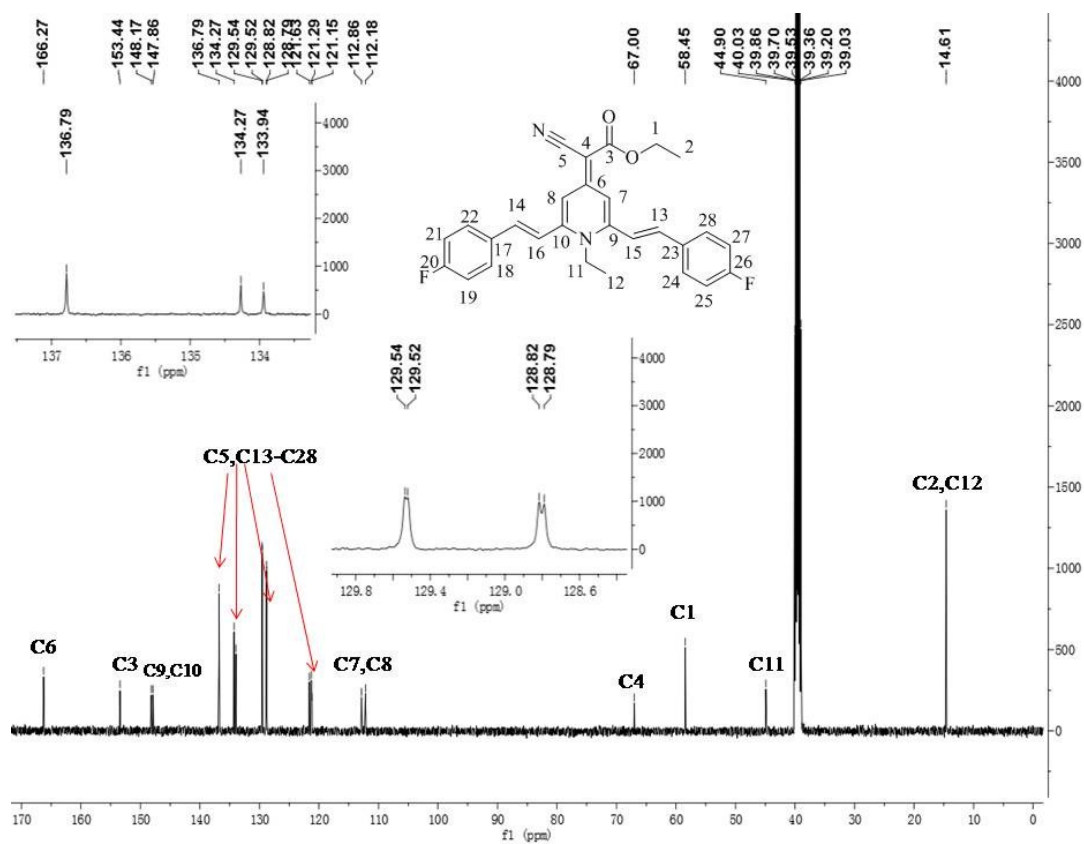


Fig. S20 ¹³C NMR of CMD-F (DMSO-*d*₆, 125 MHz).

