Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information for

Synthesis and Self-Assembly of Triphenylene-Containing Conjugated Macrocycles

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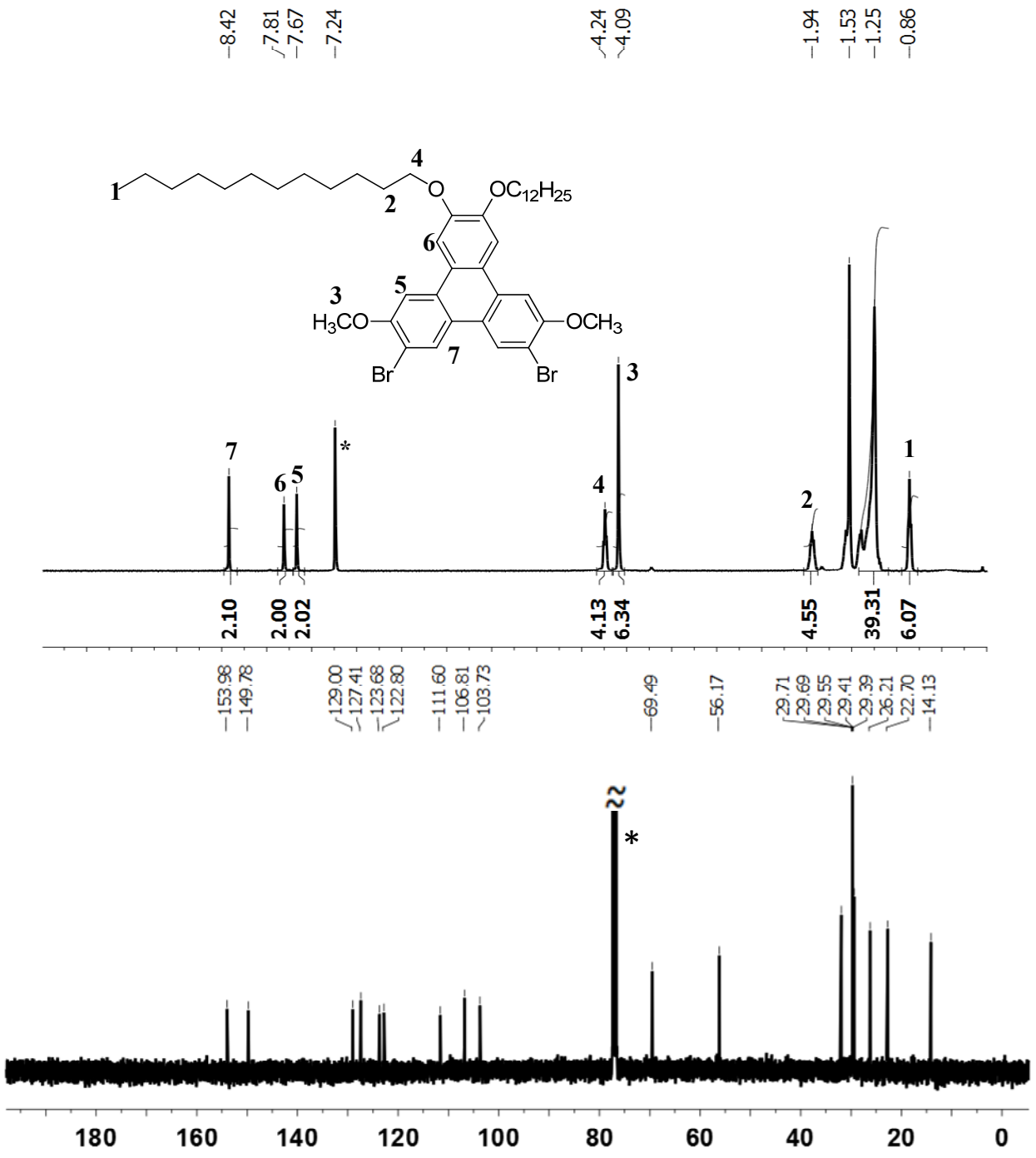

Figure S1: ^{1}H (top) and ^{13}C (bottom) NMR ($CDCl_3$, 298K) Spectra of **1** (*Solvent).

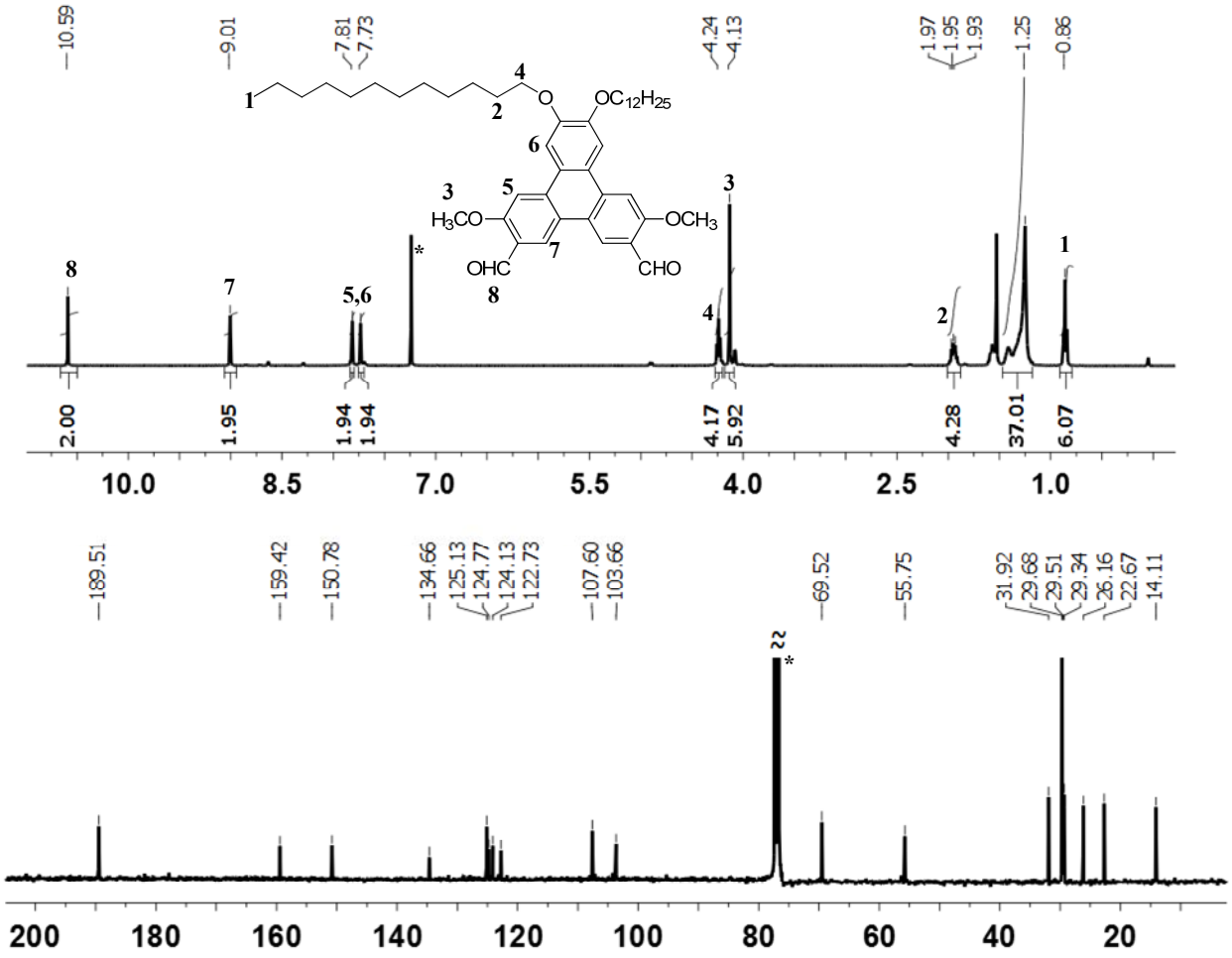

Figure S2: ^{1}H (top) and ^{13}C (bottom) NMR ($CDCl_3$, 298K) Spectra of **2** (*Solvent).

