Electronic Supplementary Information

Twisted coumarin dyes for dye-sensitized solar cells with high photovoltage: Adjustment of optical, electrochemical, and photovoltaic properties by molecular structure

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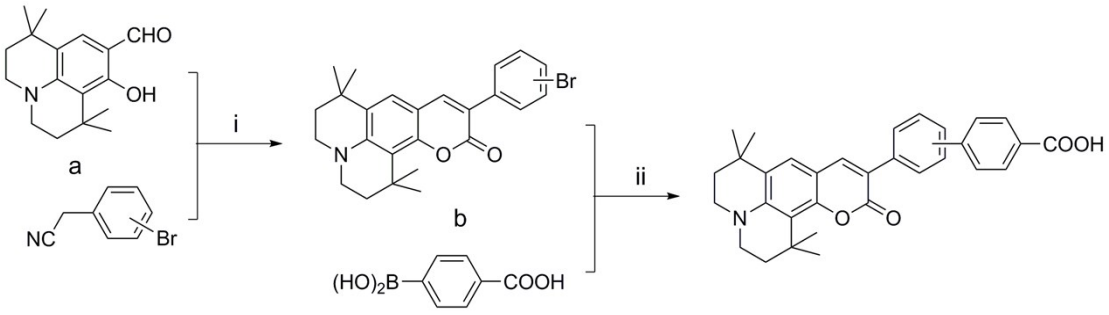

ortho-isomer: **CS-3** *meta*-isomer: **CS-4** *para*-isomer: **CS-5**

Scheme S1. Synthetic routes of coumarin dyes **CS-3, CS-4**, and **CS-5**. i: toluene, piperidine, reflux for 12h; ii: $Pd(PPh_3)_4$, K_2CO_3, dioxane, reflux for 12h.

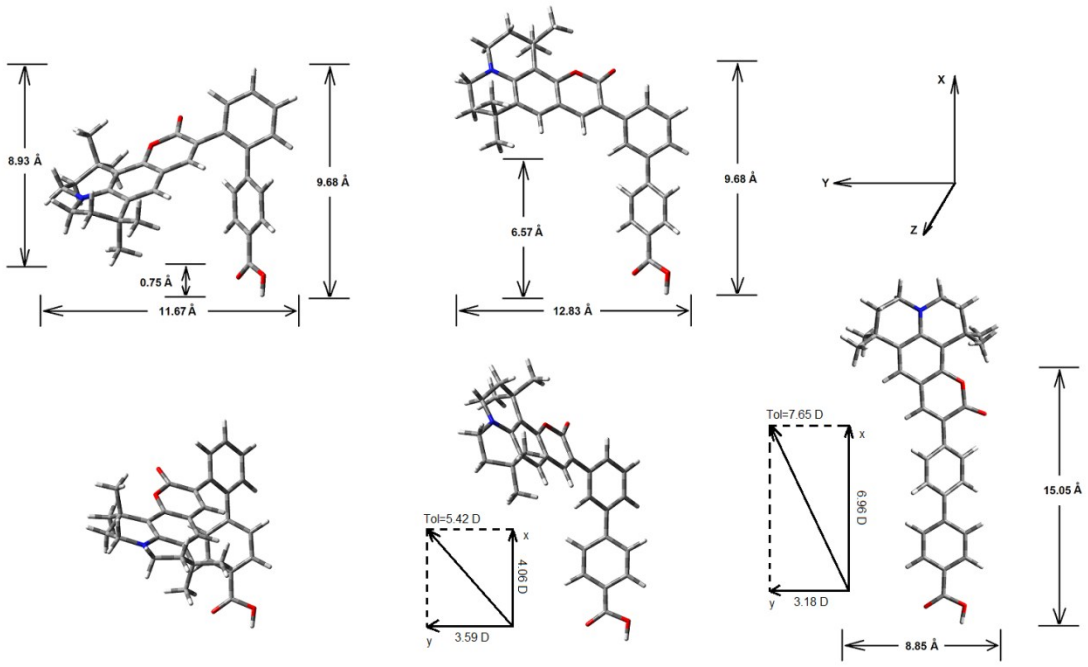

Fig.S1 The optimized ground-state geometries of **CS-3**, **CS-4**, and **CS-5** simulated on the basis of hybrid density functional theory (B3LYP) with the 6-31G* basis set as implemented in the Gaussian 09 program.

