

## **Di-branched Di-anchoring Organic Dyes for Dye-Sensitized Solar Cells**

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### **Electronic Supplementary Information**

- Table S1. Calculated excitation energies and oscillator strengths for the protonated form of D5 in vacuo and in ethanol solution.
- Figures S1 – S6. <sup>1</sup>H and <sup>13</sup>C NMR spectra of DB-1 and DB-2.
- Figure S7. UV-Vis and emission spectra of DB-1.
- Figure S8. ATR-FTIR spectra of free dyes D5, DB-1 and DB-2.
- Figure S9. ATR-FTIR spectra of D5, DB-1 and DB-2 stained TiO<sub>2</sub> films

Table S1. Calculated excitation energies (eV) and oscillator strengths (data in parentheses) for the protonated form of D5 in vacuo and in ethanol solution. The experimental absorption maximum is measured at 2.63 eV.

|                       | B3LYP       |             | MPW1K       |             |
|-----------------------|-------------|-------------|-------------|-------------|
|                       | Vacuo       | Solution    | Vacuo       | Solution    |
| $S_0 \rightarrow S_1$ | 2.23 (1.11) | 2.00 (1.20) | 2.70 (1.61) | 2.47 (1.67) |

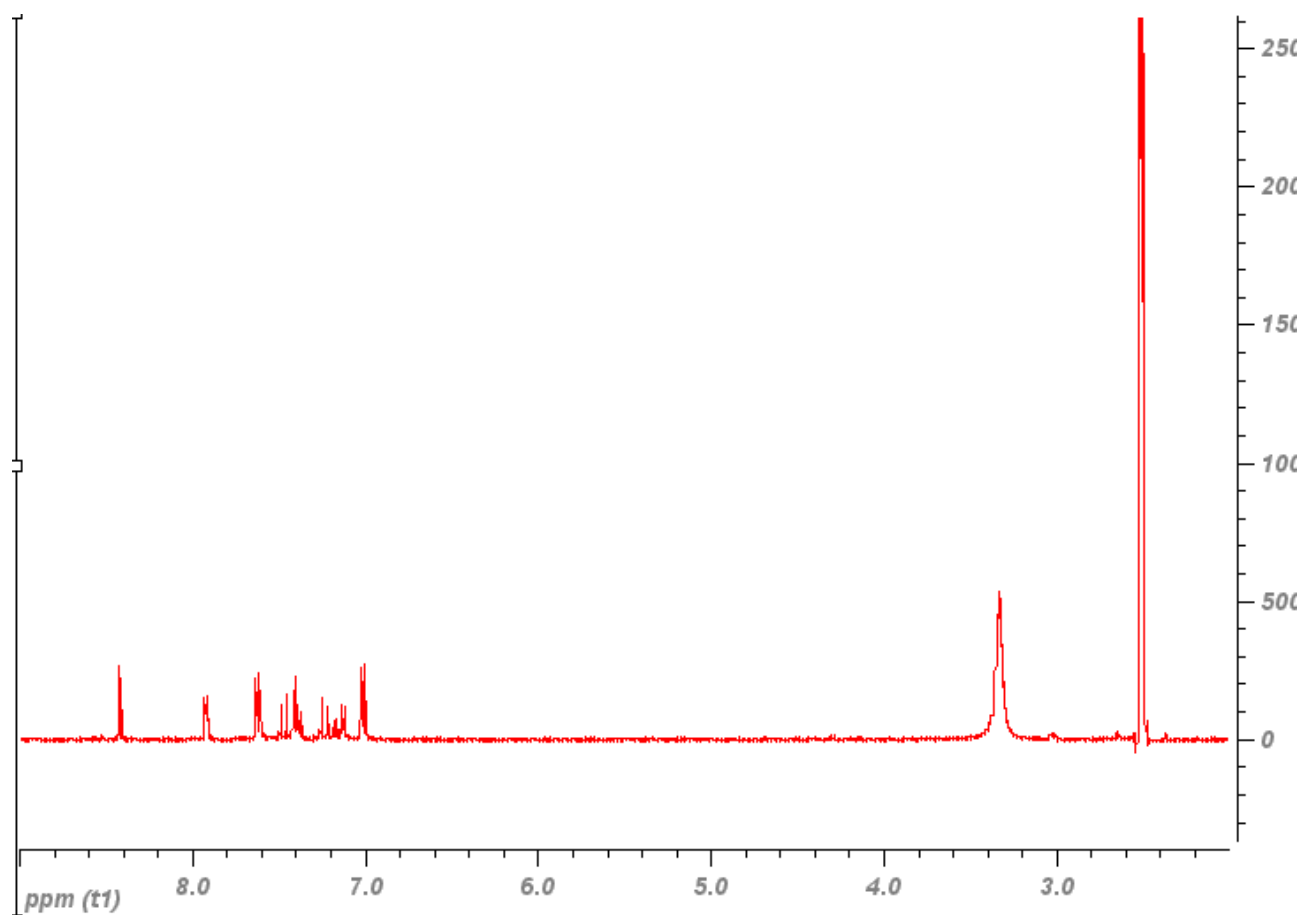


Figure S1.  $^1\text{H}$  NMR of DB-1 (500 MHz,  $\text{DMSO-}d_6$ )

