Supplementary Materials: Molecular Level Factors Affecting the Efficiency of Organic Chromophores for *p*-Type Dye Sensitized Solar Cells

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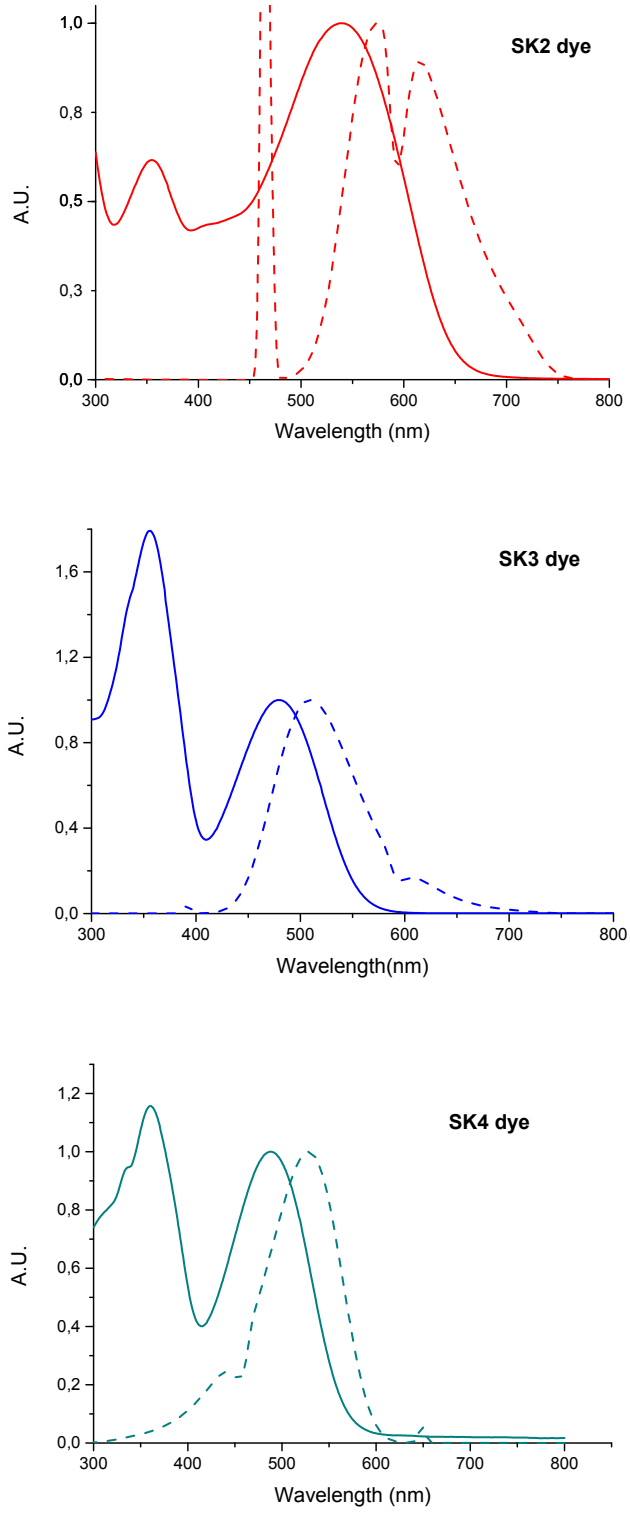


Figure S1. Normalized absorption and emission spectra of the SK dye series.