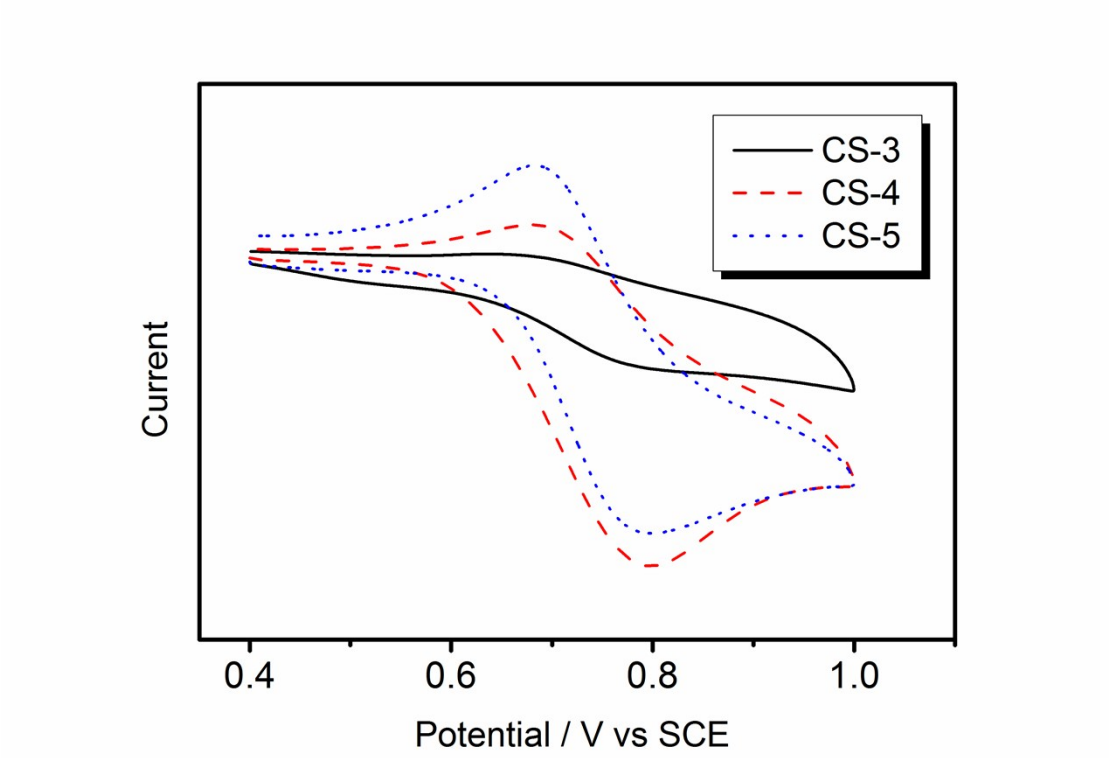

Fig. S2 Oxidative cyclic voltammetry plots of **CS-3**, **CS-4**, and **CS-5** measured with using dye-loaded TiO_2 film as the working electrode, a saturated calomel (SCE) reference electrode, and a platinum wire as the counter electrode.