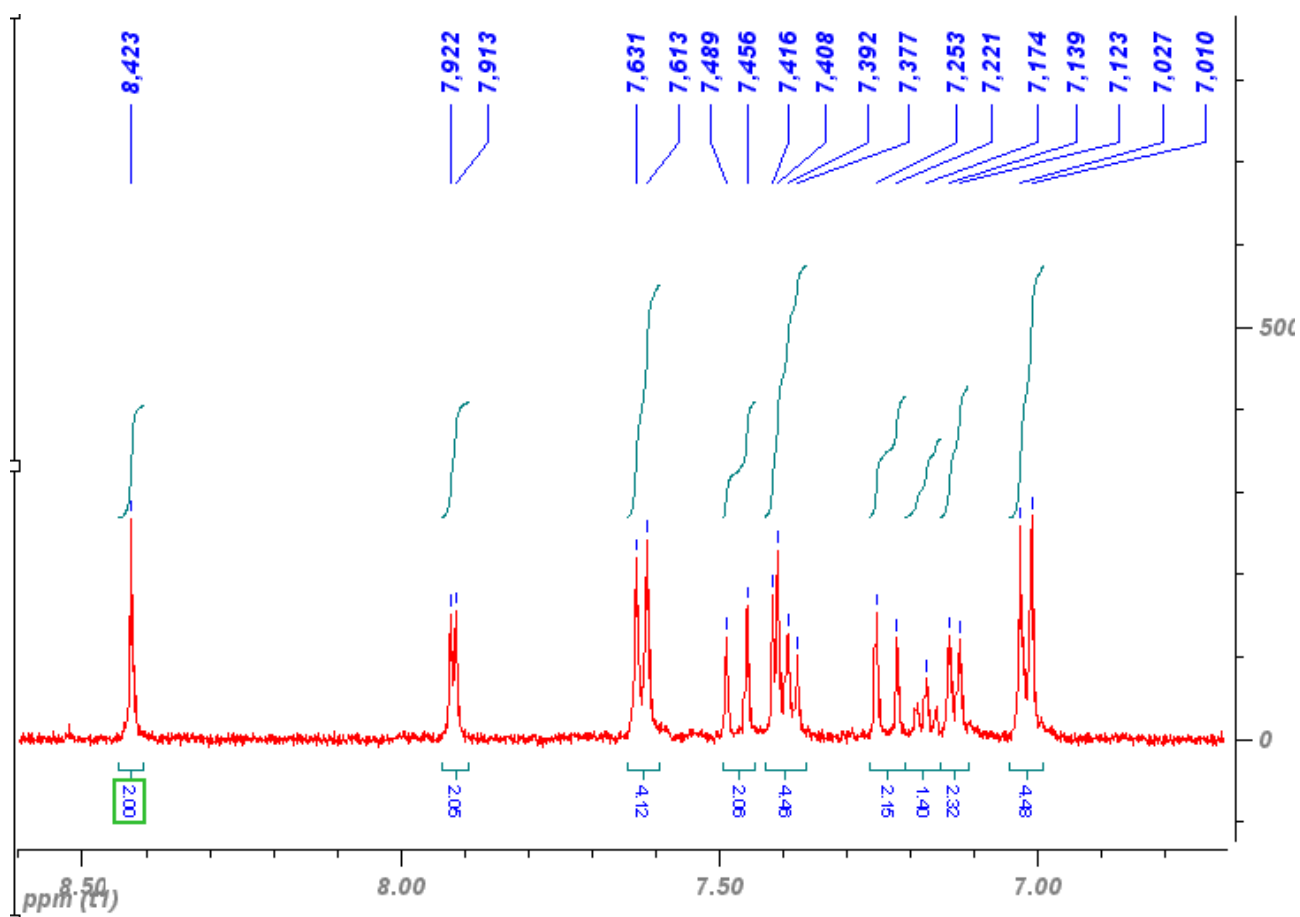


Figure S2.  $^1\text{H}$  NMR of DB-1 (500 MHz,  $\text{DMSO}-d_6$ ) (aromatic region)