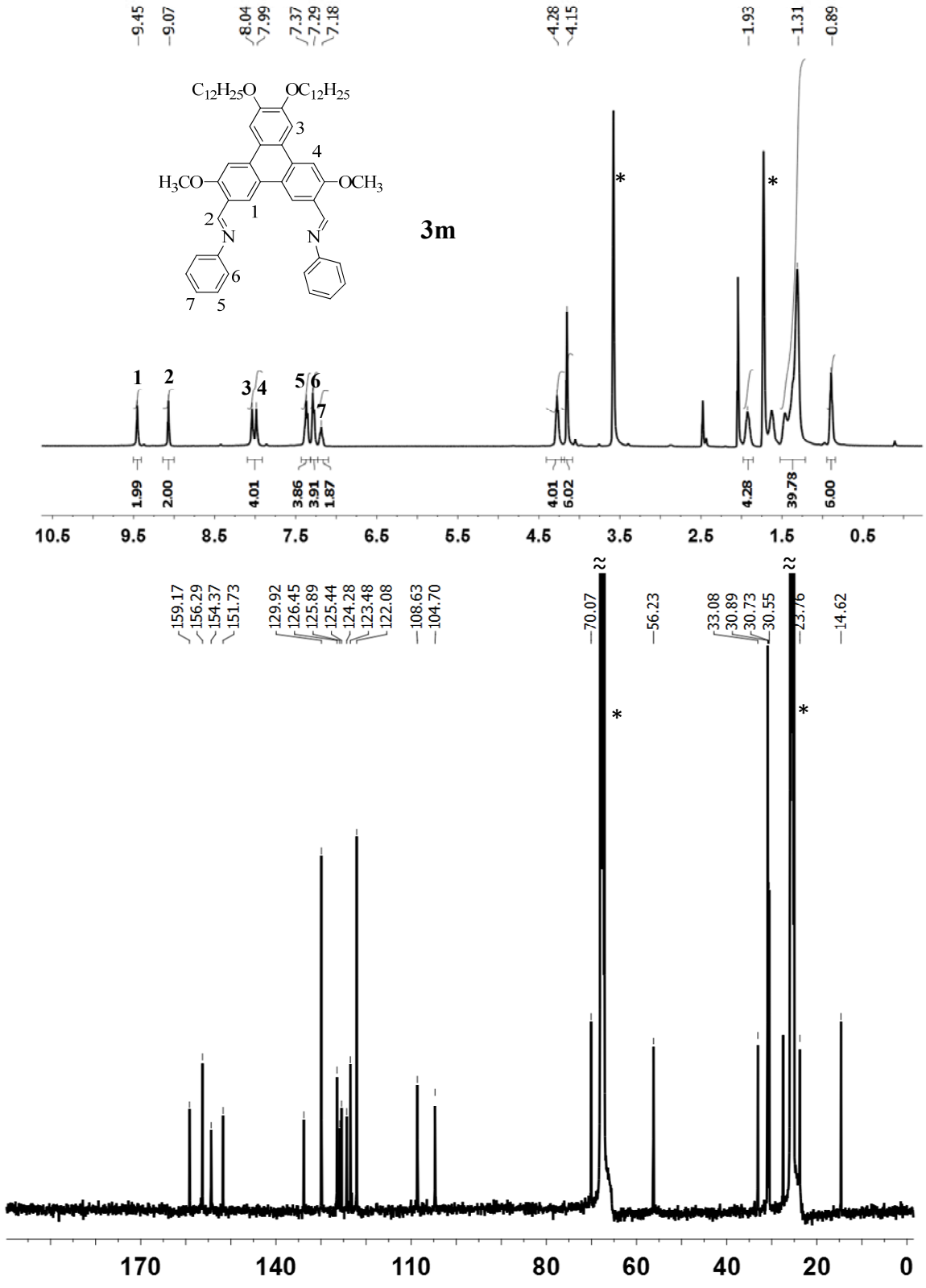

Figure S3: ^{1}H (top) and ^{13}C (bottom) NMR (THF-*d8*, 298K) Spectra of **3m** (* Solvent).

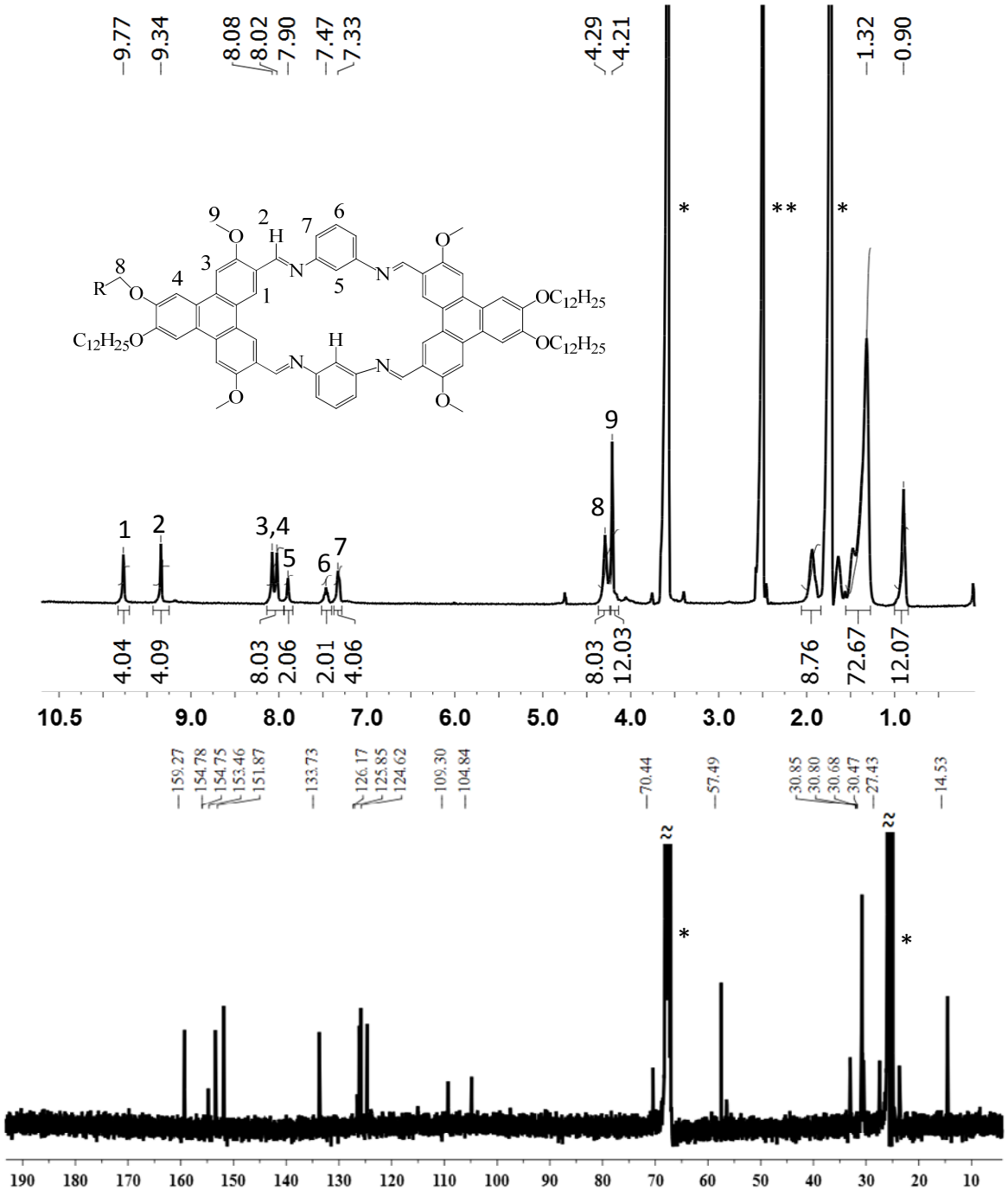

Figure S4: ^{1}H (top) and ^{13}C (bottom) NMR (THF-*d8*, 298K) Spectra of **3** (*Solvent, ** Water).

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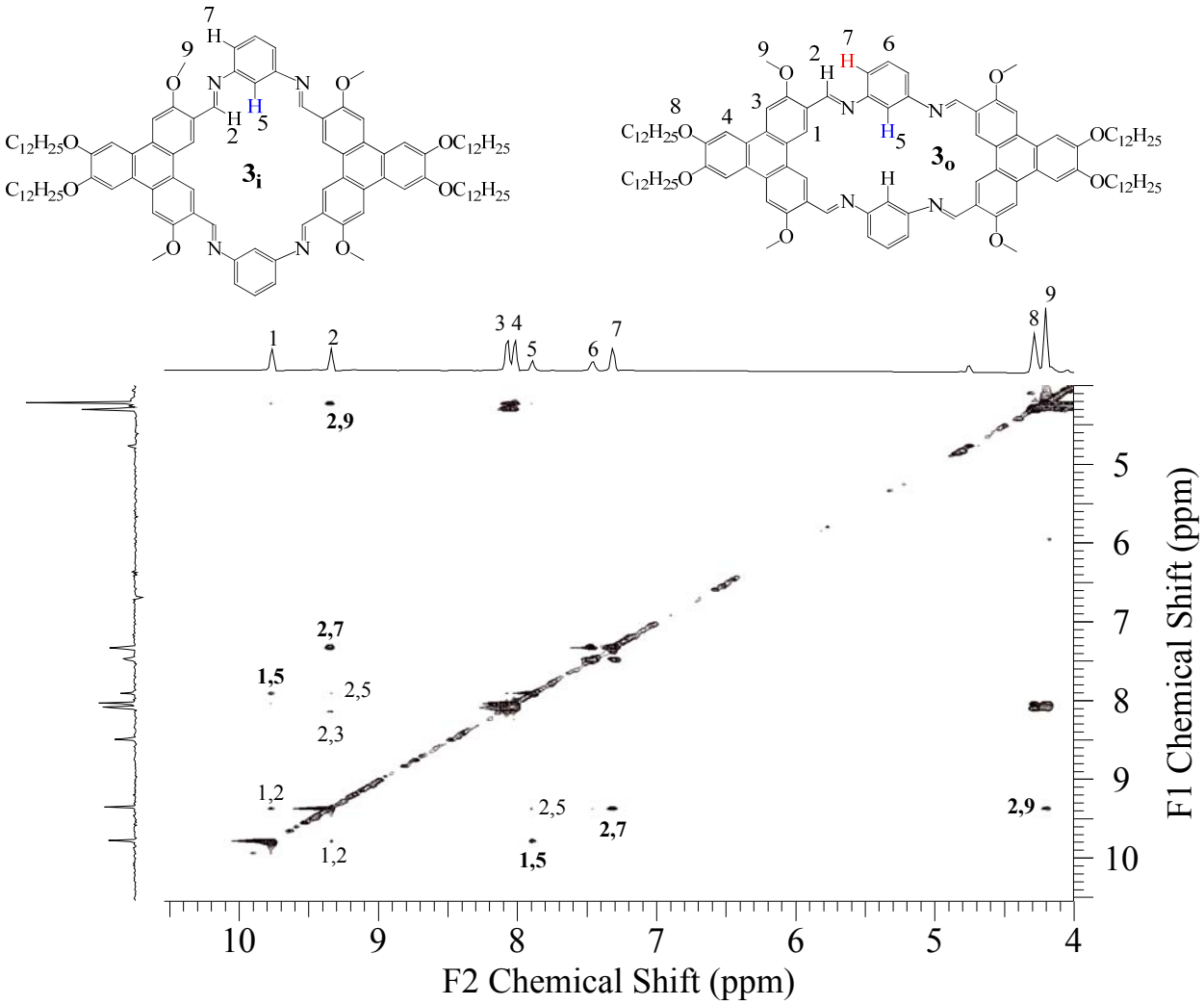