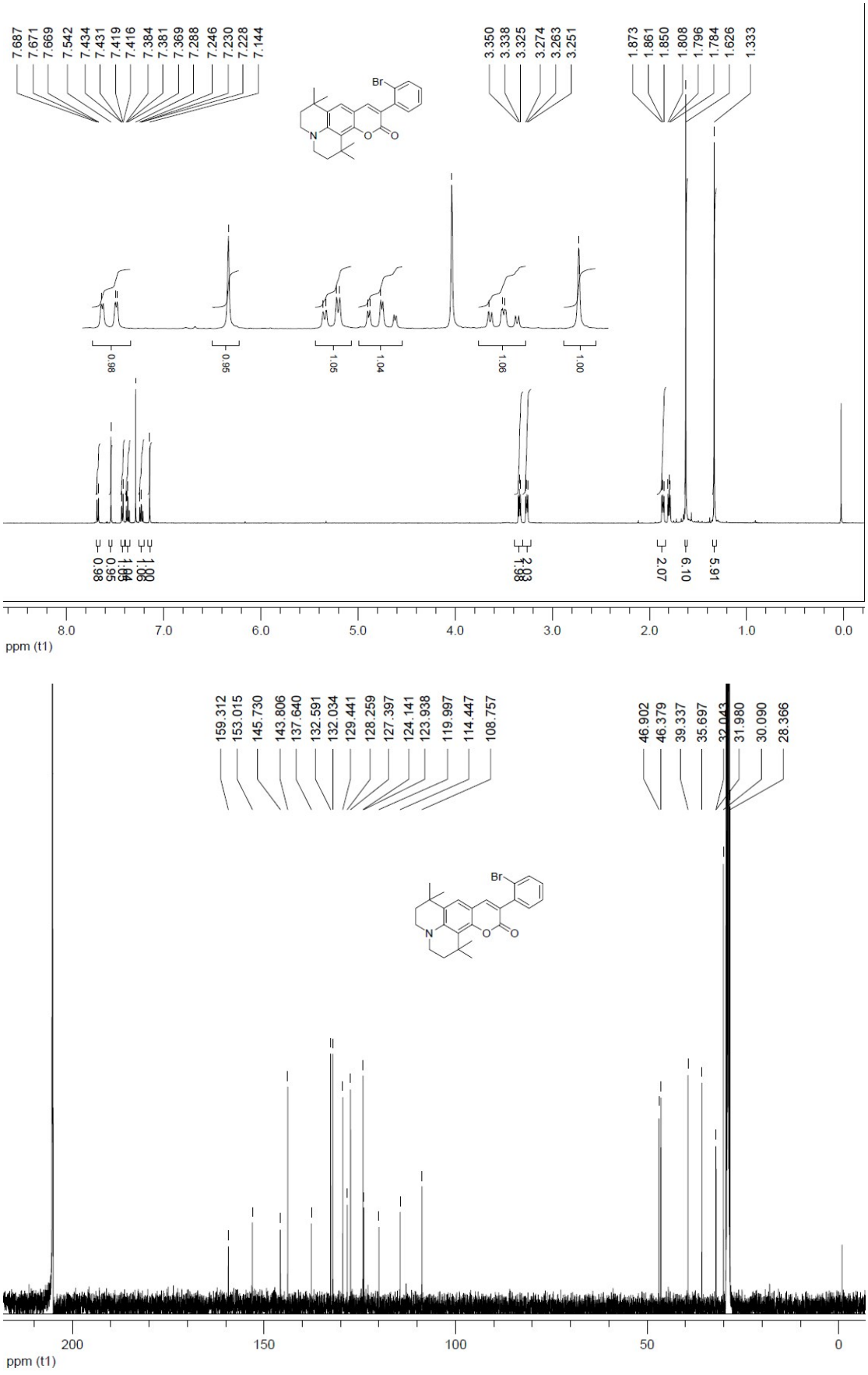

Fig. S3 ^{1}H and ^{13}C NMR spectra of intermediate **b-3**.