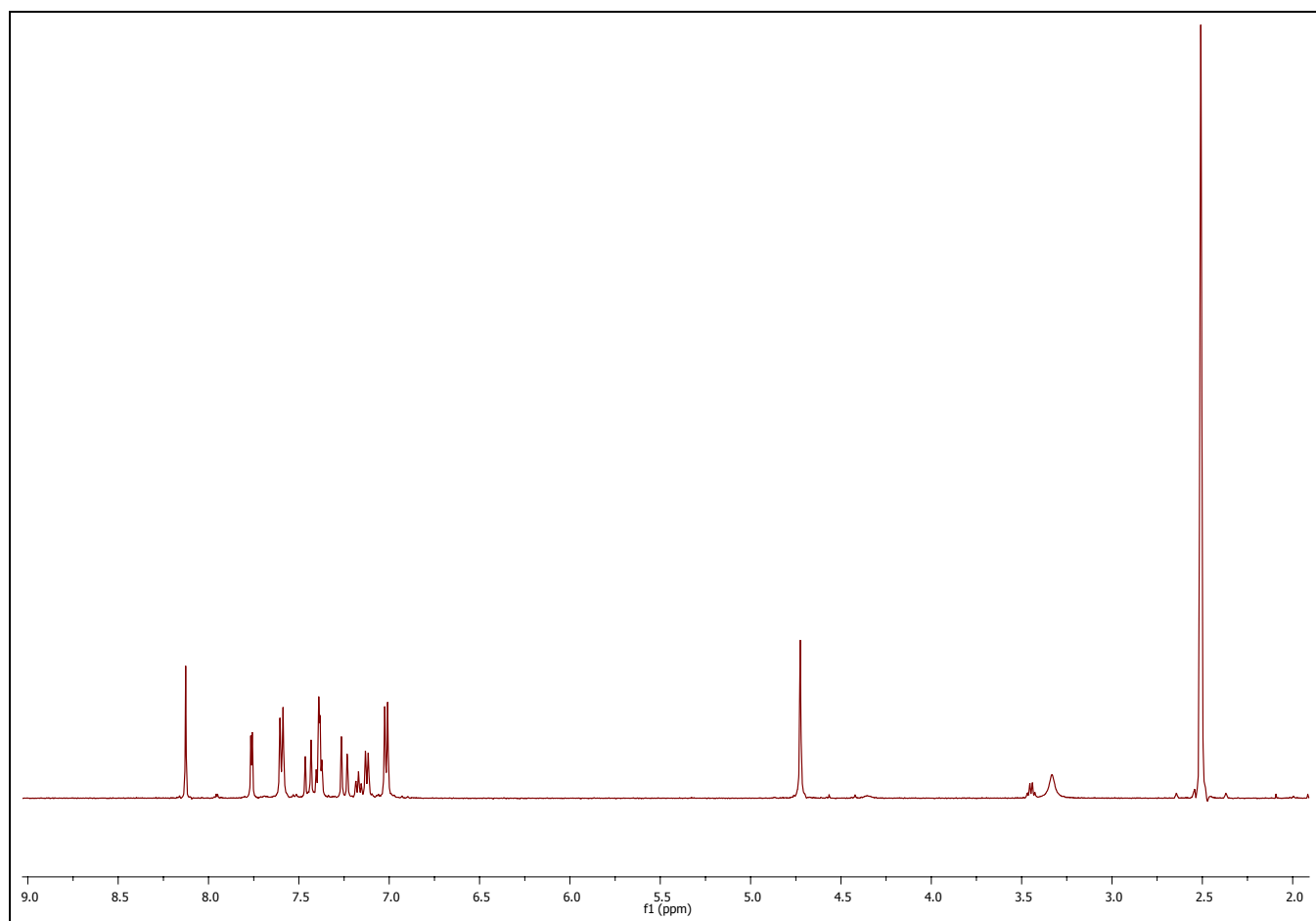


Figure S3. <sup>1</sup>H NMR of DB-2 (500 MHz, DMSO-*d*<sub>6</sub>)