Figure S5: Selected region from 2D watergate NOESY 600MHz ^{1}H NMR spectrum of **3** which was recorded in THF-*d8* at 298K usng a 400 ms NOE mixing time (Strong NOE contacts are shown in bold).

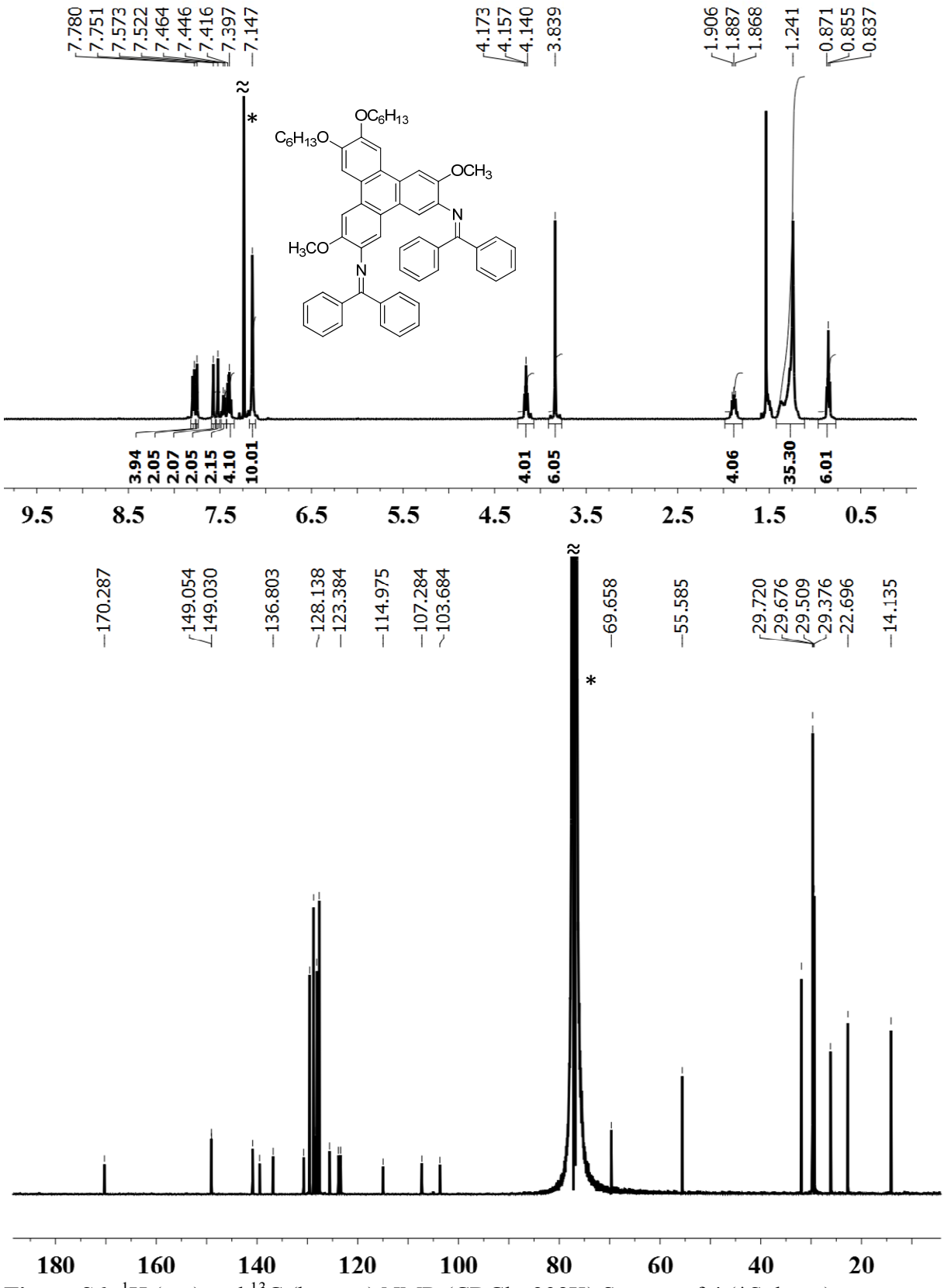

Figure S6: ^{1}H (top) and ^{13}C (bottom) NMR ($CDCl_3$, 298K) Spectra of **4** (*Solvent).

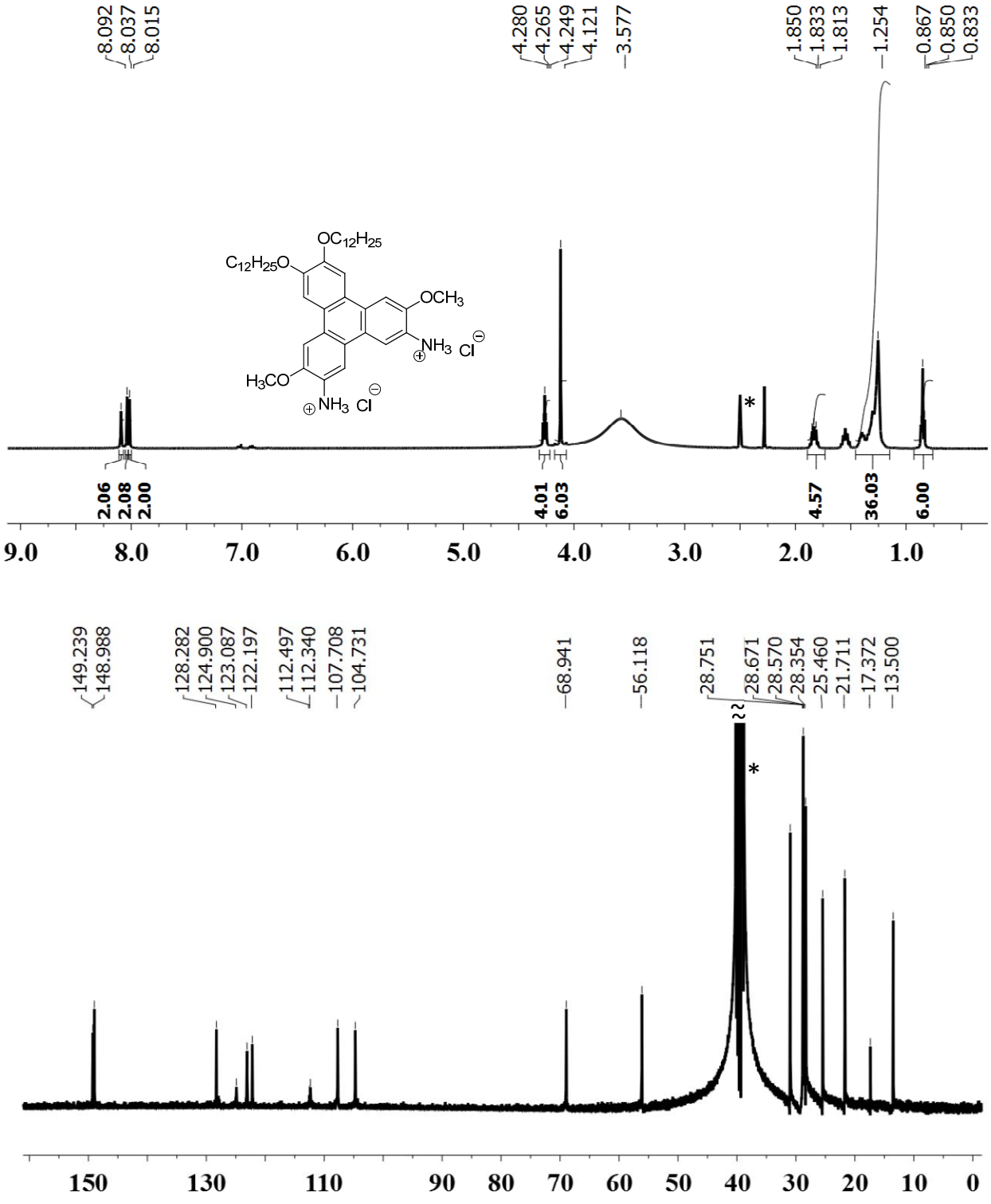

Figure S7: ^{1}H (top) and ^{13}C (bottom) NMR (DMSO-*d6*, 298K) Spectra of **5** (*Solvent).