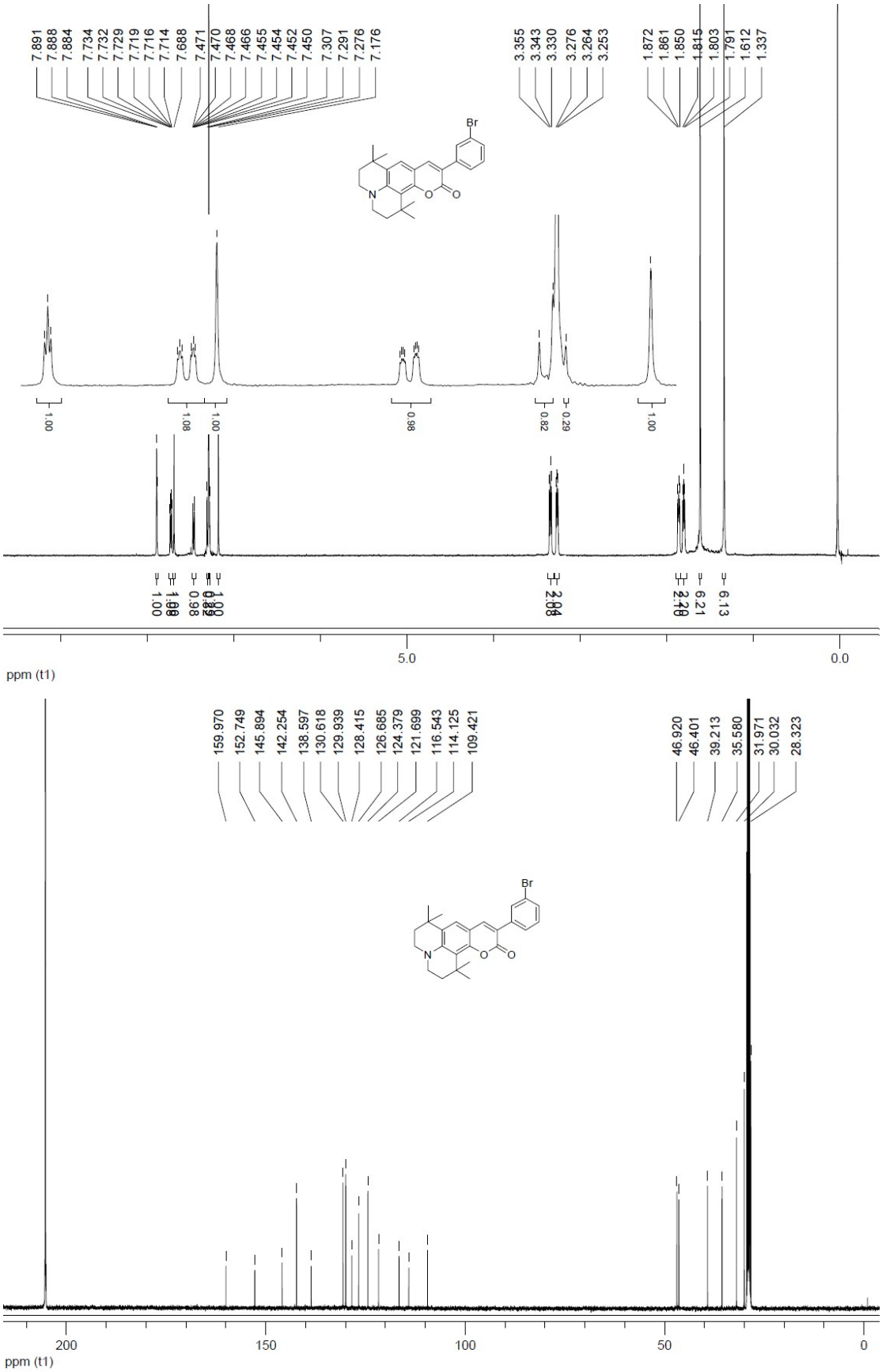

Fig. S4 ^{1}H and ^{13}C NMR spectra of intermediate **b-4**.