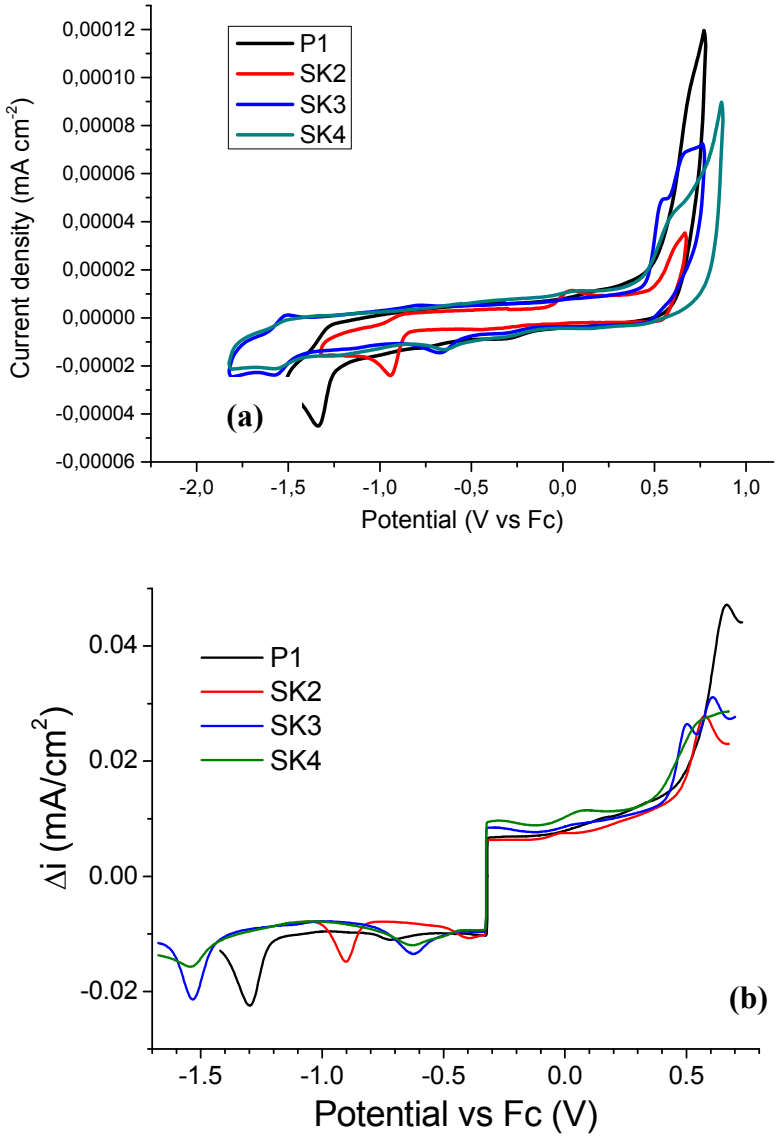


Figure S2. Dyes Electrochemistry: (**a**) Cyclic voltammetry (scan rate of 50 mVs^{-1}) and (**b**) DPVs (scan rate 20 mVs^{-1}) of **P1**, **SK2**, **SK3,** and **SK4** in 0.1 M solution of tetrabutylammonium perchlorate in anhydrous DMSO.

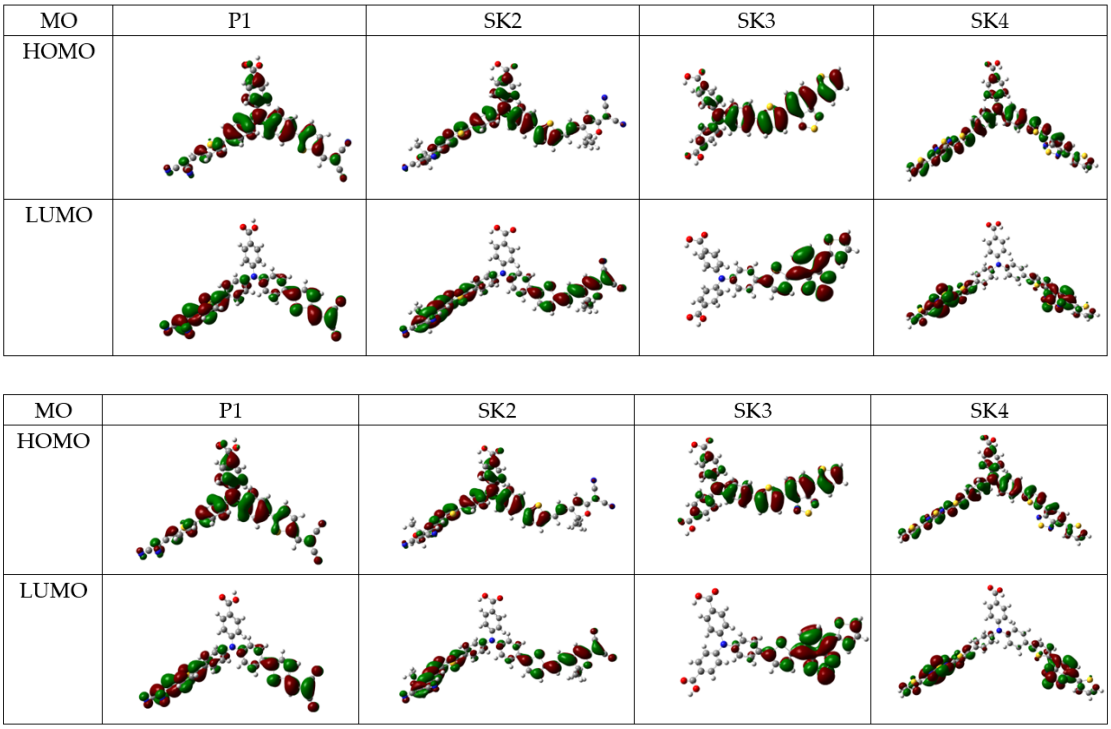


Figure S3. Isodensity (0.02) plots of HOMOs and LUMOs calculated at the DFT 6311G,d,+ level employing the BH&H (top) and the B3LYP (bottom) functionals.

Table S1. HOMO-LUMO energy gap ($\Delta E_{(HOMO\text{-}LUMO)}$) and Exciton Binding Energy (EBE) calculated according to EBE = $\Delta E_{(HOMO\text{-}LUMO)} - E^{op}$. [a]

Dye	$\Delta E_{(HOMO\text{-}LUMO)}$(eV) BH & H	$\Delta E_{(HOMO\text{-}LUMO)}$(eV) B3LYP	EBE BH & H	EBE B3LYP
P1	4.20	2.47	1.41	0.17
SK2	4.17	2.41	1.31	0.33
SK3	4.20	2.52	1.58	0.38
SK4	3.90	2.27	1.42	0.35

[a] E^{op} is the lowest vertical excitation energy calculated with the B3LYP and BH&H functionals.