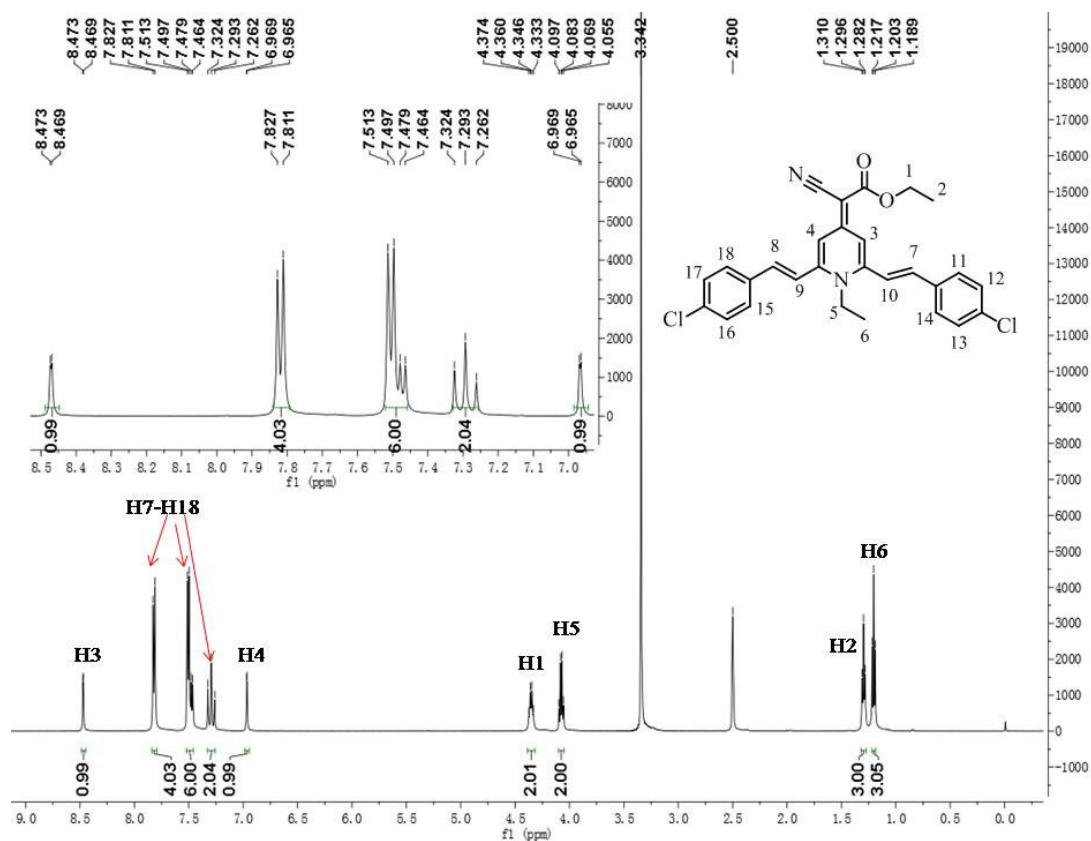


Fig. S21 ¹H NMR of CMD-Cl (DMSO-*d*₆, 500 MHz).