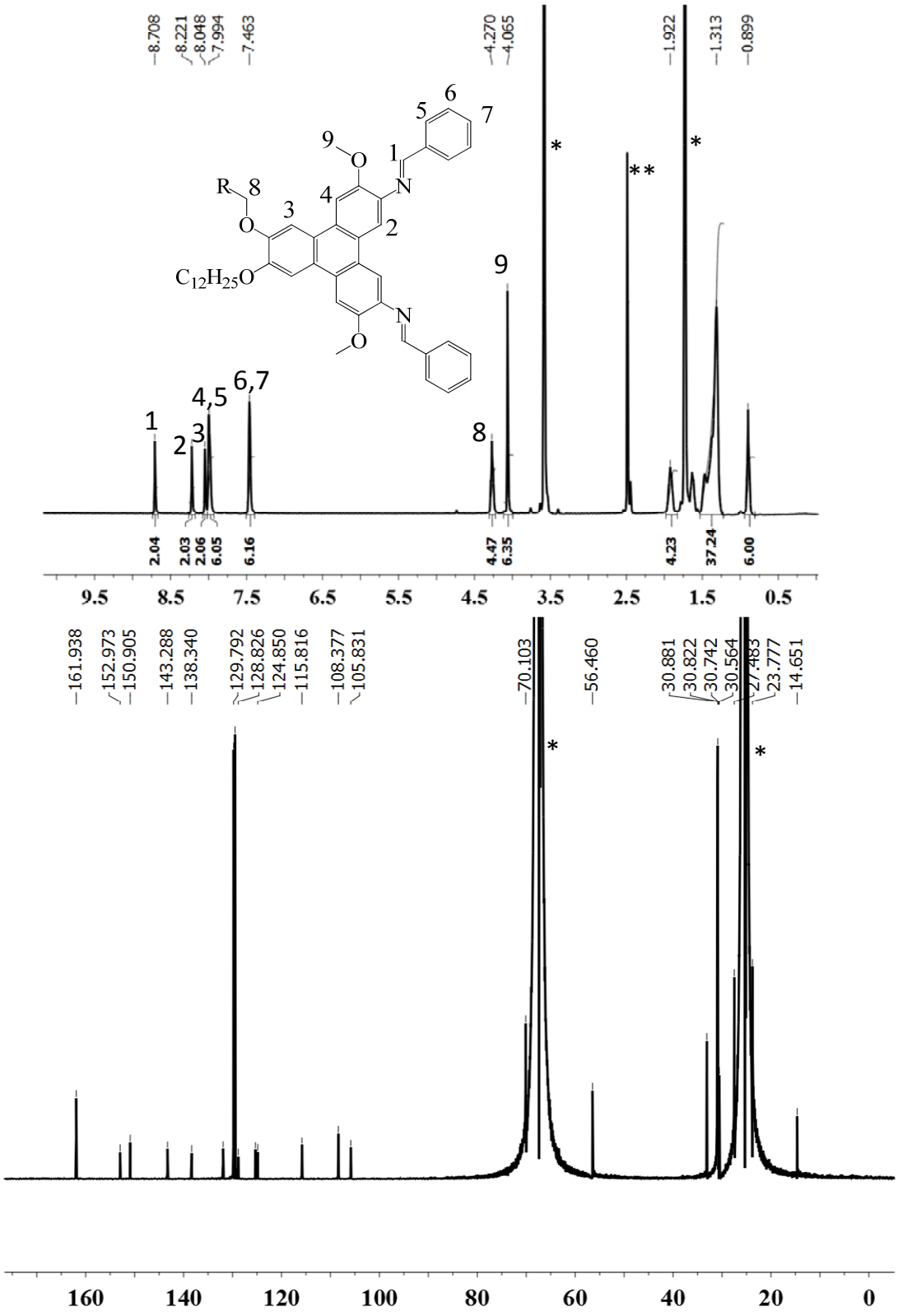

Figure S8: ^{1}H (top) and ^{13}C (bottom) NMR (THF-*d8*, 298K) Spectra of **6m** (*Solvent, ** Water).

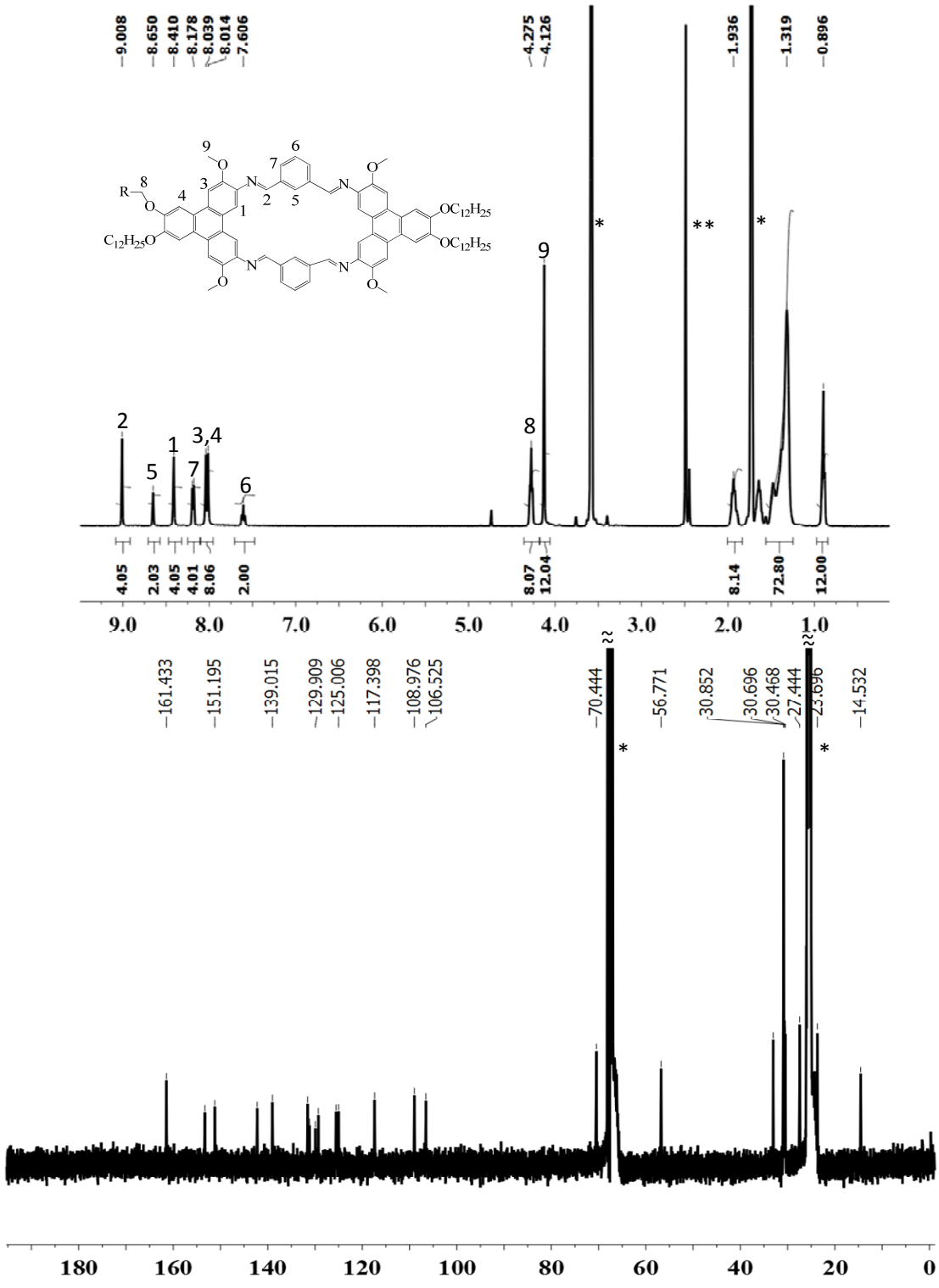

Figure S9: ^{1}H (top) and ^{13}C (bottom) NMR (THF-*d8*, 298K) Spectra of **6** (*Solvent, ** Water).