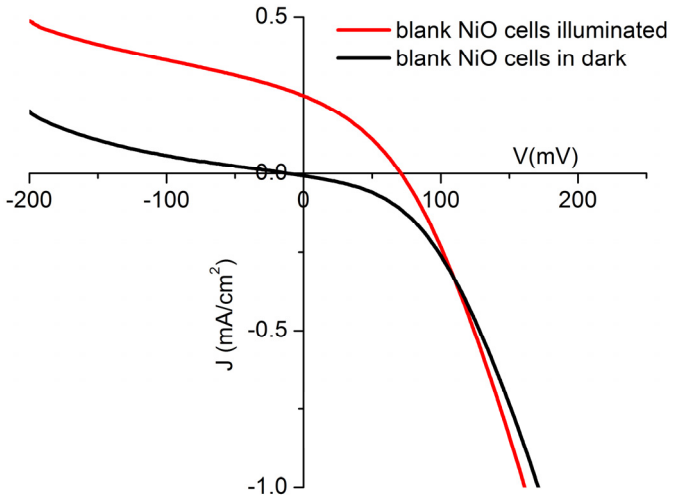


Figure S4. *J*/*V* characteristics and under AM 1.5 illumination (**red**) and in the dark (**black**) of a blank NiO cells (bare NiO in contact with iodide based electrolyte).

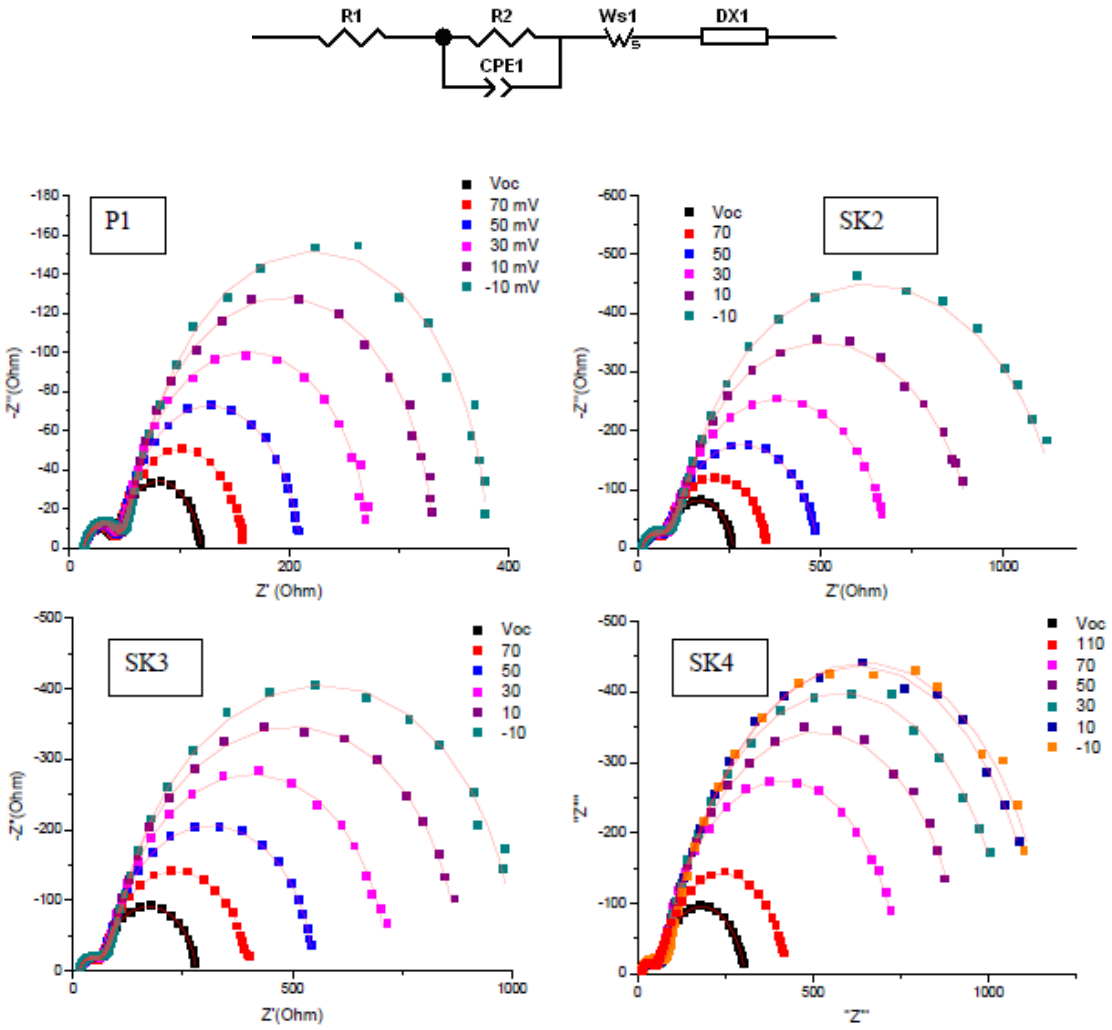


Figure S5. EIS spectra at different applied voltages.