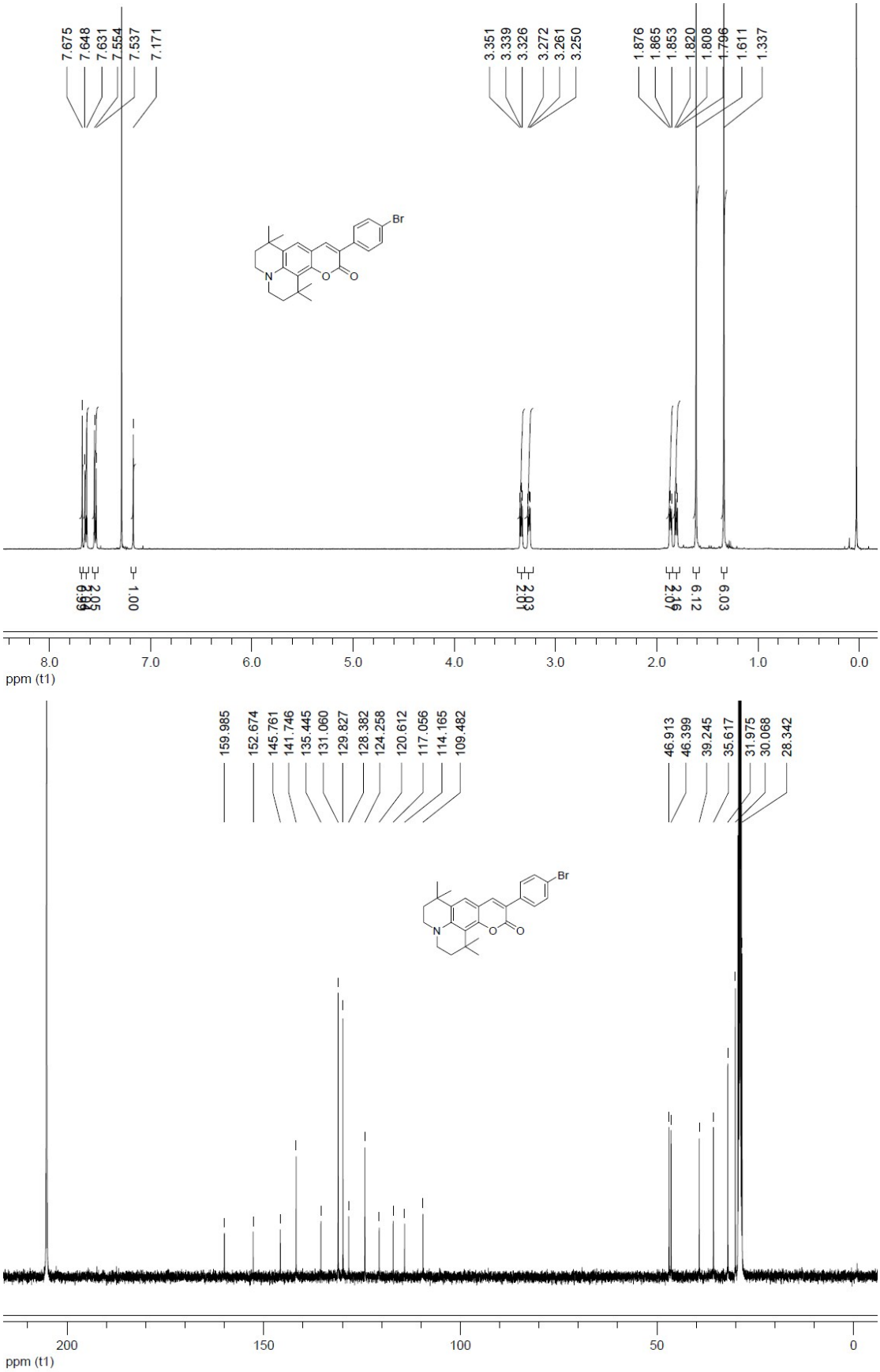

Fig. S5 ^{1}H and ^{13}C NMR spectra of intermediate **b-5**.