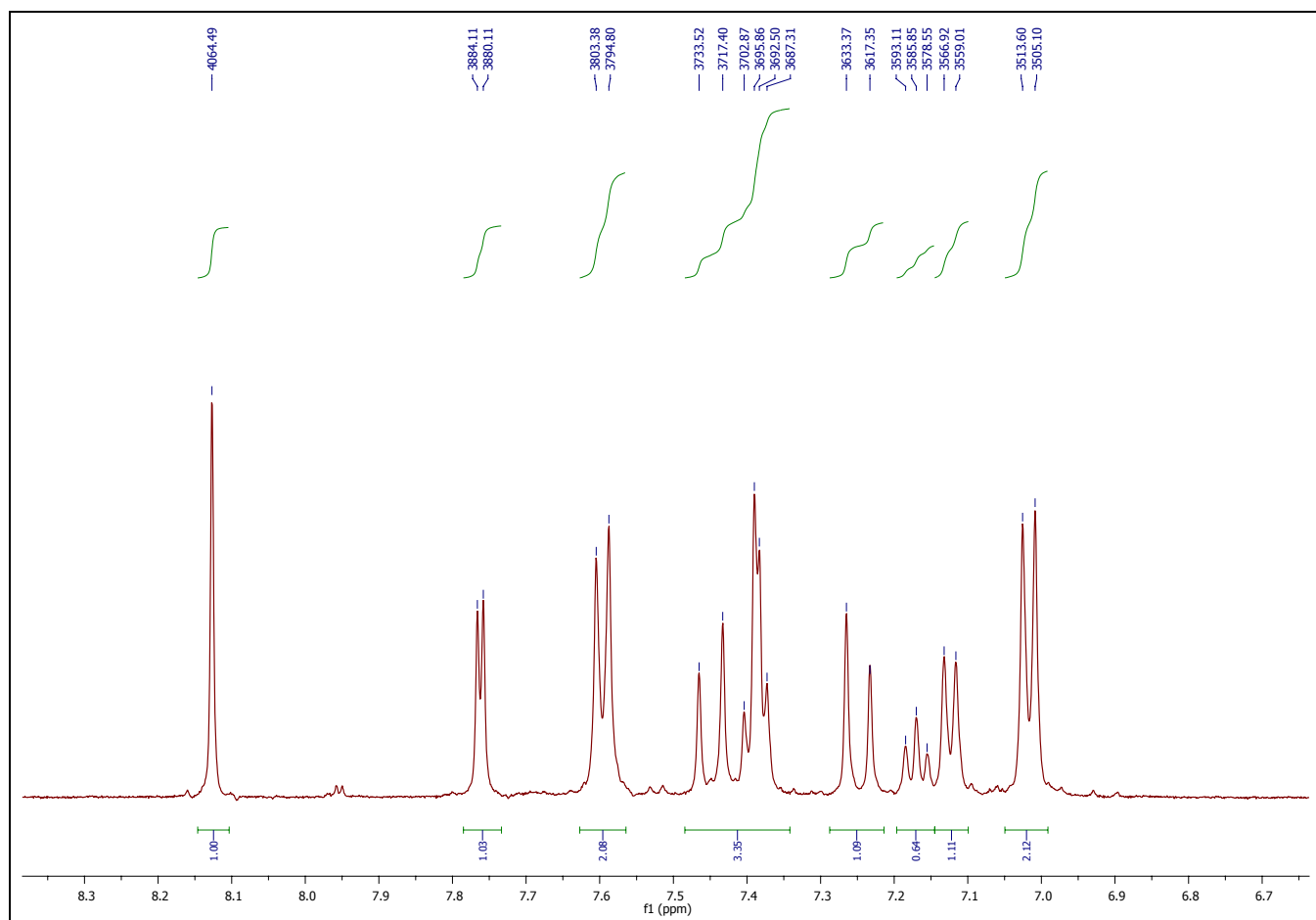


Figure S4.  $^1\text{H}$  NMR of DB-2 (500 MHz,  $\text{DMSO}-d_6$ ) (aromatic region)