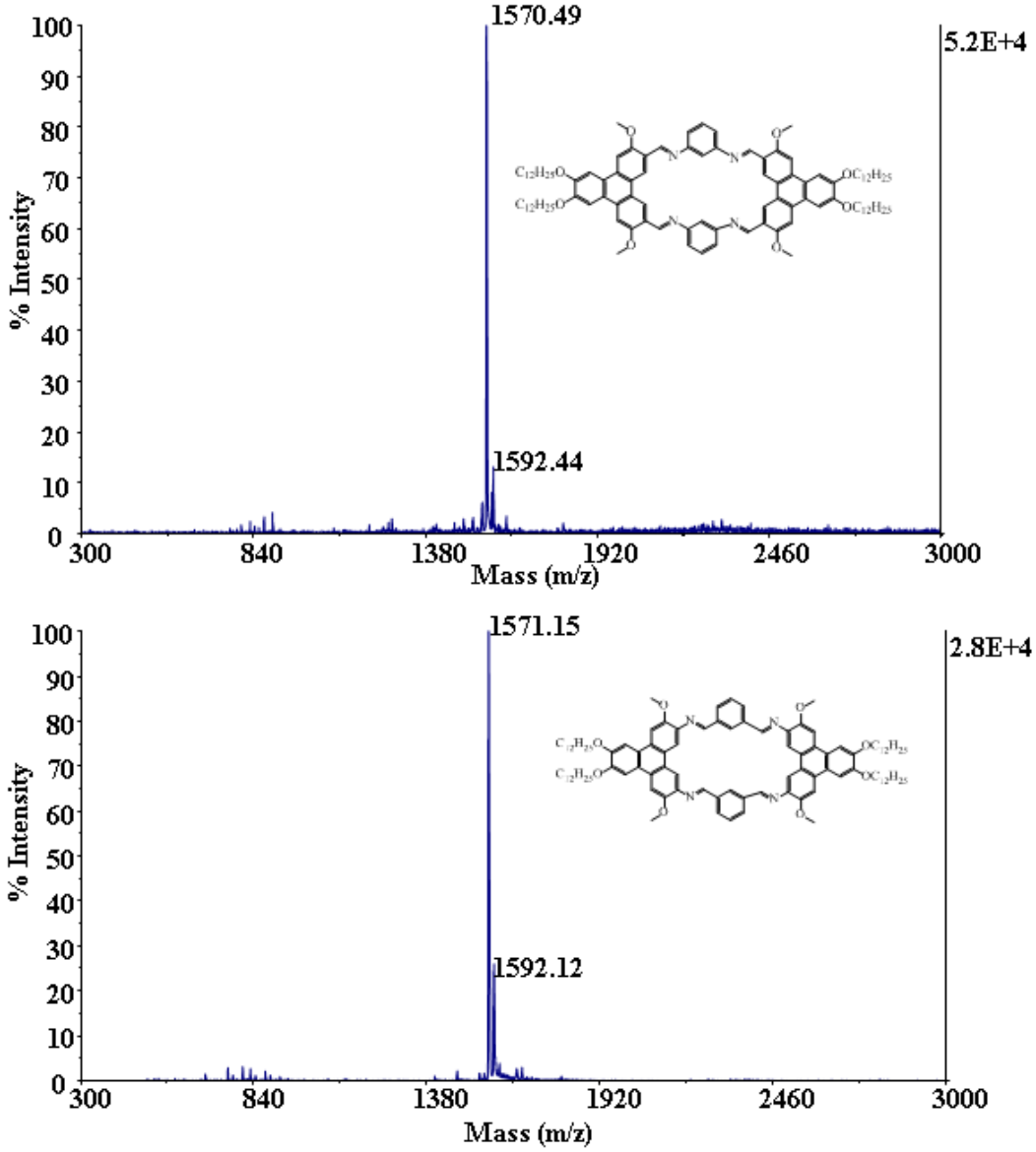

Figure S10: MALDI-TOF Spectra of **3** and **6**.

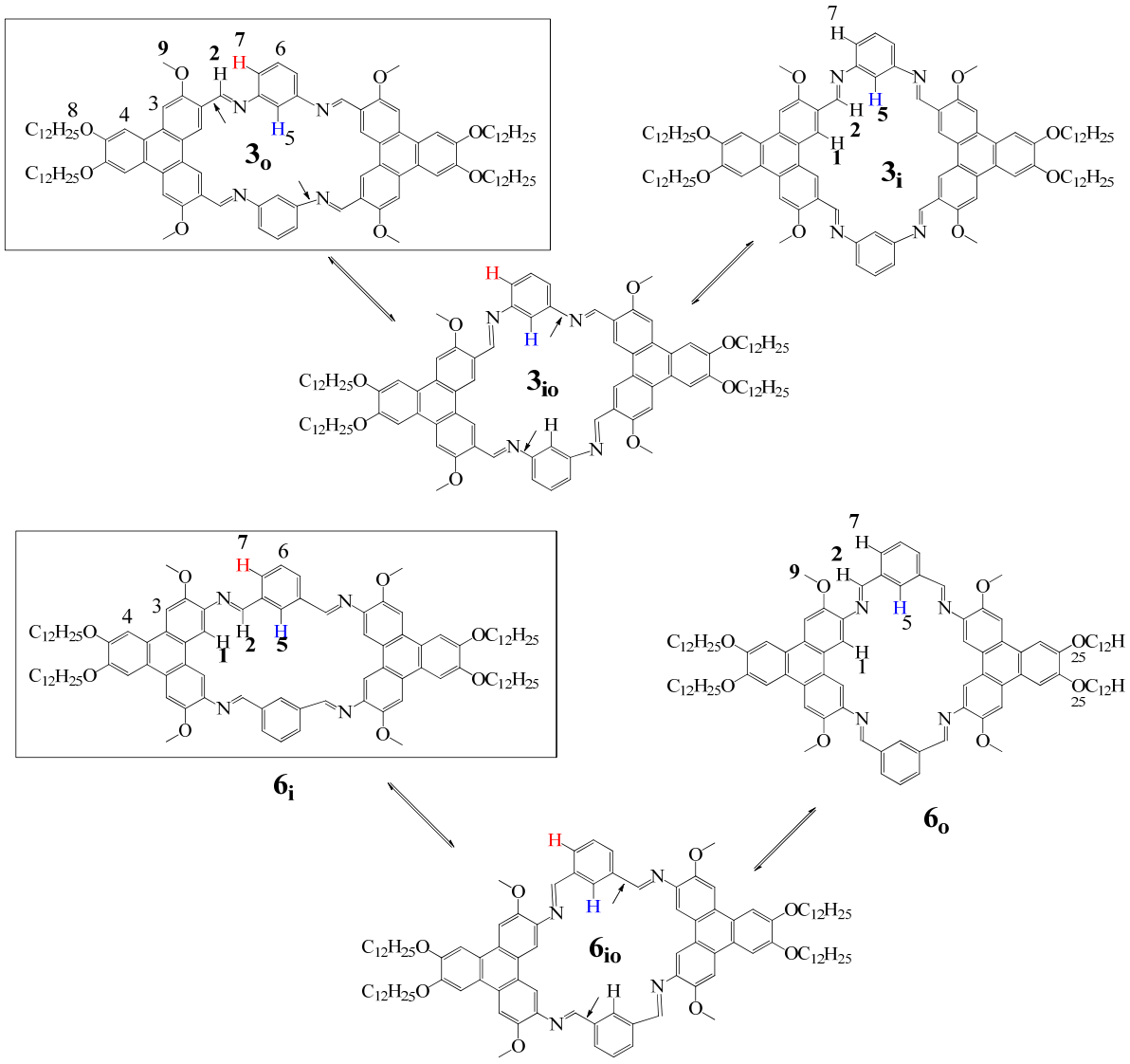

Figure S11. Structures of various conformers of **3** and **6**.

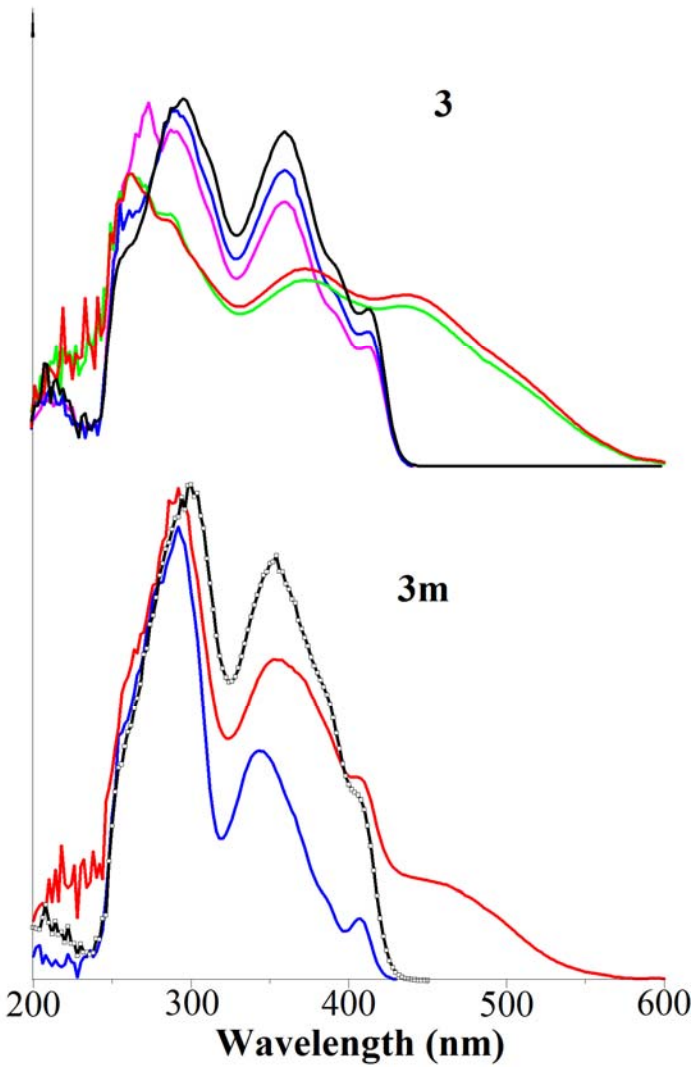

Figure S12. UV/Vis absorption spectra of 3 (top) and 3m (bottom) in original THF solutions (black), after addition of TsOH (red), after subsequent neutralization with Et_3N (blue), and another addition of TsOH (green) and neutralization (pink).