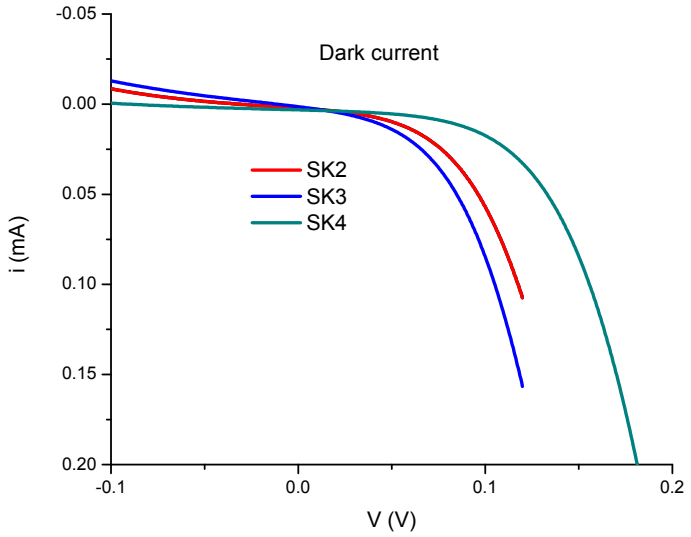


Figure S6. Dark currents of the sensitized NiO DSSCs (SK series).