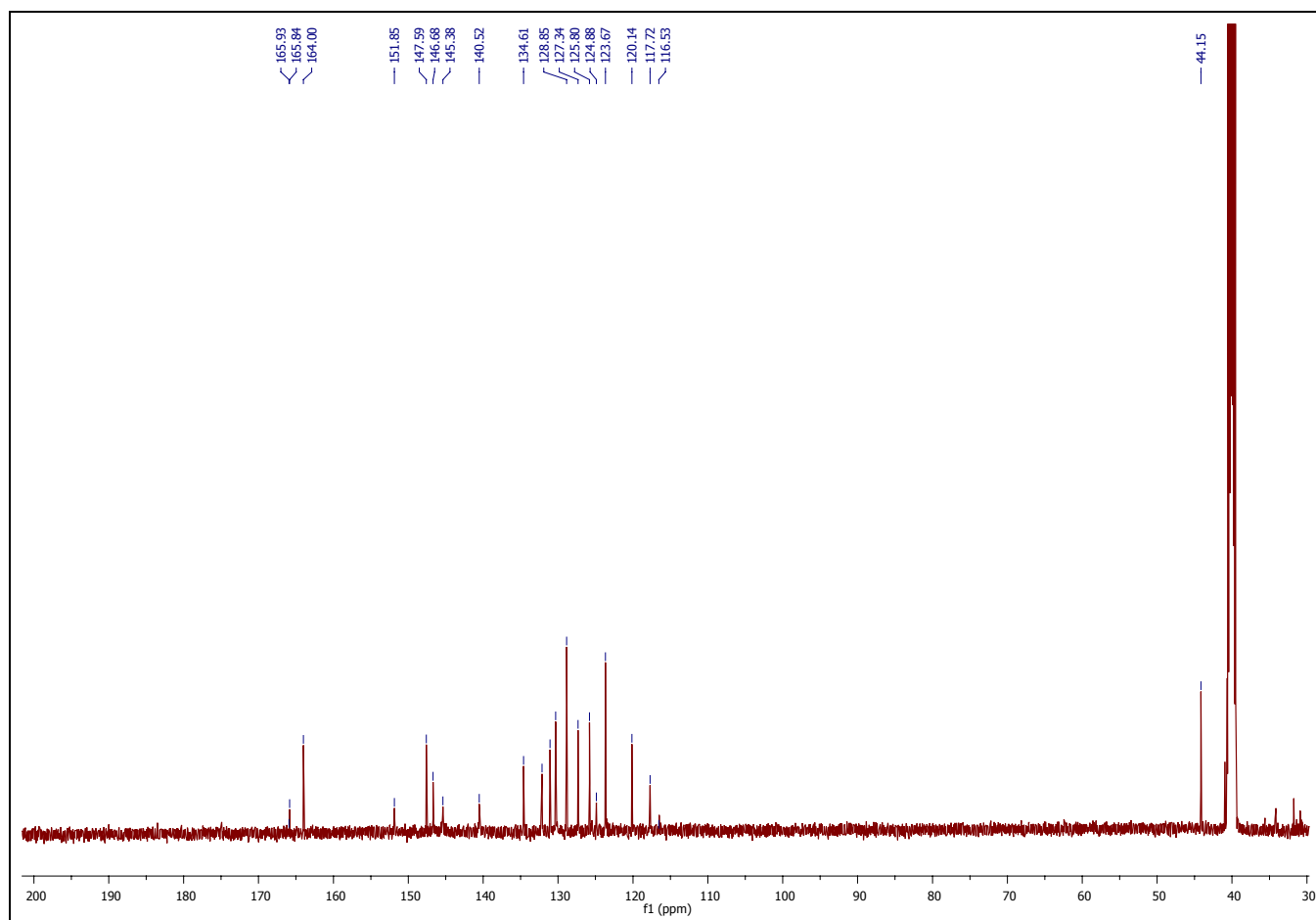


Figure S5.  $^{13}\text{C}$  NMR of DB-1 (125.77 MHz,  $\text{DMSO-}d_6$ )