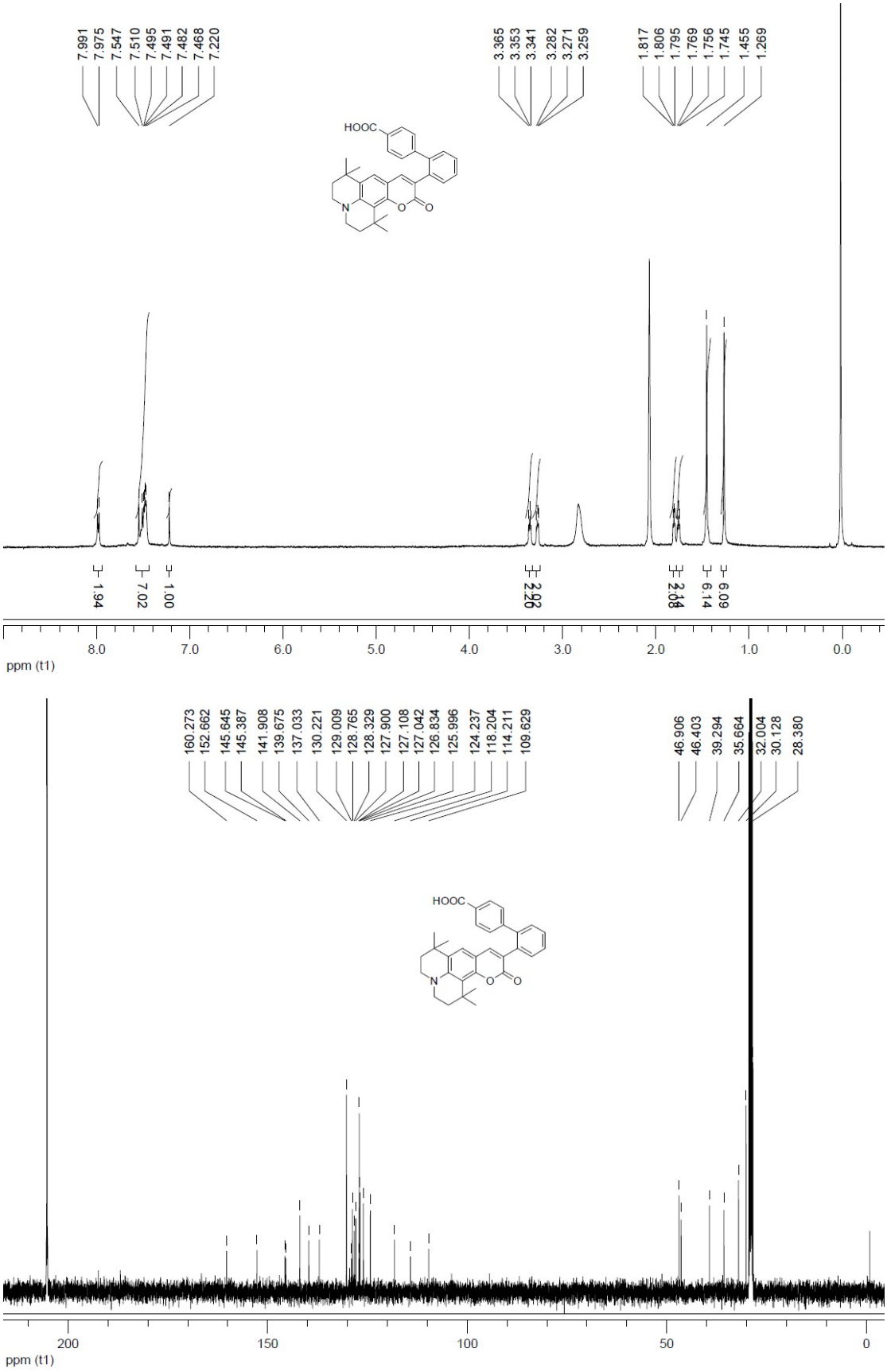

Fig. S6 ^{1}H and ^{13}C NMR spectra of intermediate **CS-3**.