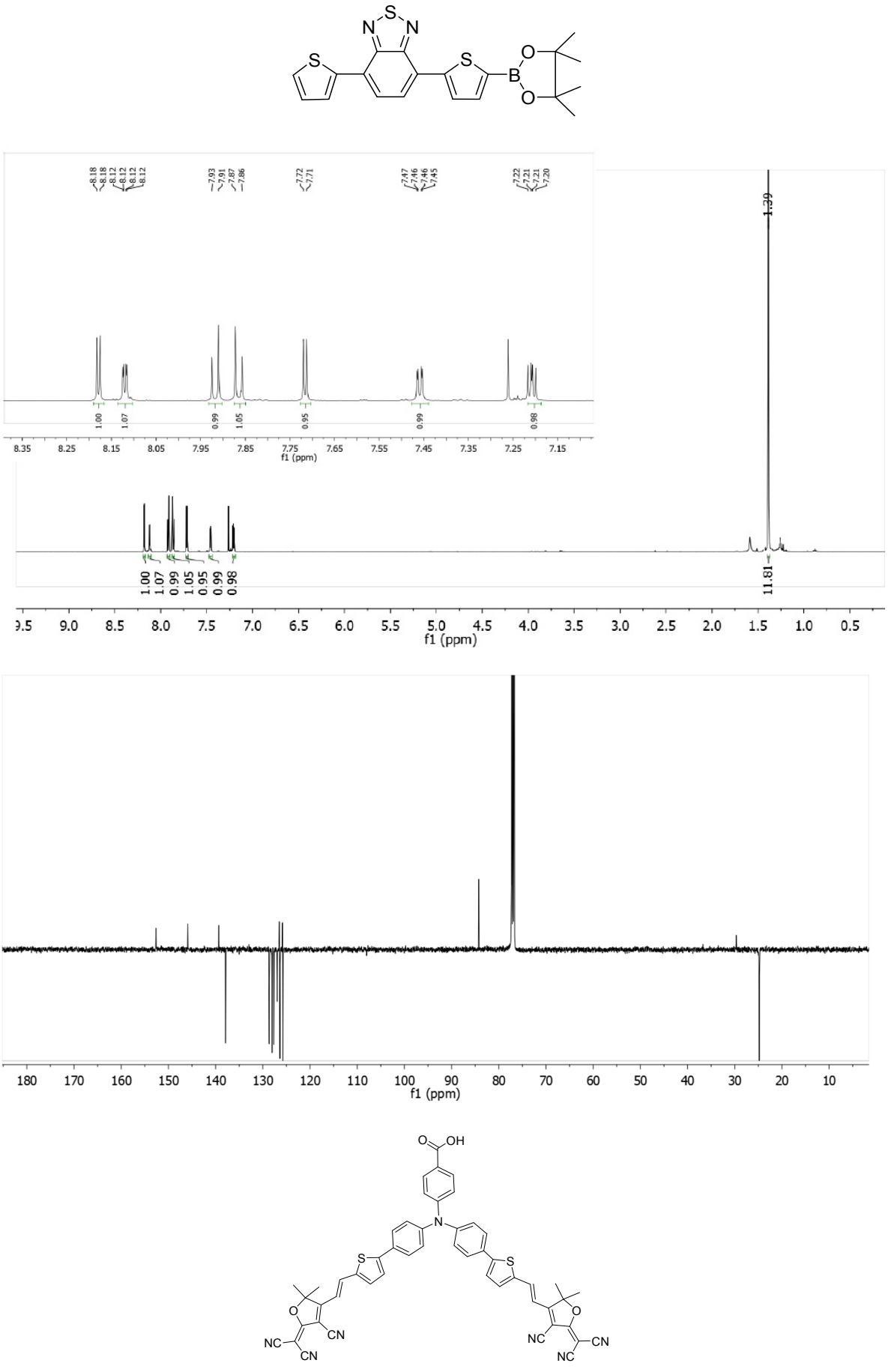


Figure S7. *Cont.*