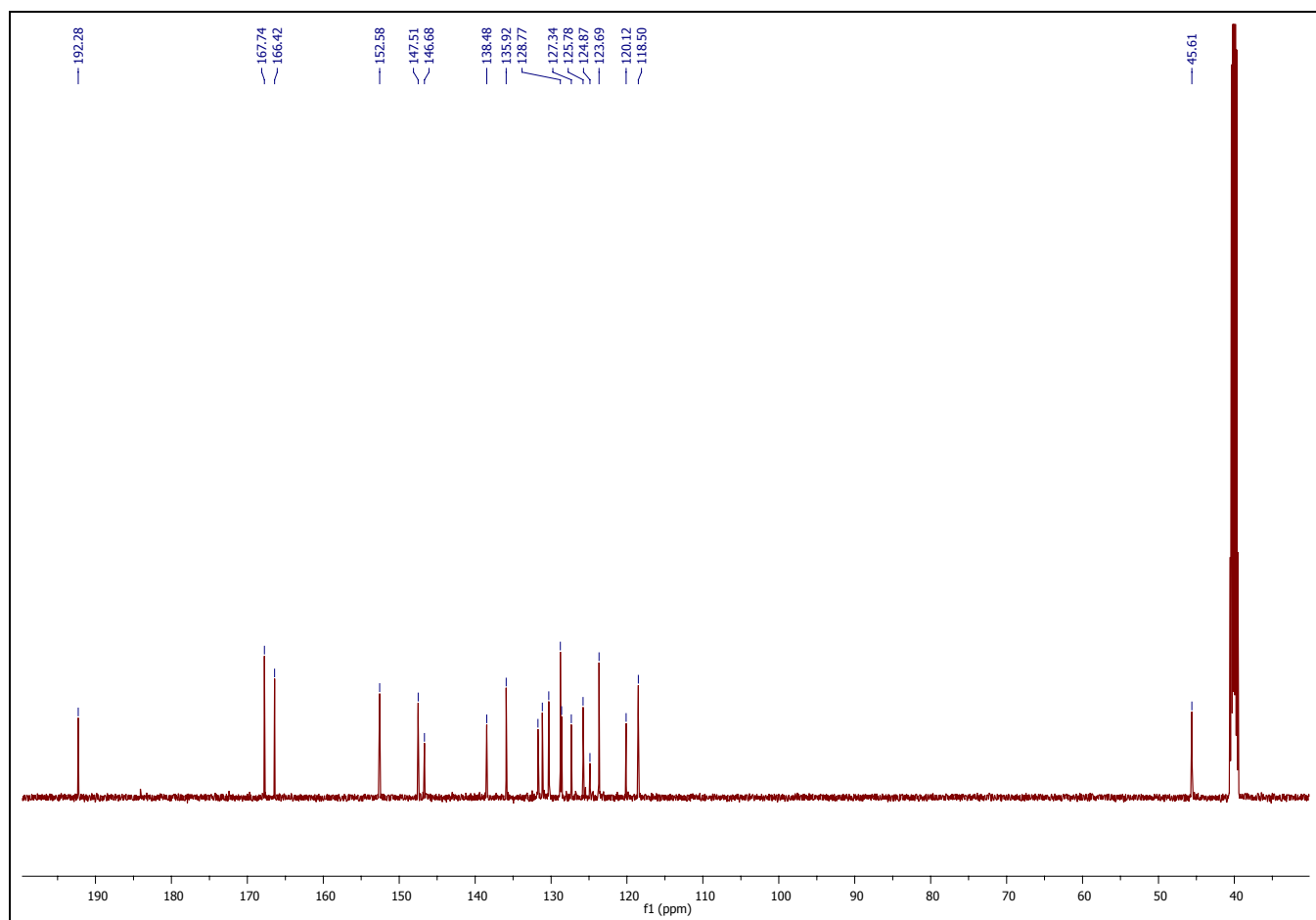


Figure S6.  $^{13}\text{C}$  NMR of DB-2 (125.77 MHz,  $\text{DMSO-}d_6$ )



