

## Supplementary Material

### Reversible Fluorescence Switching of Donor-Acceptor Type Bipyridines by Simple Protonation-Deprotonation Equilibria

*Shaik Mubeena,<sup>A</sup> Meghana N,<sup>A</sup> Gayatri Annapareddy,<sup>A</sup> Yi-Sheng Chen,<sup>B</sup> Monima Sarma,<sup>A,C</sup> and Ken-Tsung Wong<sup>B,C</sup>*

<sup>A</sup>Department of Chemistry, KL Deemed to be University (KLEF), Greenfields, Vaddeswaram, Andhra Pradesh 522502, India.

<sup>B</sup>Department of Chemistry, National Taiwan University, Taipei 10617, Taiwan.

<sup>C</sup>Corresponding authors. Email: monima.22@gmail.com; kenwong@ntu.edu.tw

# NMR Spectra

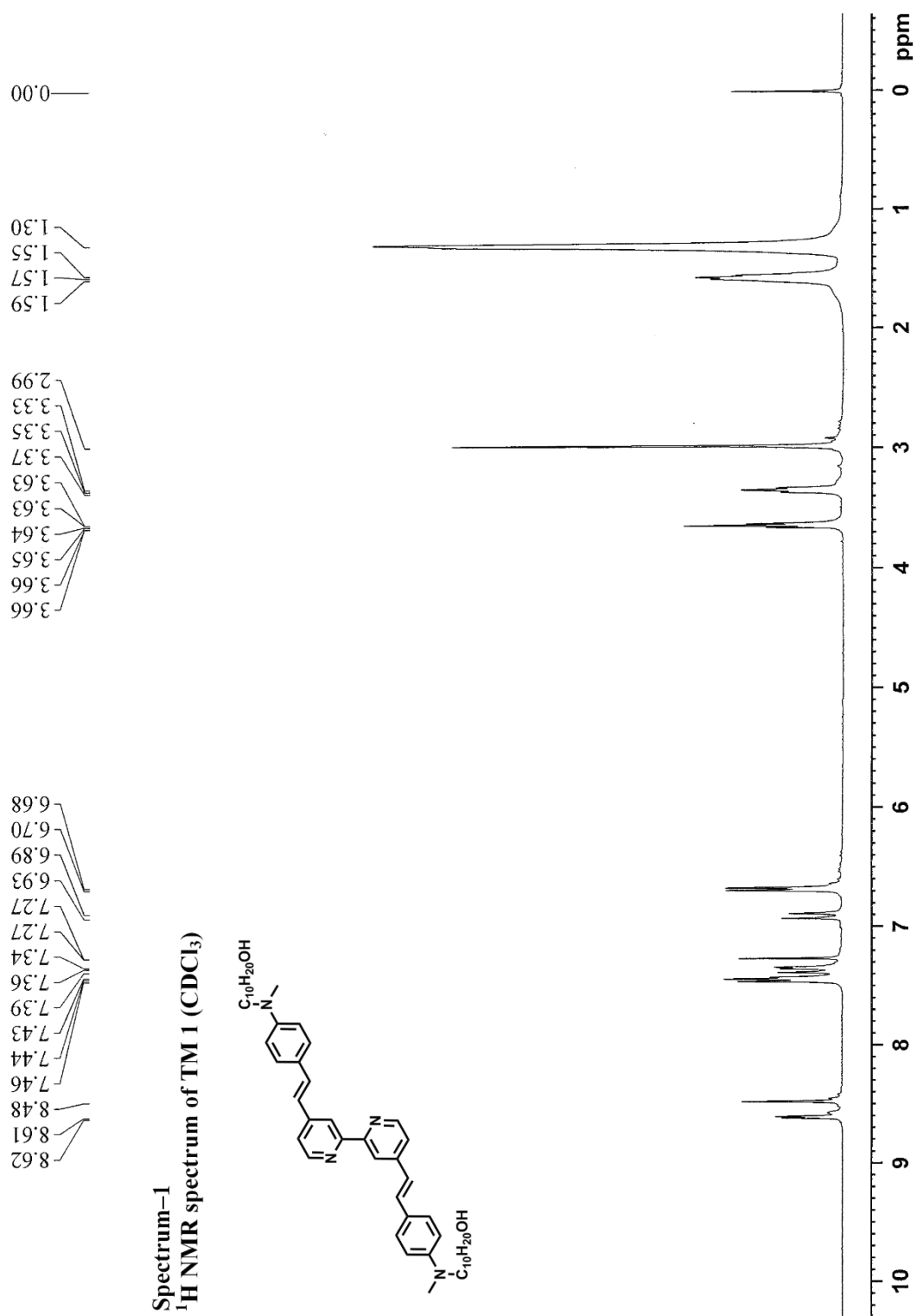


Figure S1. <sup>1</sup>H NMR Spectrum of TM1 (CDCl<sub>3</sub>, 400 MHz)