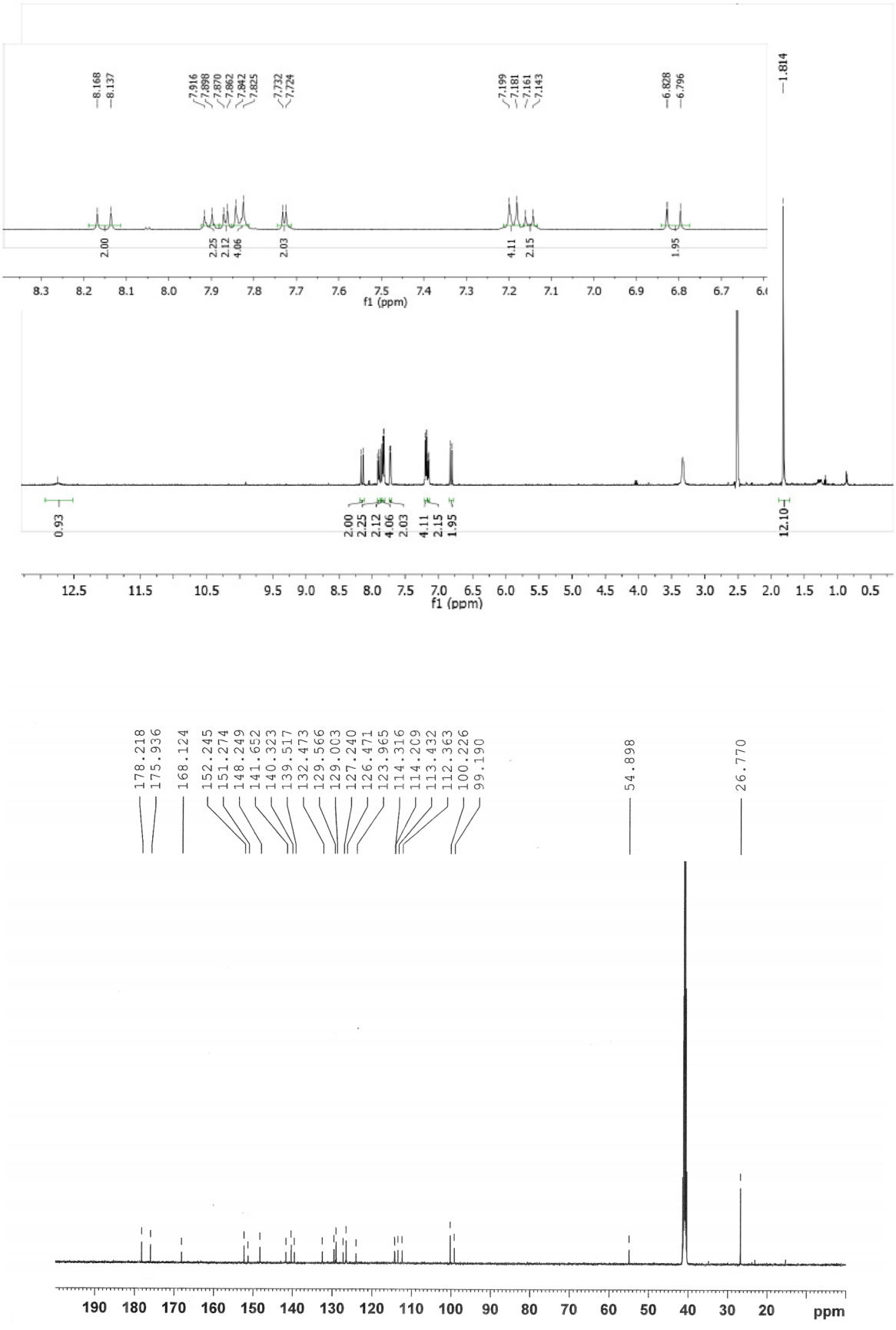
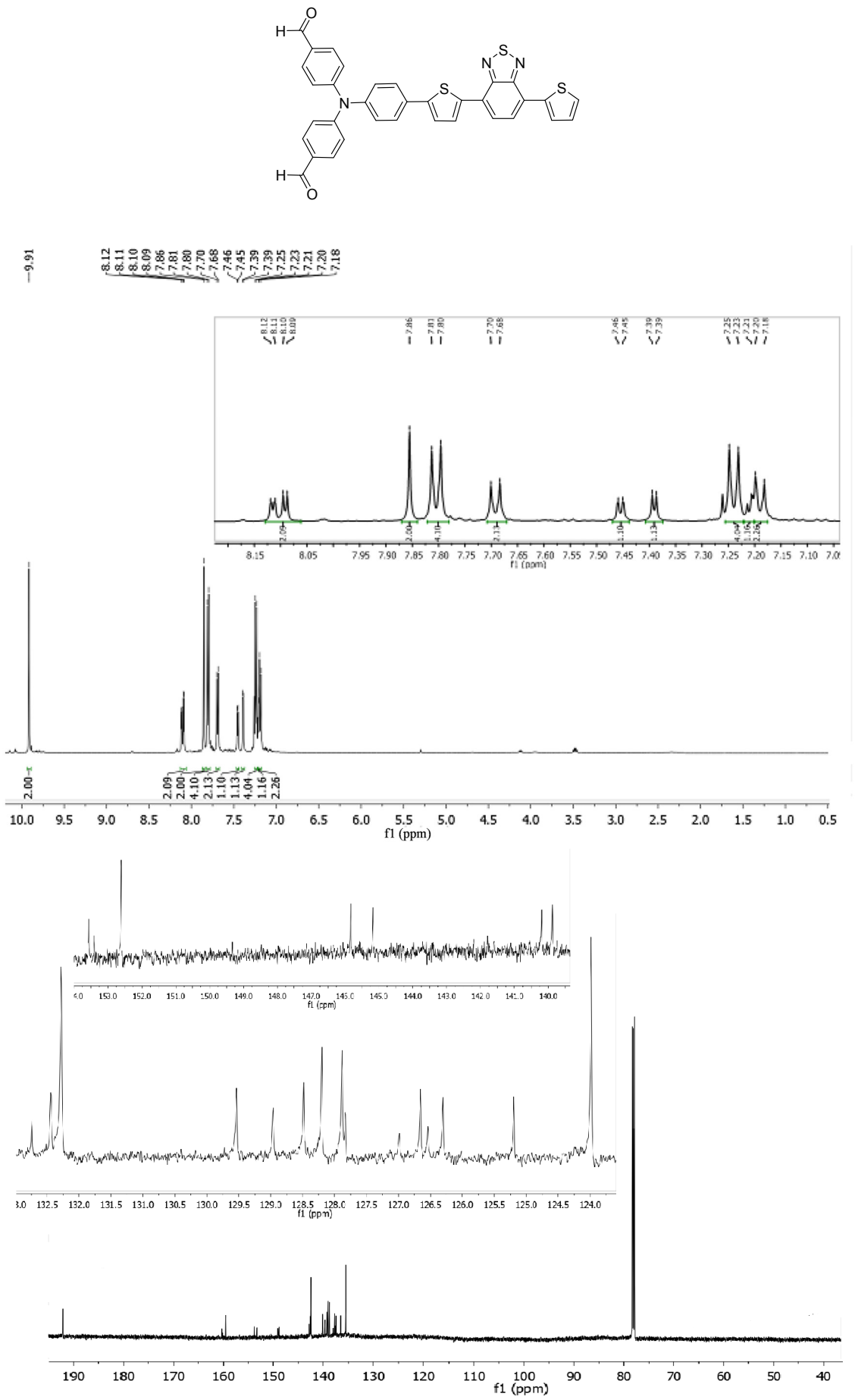