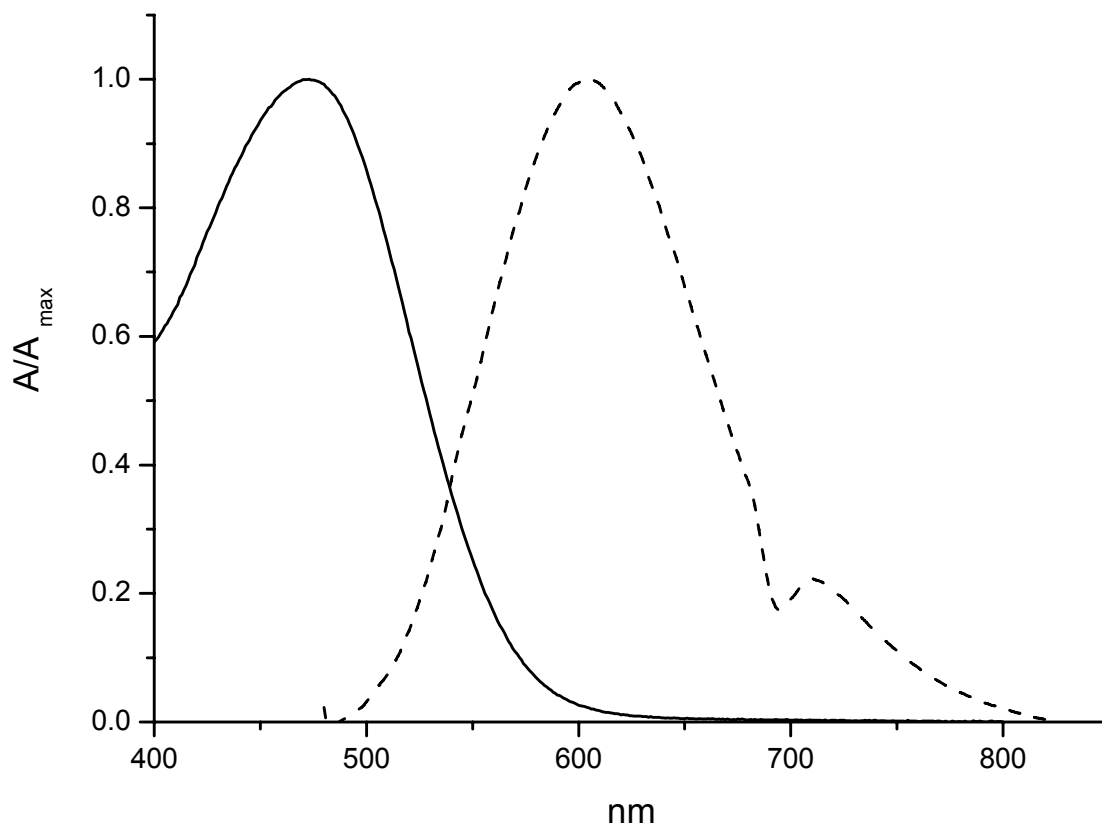


Figure S7. Normalized linear absorption (solid line) and emission (dashed line) spectra of DB-1 in EtOH.

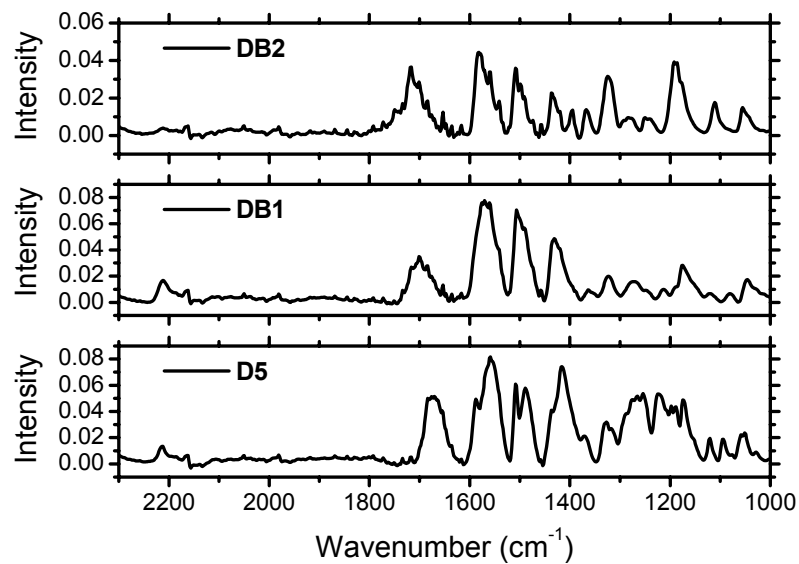