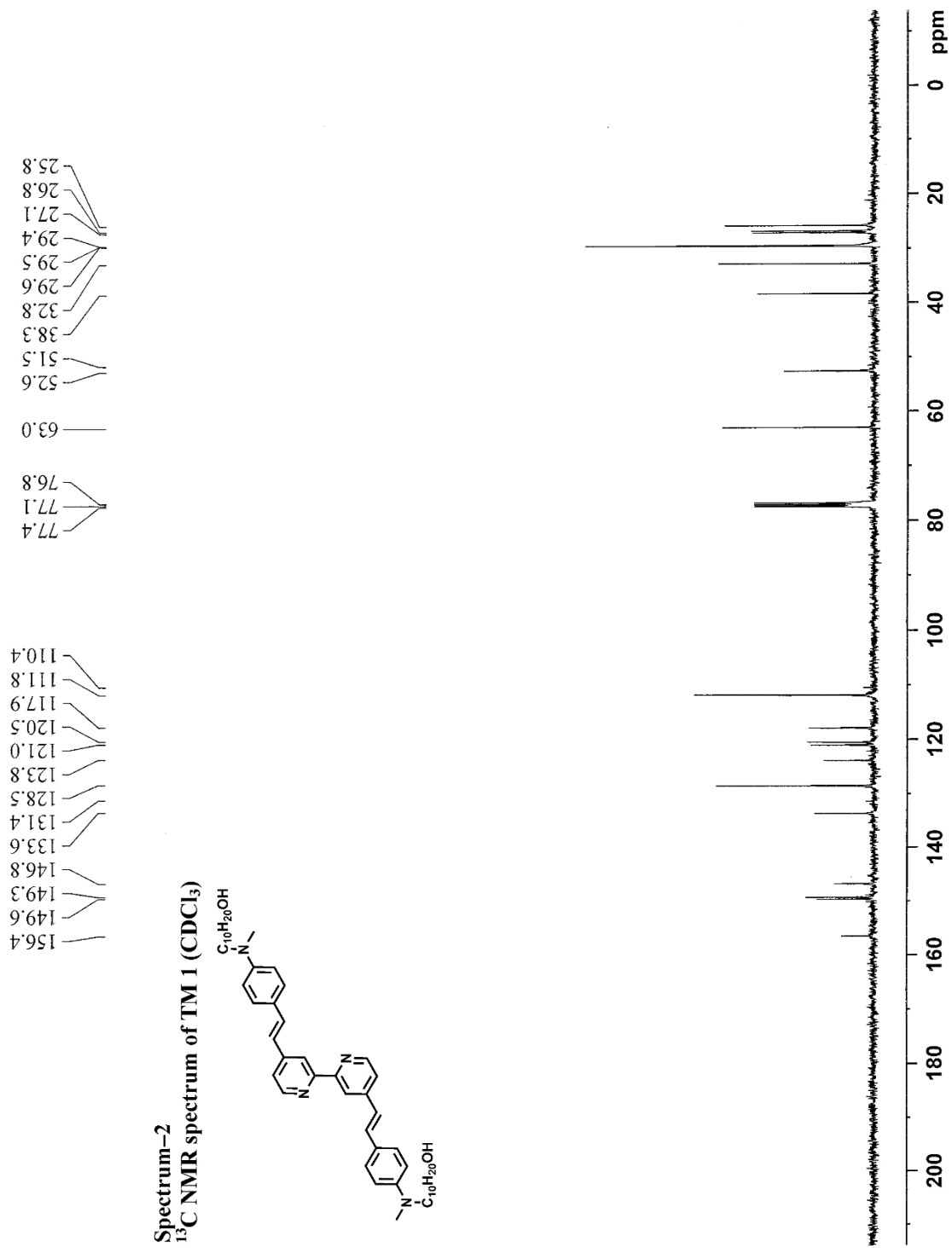