Figure S7. *Cont.*



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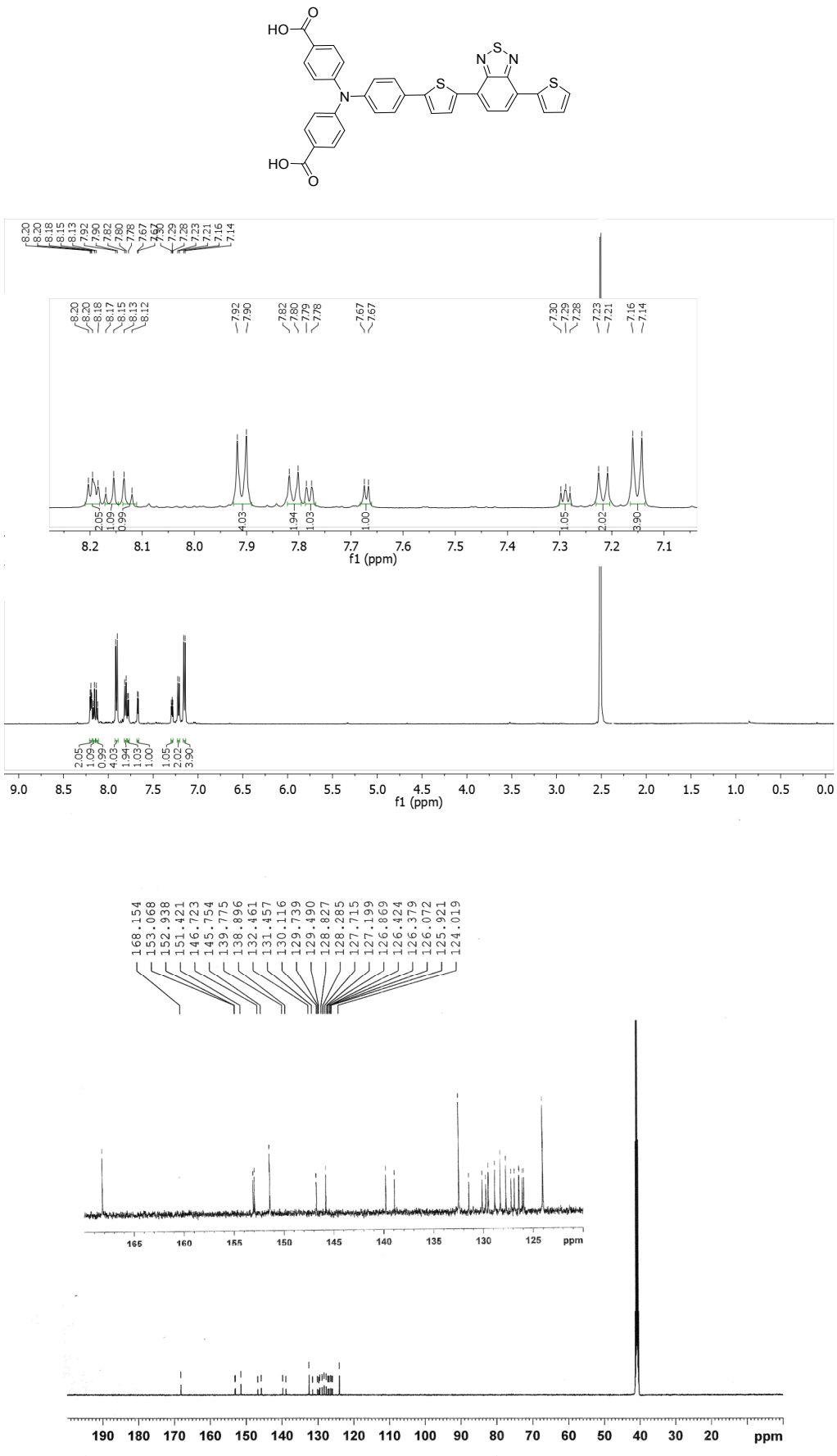

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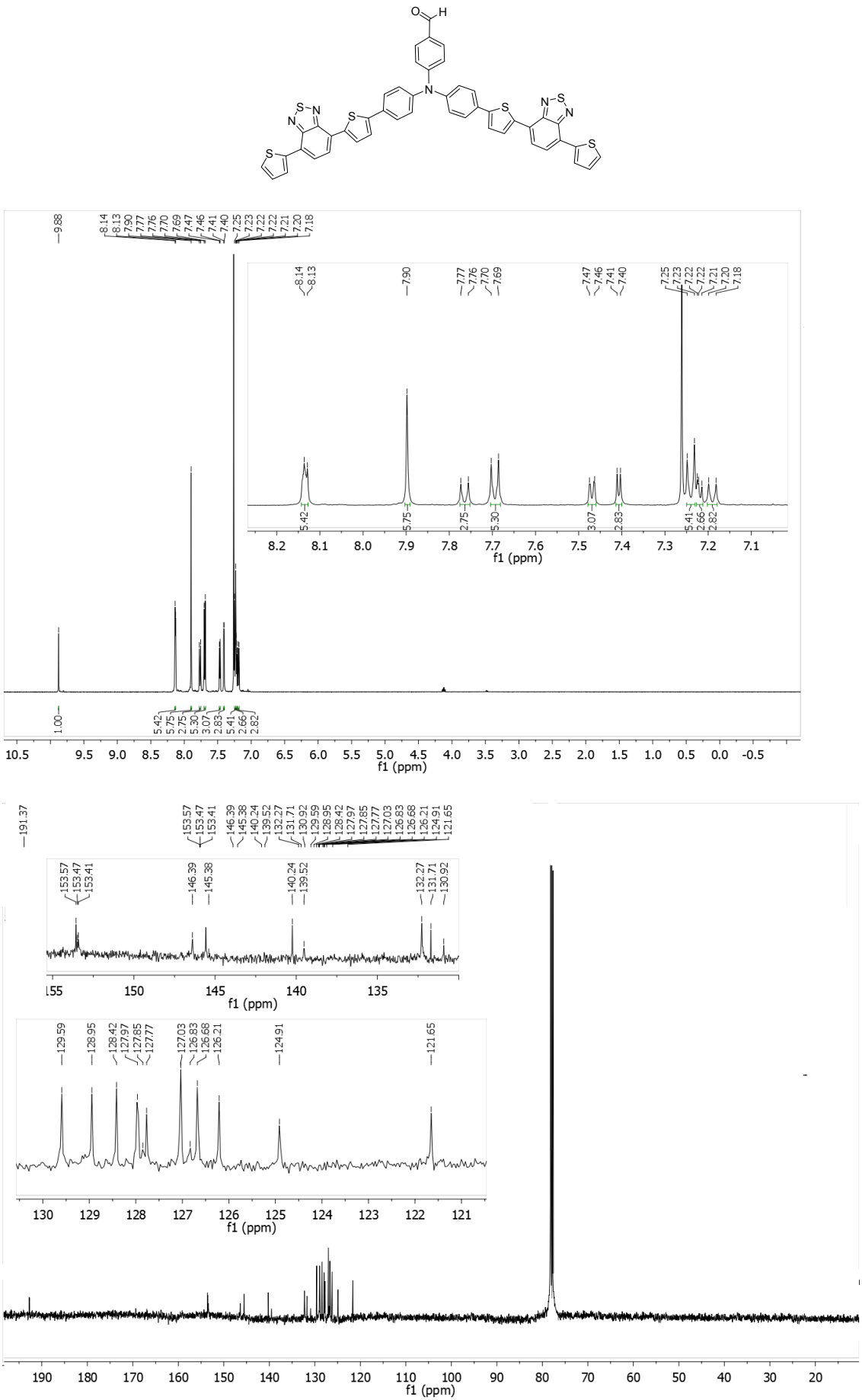