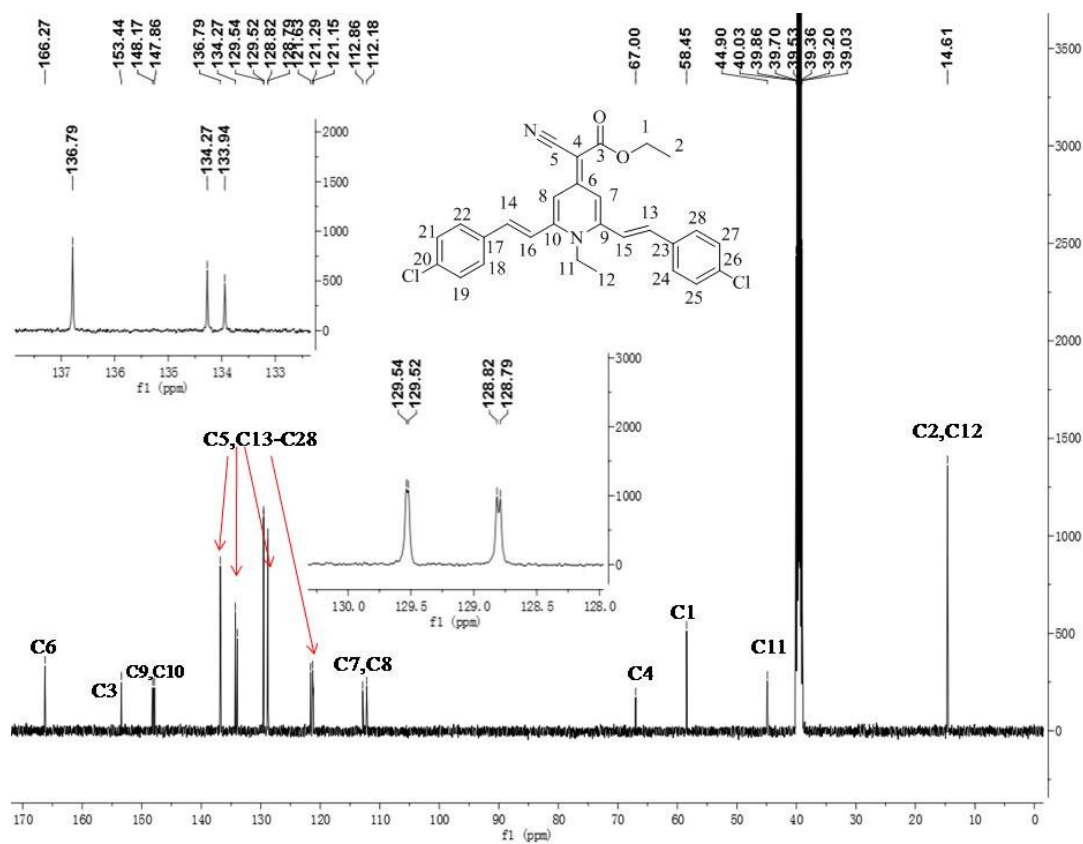


Fig. S22 ¹³C NMR of CMD-Cl (DMSO-*d*₆, 125 MHz).