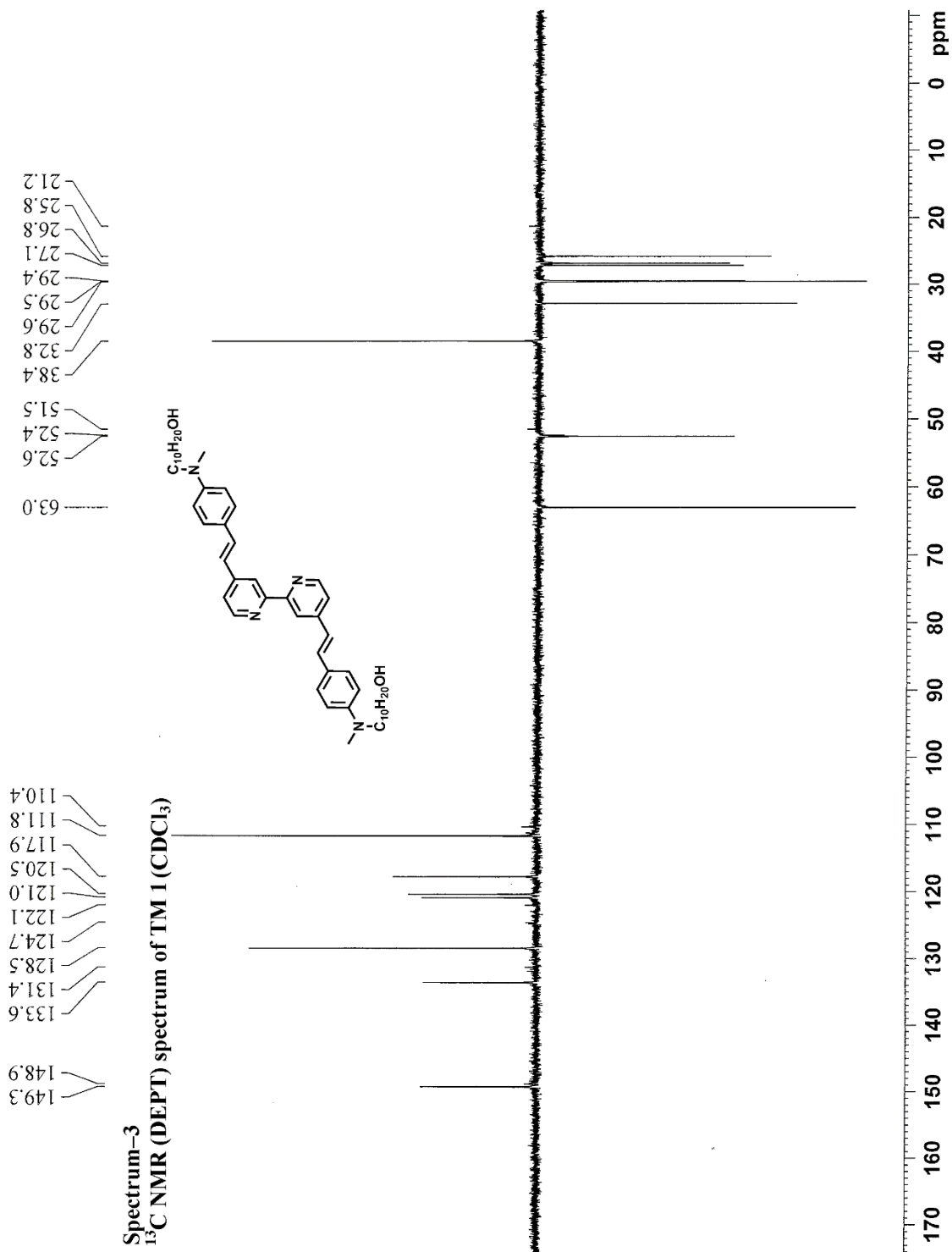