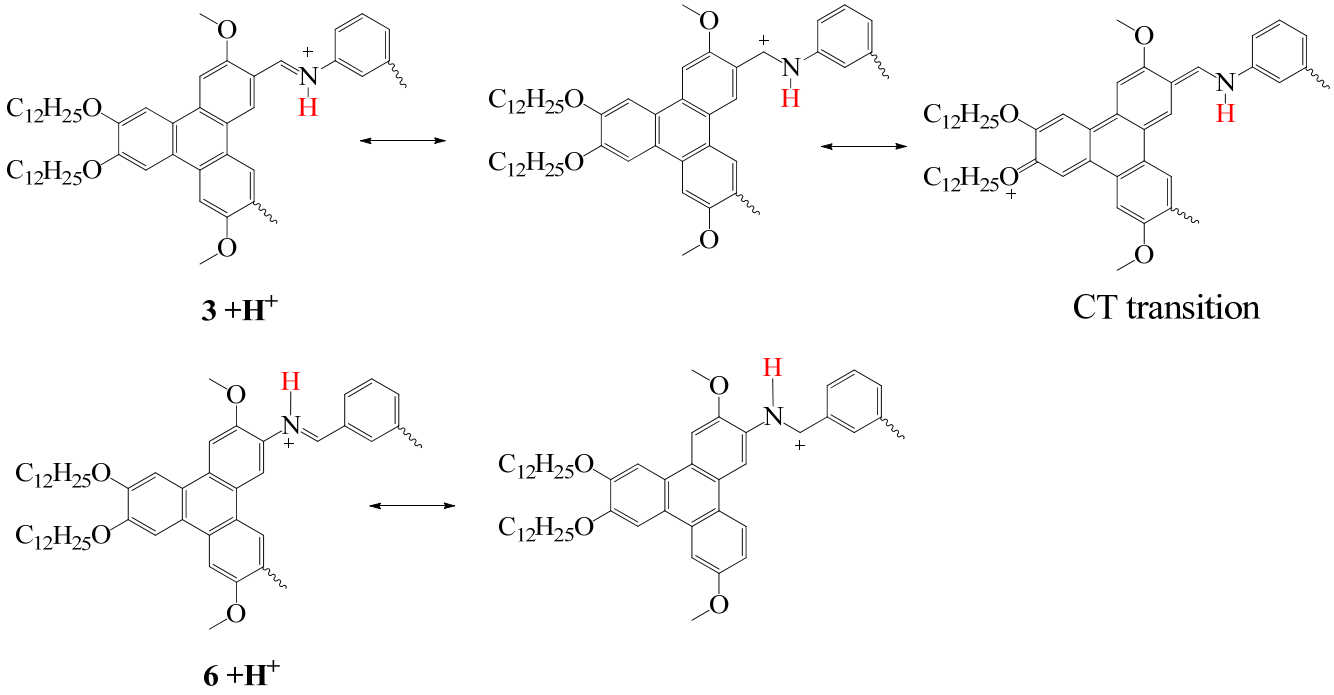

Figure S13. Proposed charge transfer transition which accounts for the red-shifted absorption of macrocycle **3** under acidic conditions.

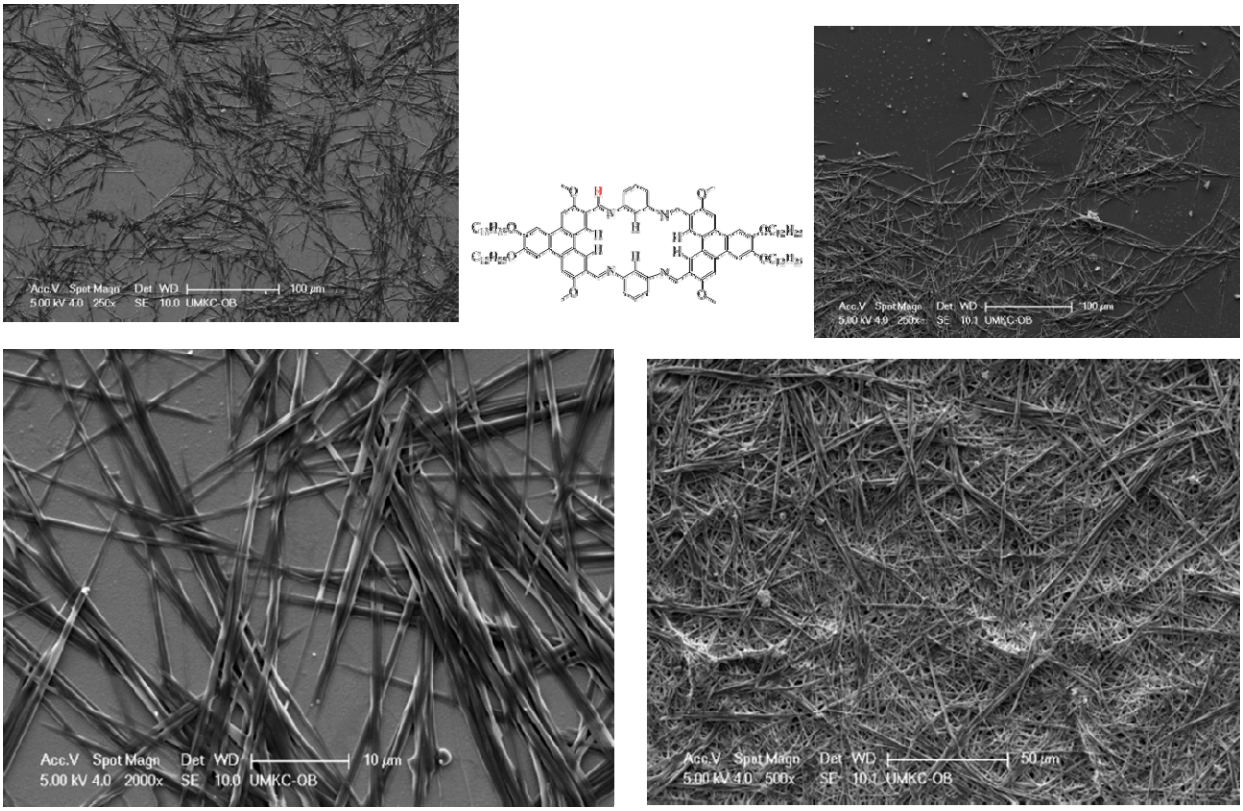

Figure S14: SEM pictures of **3**.

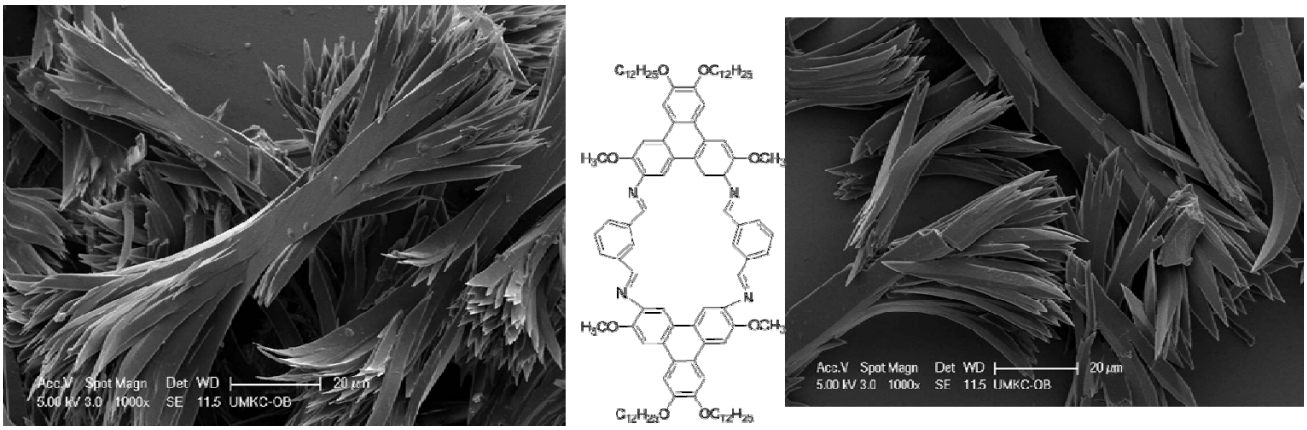

Figure S15: SEM pictures of **6**.