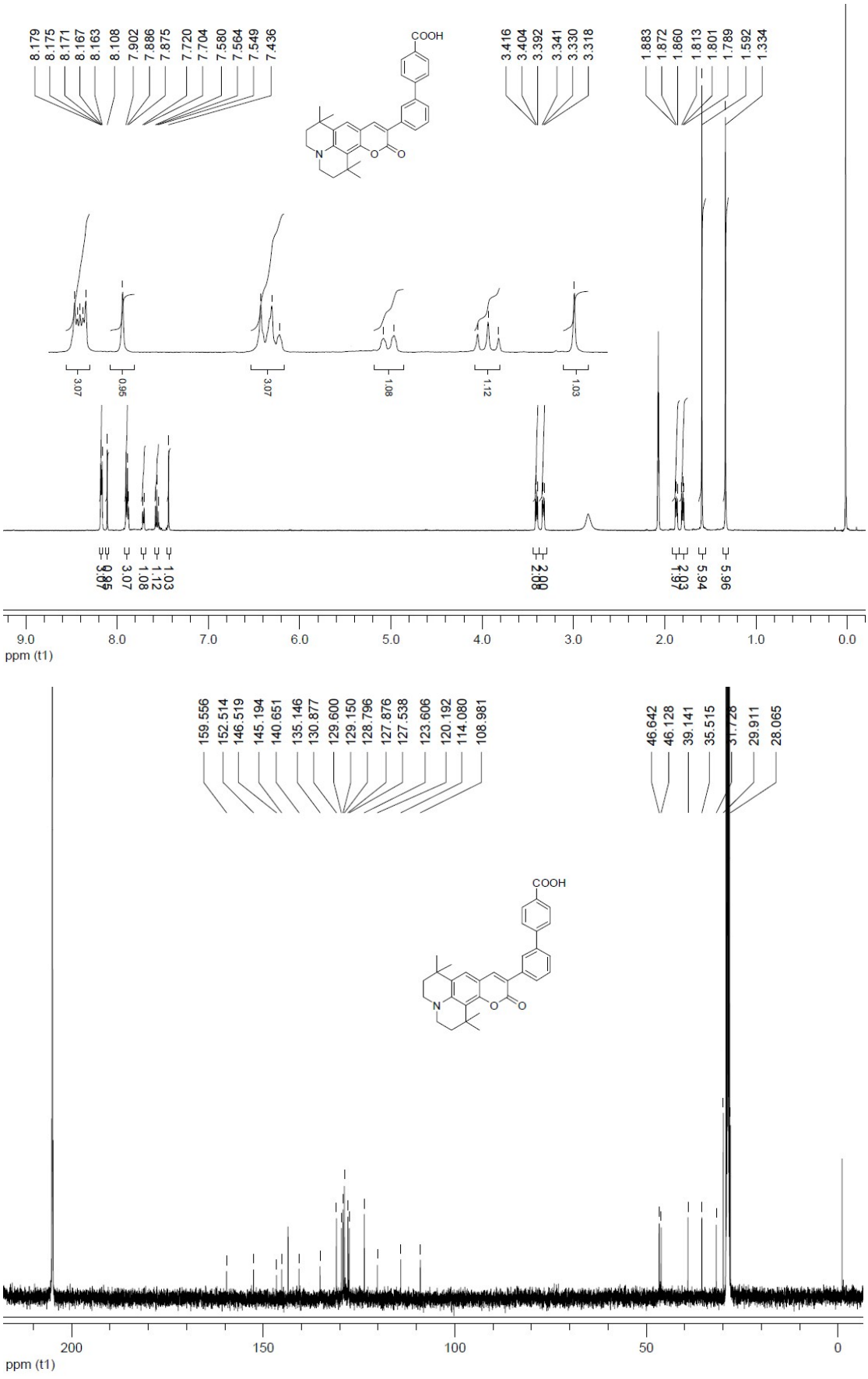

Fig. S7 ^{1}H and ^{13}C NMR spectra of intermediate **CS-4**.