Figure S2. <sup>13</sup>C NMR Spectrum of TM1 (CDCl<sub>3</sub>, 100 MHz)



**Figure S3.** <sup>13</sup>C NMR Spectrum (DEPT) of TM1 (CDCl<sub>3</sub>, 100 MHz)

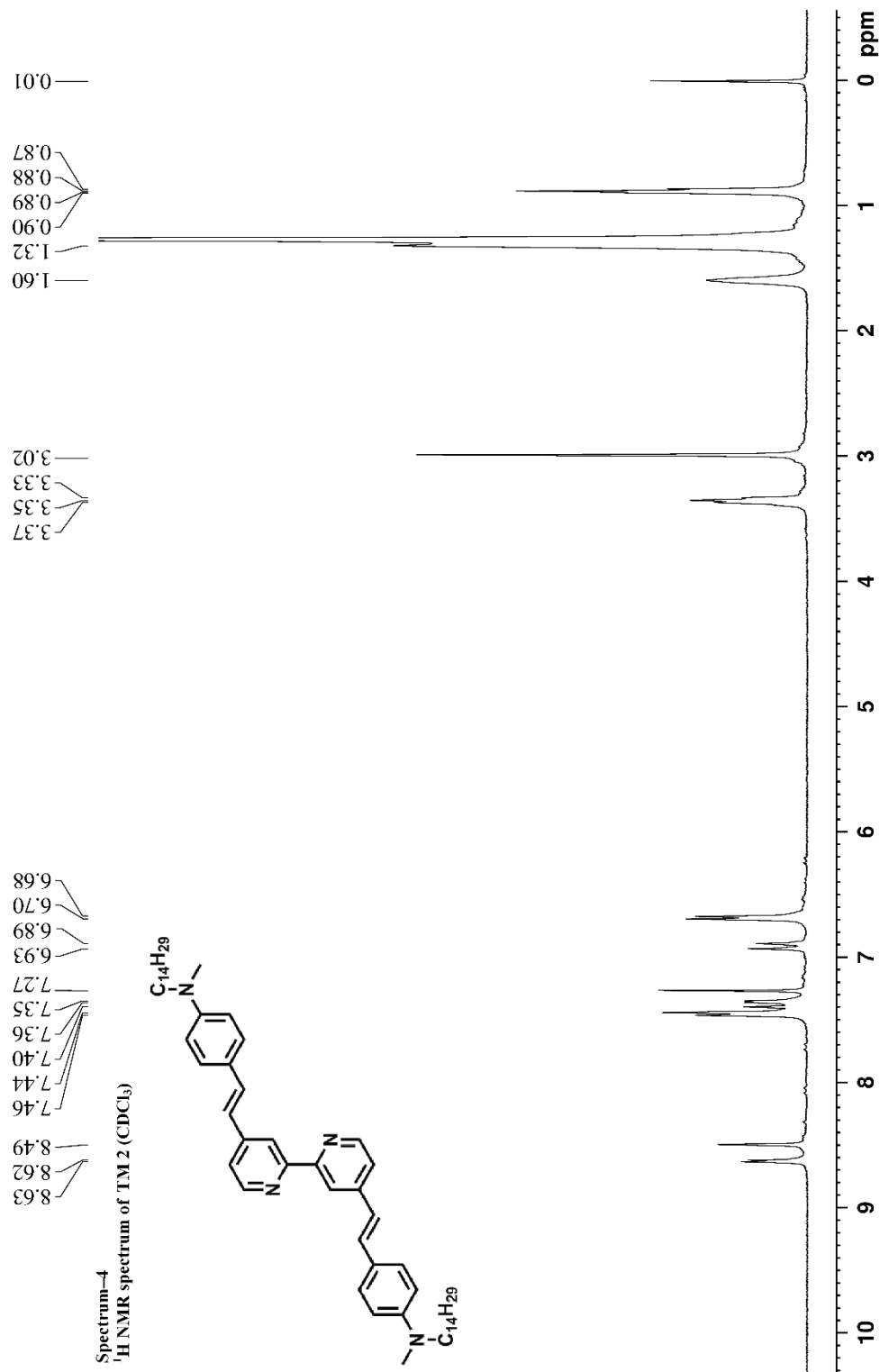


Figure S4. <sup>1</sup>H NMR Spectrum of TM2 (CDCl<sub>3</sub>, 400 MHz)