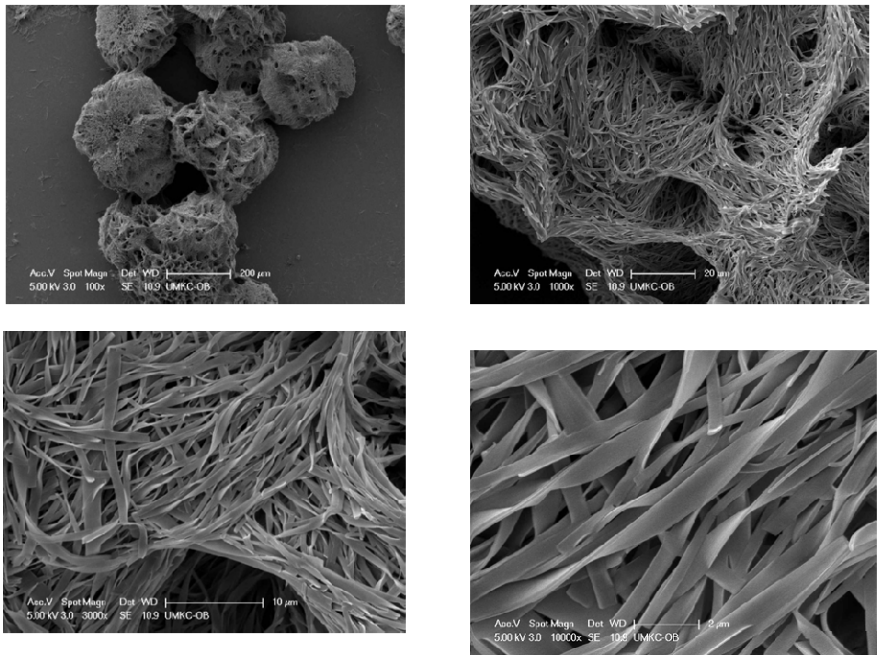

Figure S16: SEM images of self-assembled objects of **6m**.

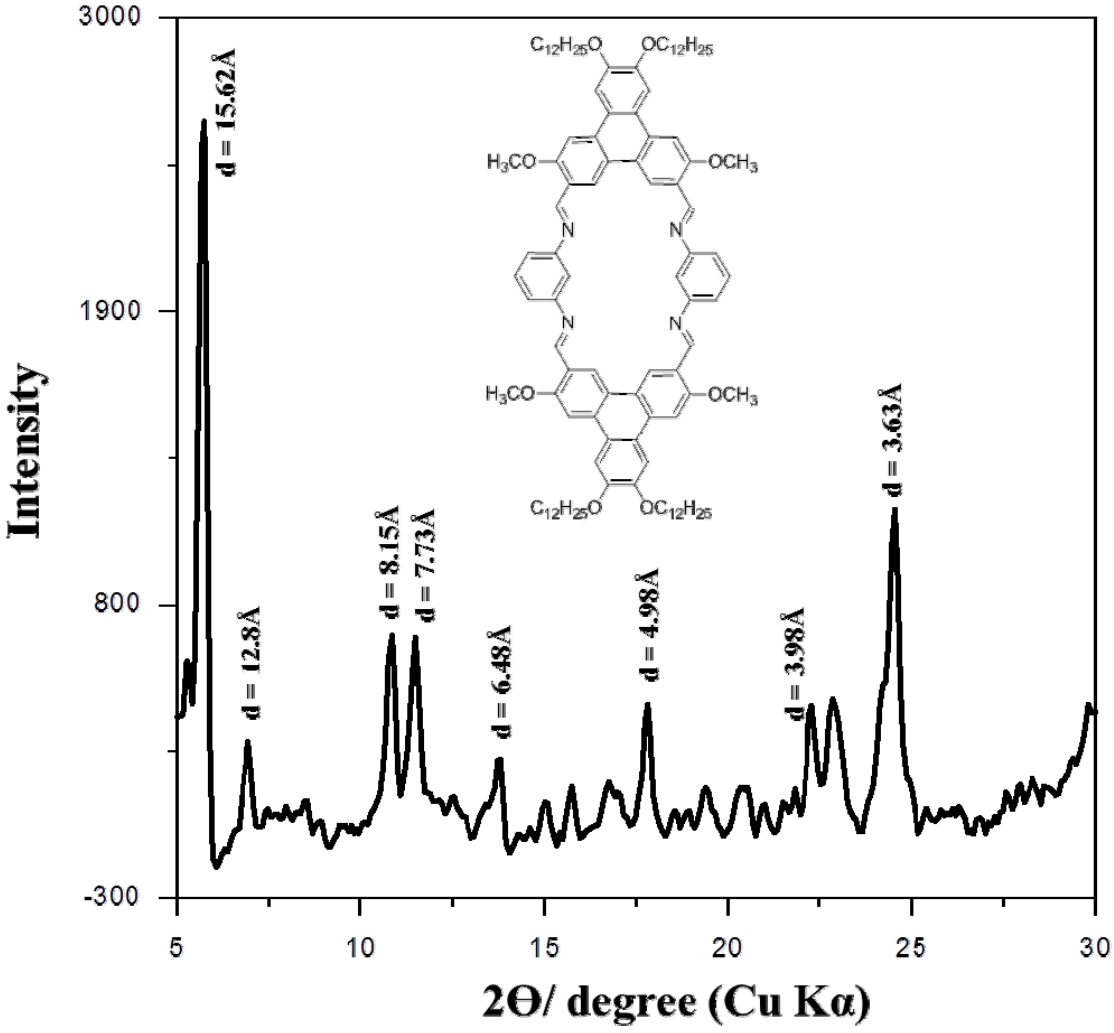

Figure S17: X-ray diffraction pattern of the micro-rods of **3**.

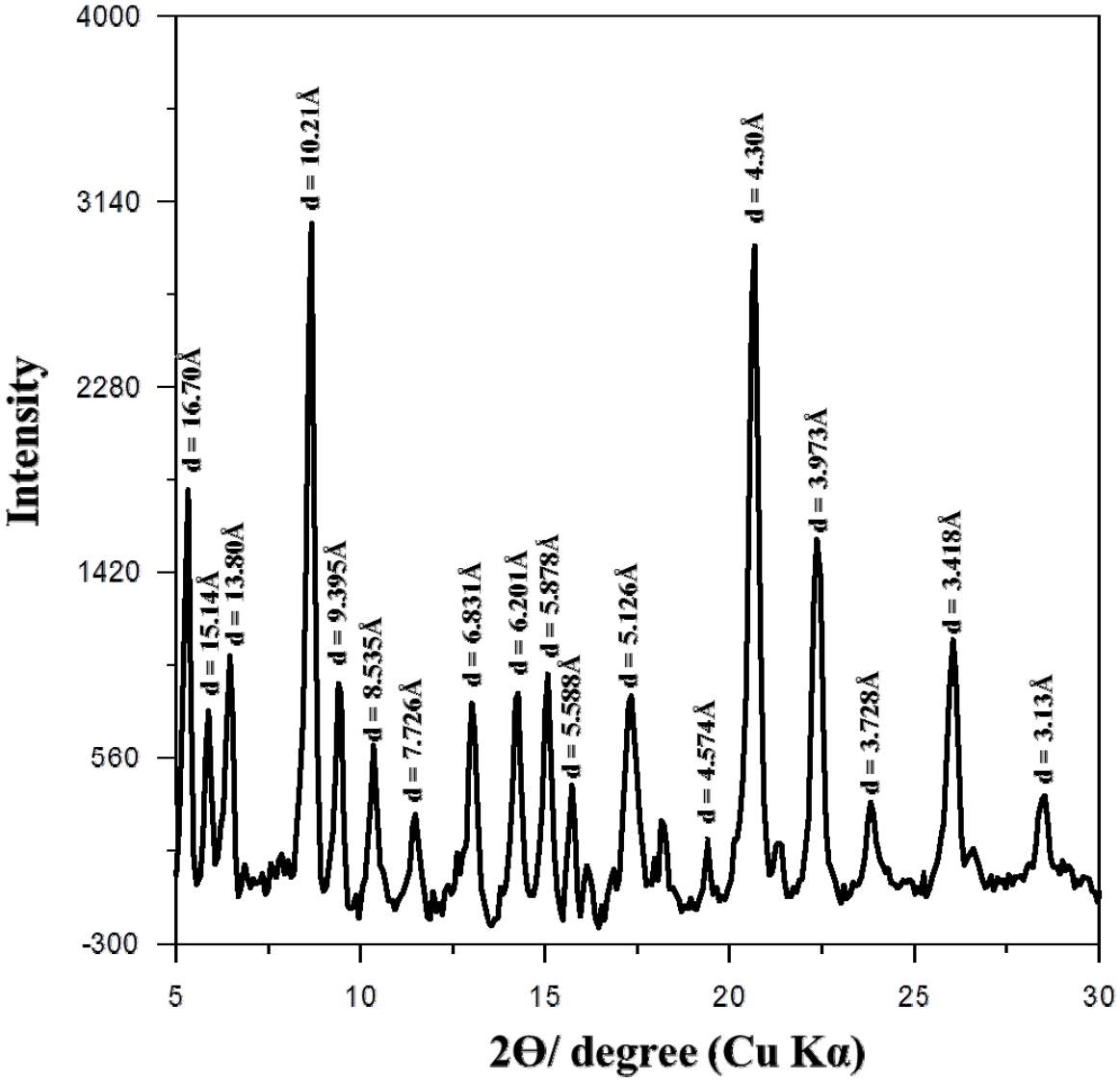

Figure S18: X-ray diffraction pattern of the micro panels of **6**.