Figure S8. ATR-FTIR spectra of D5, DB-1, and DB-2 measured as solid powders.

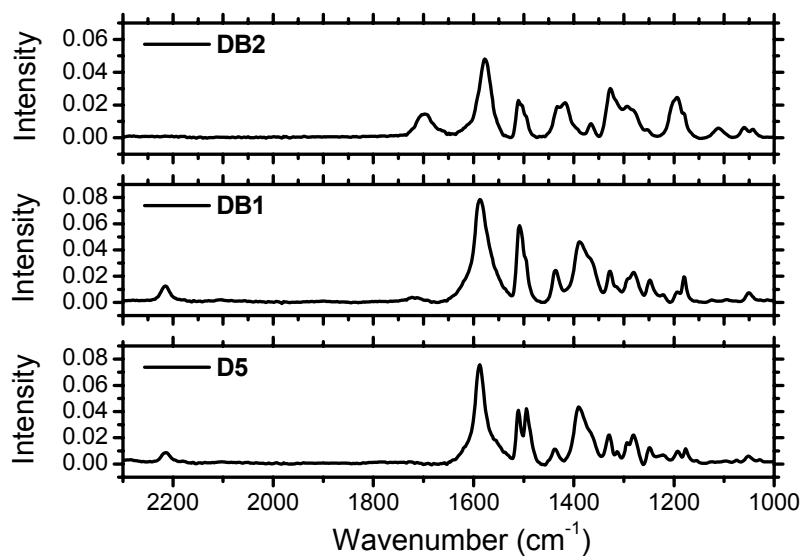


Figure S9. ATR-IR spectra of D5, DB-1, and DB-2 stained TiO<sub>2</sub> (~7 μm) films.