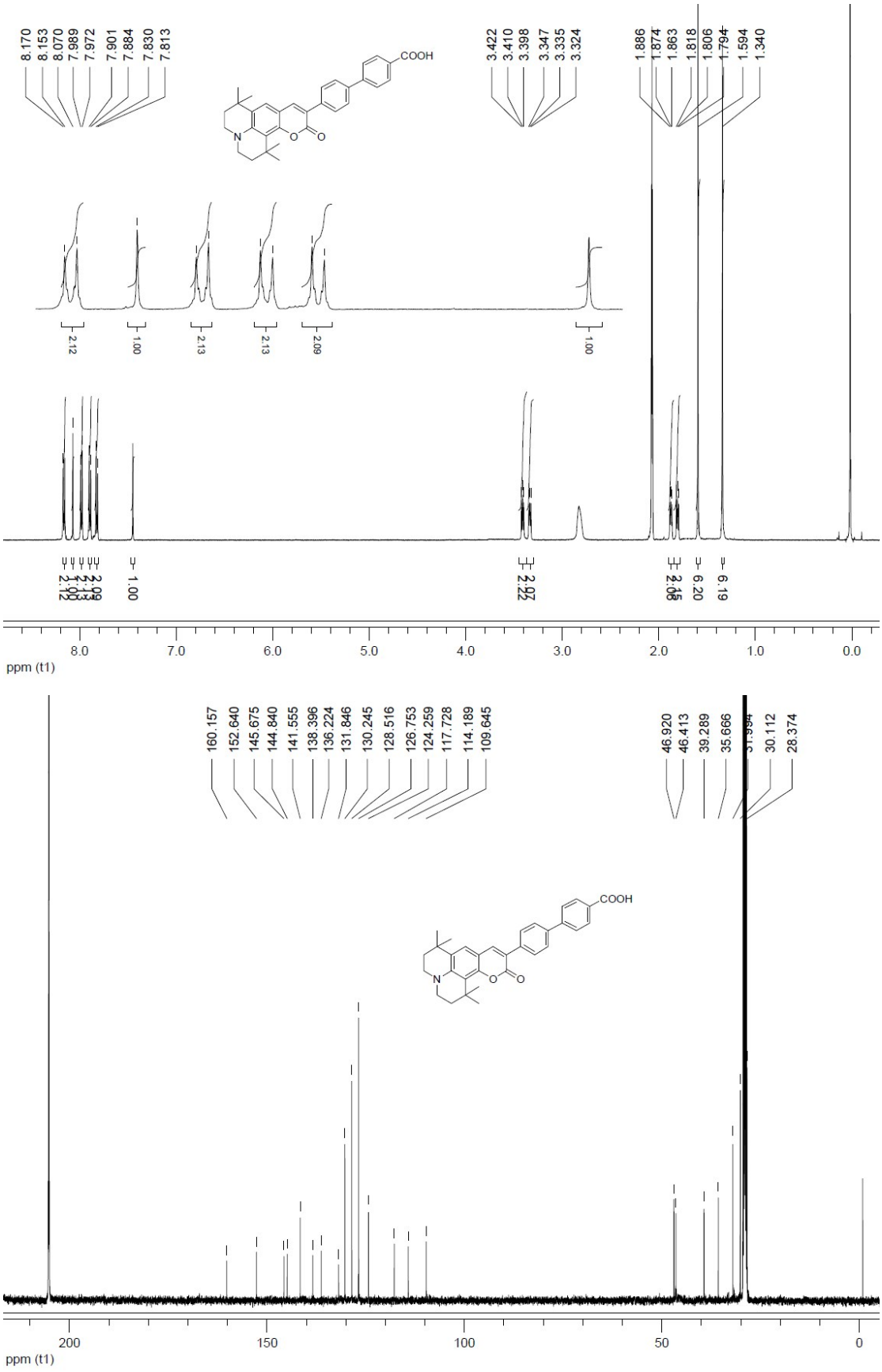

Fig. S8 ^{1}H and ^{13}C NMR spectra of intermediate **CS-5**.