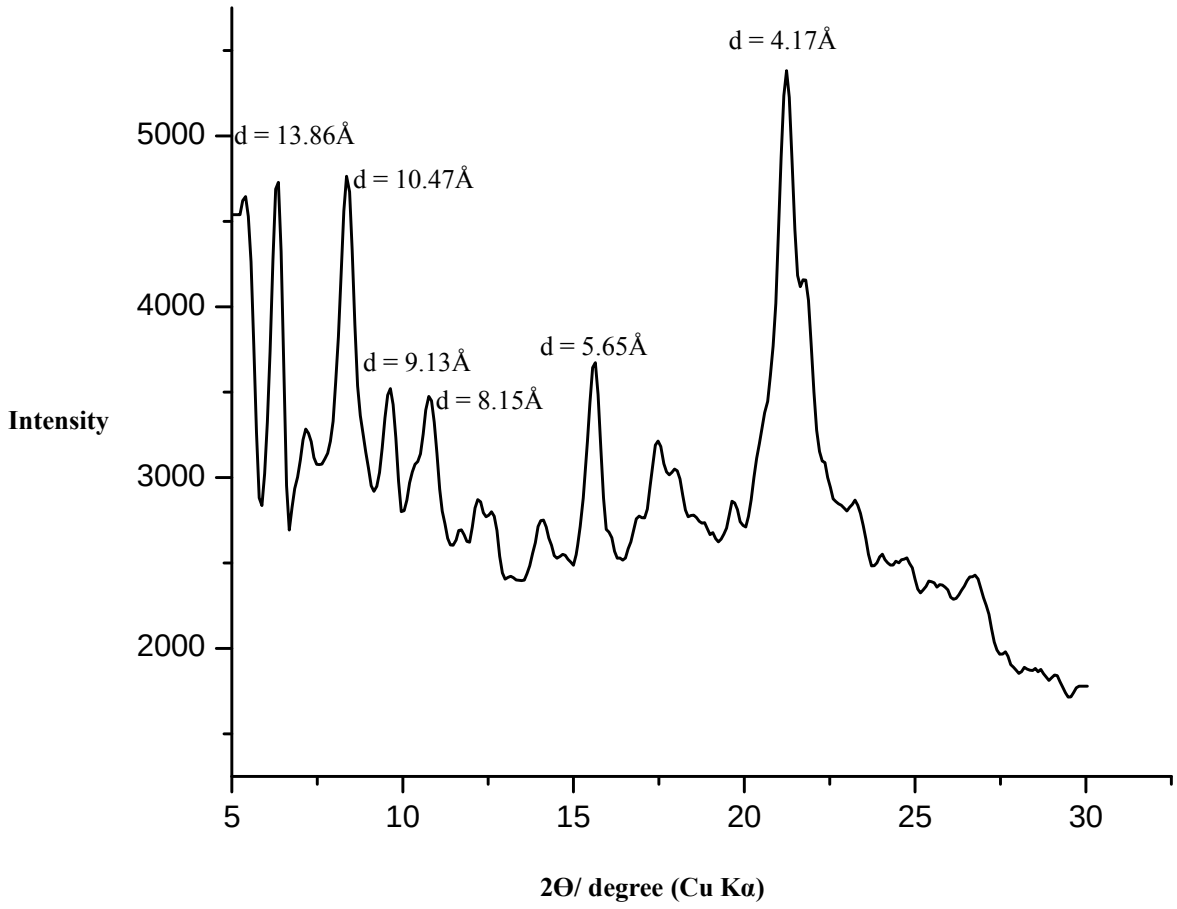

Figure S19: X-ray diffraction pattern of **3m**.

Description on quantum mechanical calculations:

QM Energy Calculation. The model structures (ethoxy analogs) of $\mathbf{3_i}$, $\mathbf{3_o}$, $\mathbf{3_{io}}$, $\mathbf{6_i}$, $\mathbf{6_o}$, and $\mathbf{6_{io}}$ were built in Maestro and were minimized with the OPLS force field using the MacroModel software in Schrödinger software suite.[1] The DFT B3LYP[2-4] functional method with 6-31G** basis set was employed to calculate QM energy in Jaguar package in Schrödinger software. The accuracy level of SCF was selected to its highest level (fully analytic). Due to the large number of atoms in the model compounds, STO-3G level of theory was used for minimization, followed by single point energy calculations and the NMR shielding calculations using B3LYP/6-31G** level of theory, with TMS as a reference to calculate the predicted chemical shifts. The energetic of different conformations are listed in Table 1 in the main text.

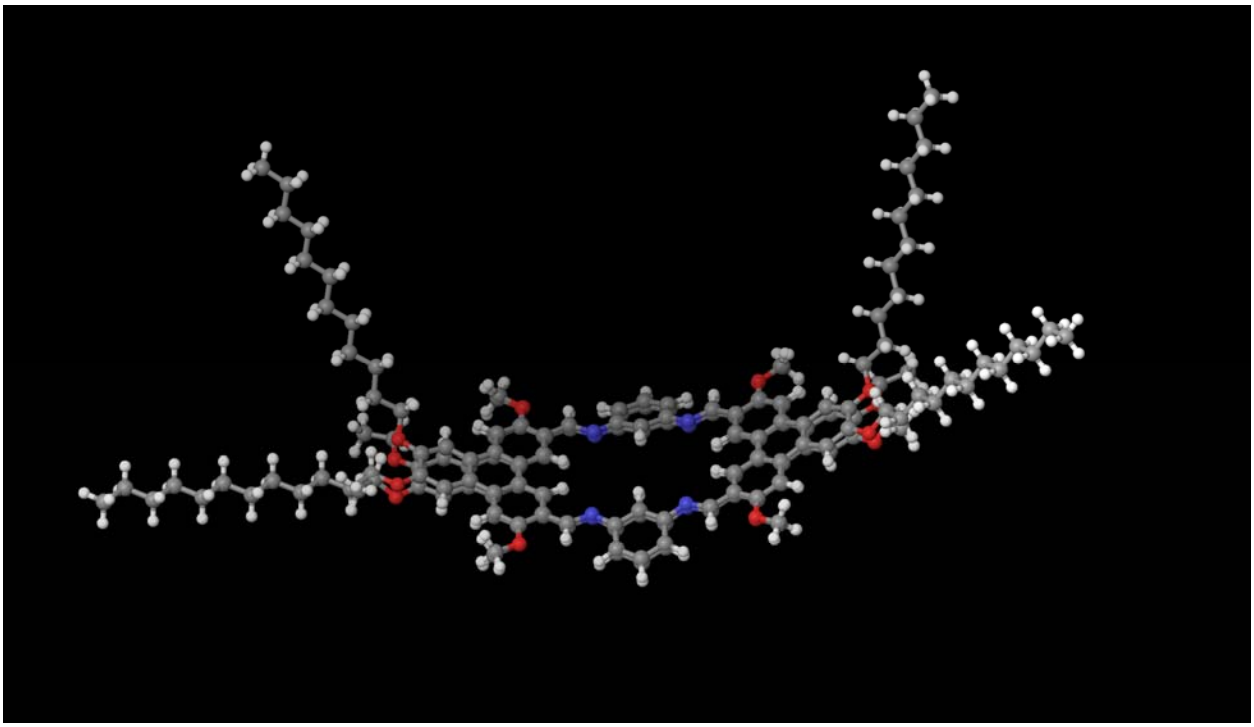

Figure S20. Superposition of $\mathbf{3_o}$ with dodecyloxy side chains vs $\mathbf{3_o}$ with ethoxy side chains.

Reference:

1. Protein Preparation Wizard, Maestro, MacroModel, Phase, Induced Fit, Jaguar, and Glide; Schrödinger, LLC: Portland, OR, **2009**.
2. Johnson, B. G.; Gill, P. M. W.; Pople, J. A. *J. Chem. Phys.* **1993**, *98*, 5612-5626.
3. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B.* **1988**, *37*, 785-789.
4. Becke, A. D. *J.Chem.Phys.* **1993**, *98*, 1372-1377.