Figure S7. *Cont.*

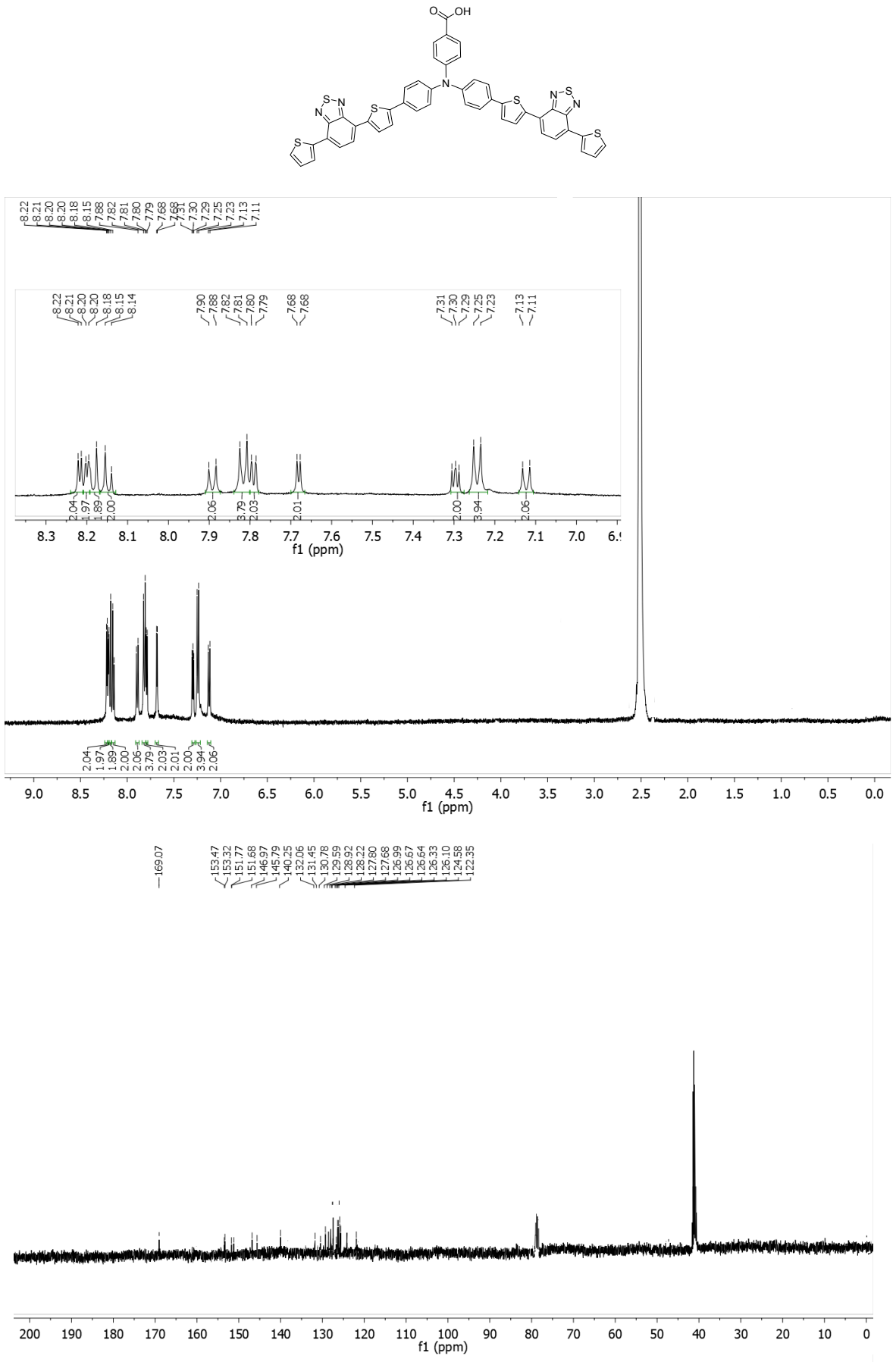

Figure S7. 1H- and 13C-NMR spectra of intermediates and dyes.