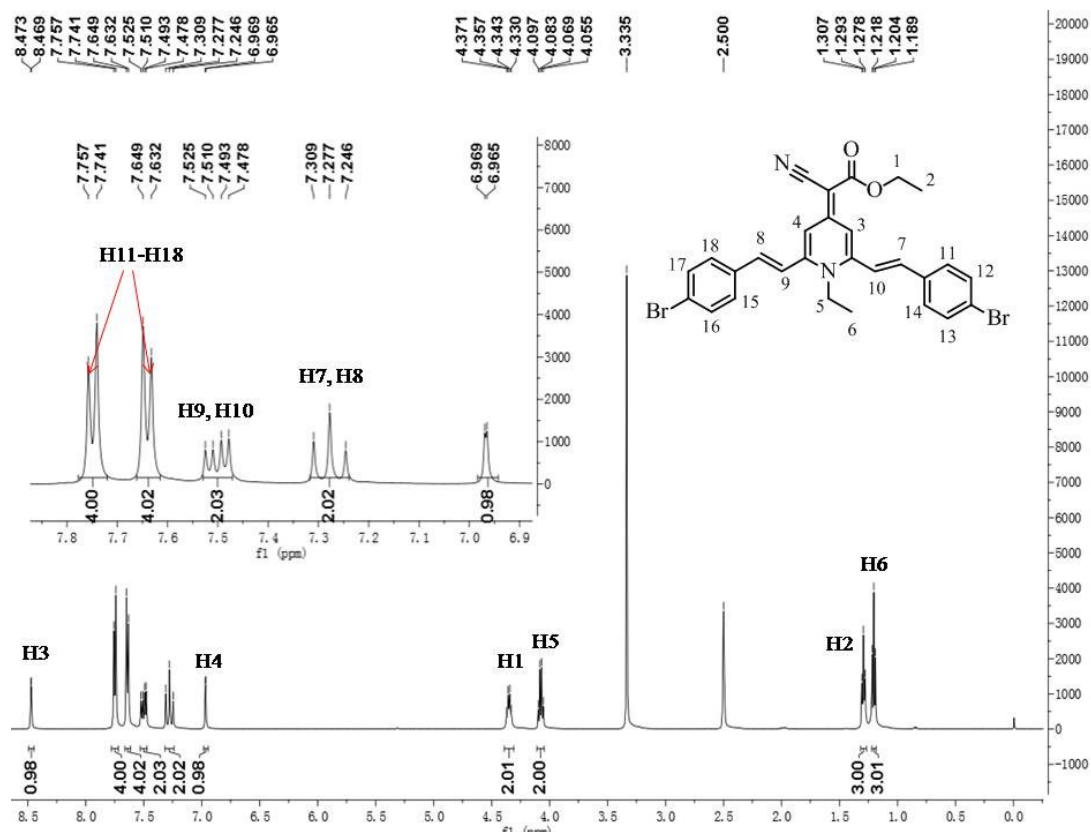


Fig. S23 ¹H NMR of CMD-Br (DMSO-*d*₆, 500 MHz).

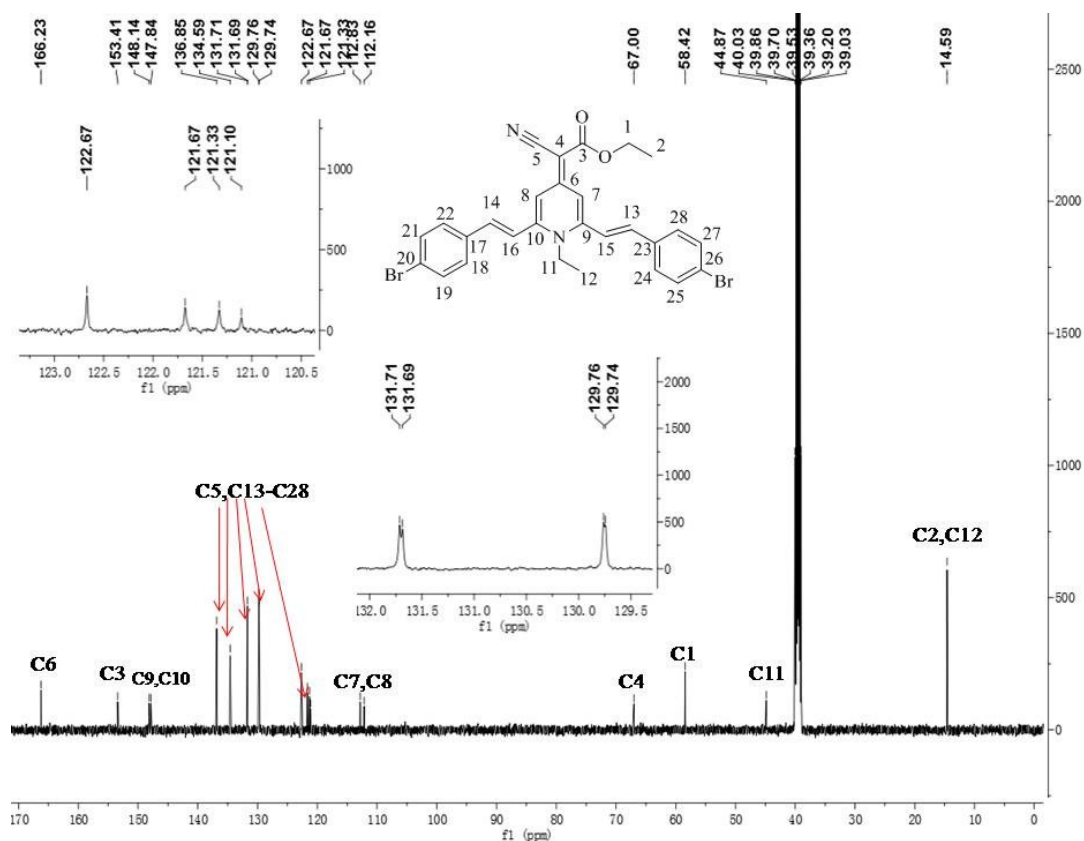


Fig. S24 ¹³C NMR of CMD-Br (DMSO-*d*₆, 125 MHz).