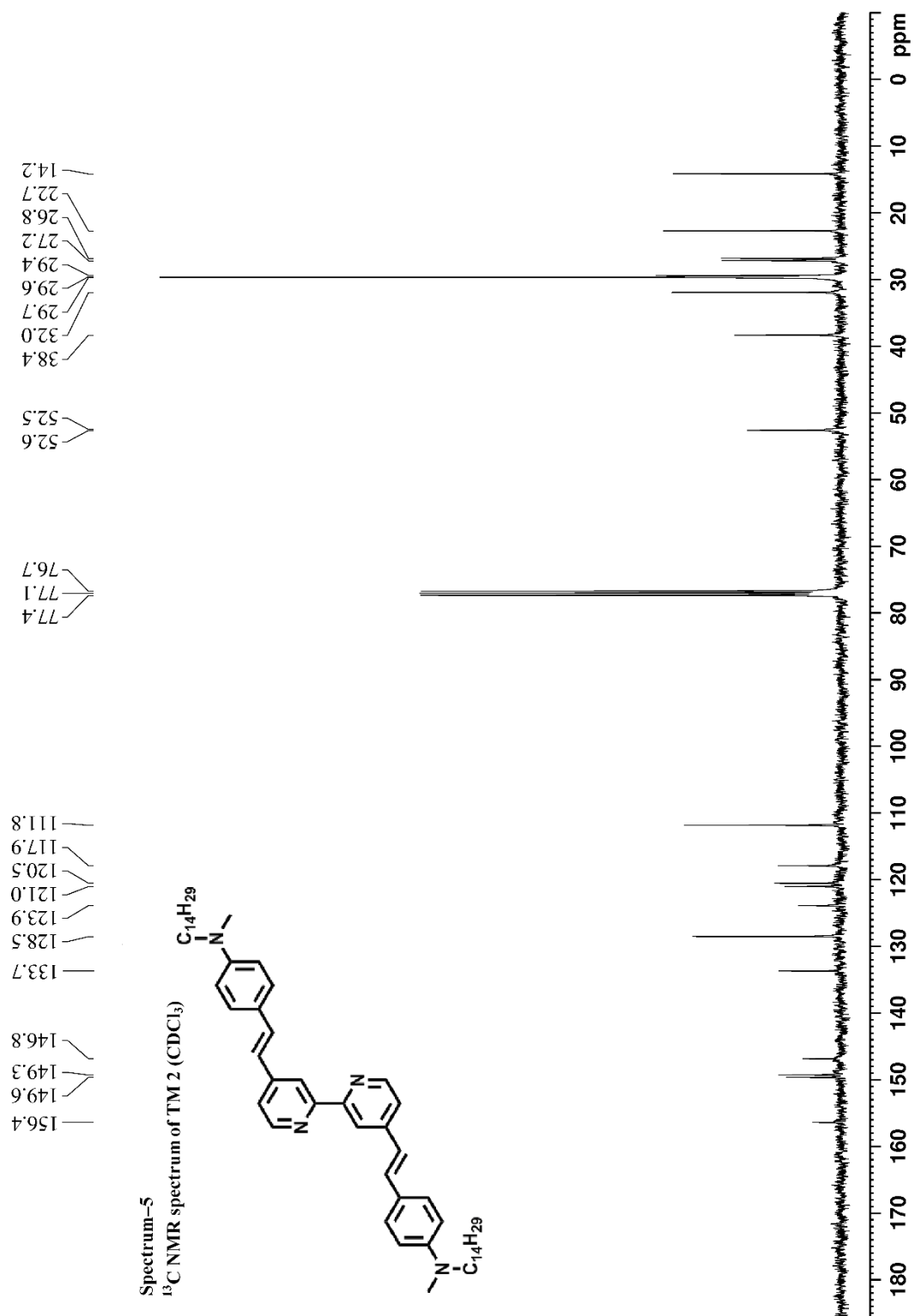
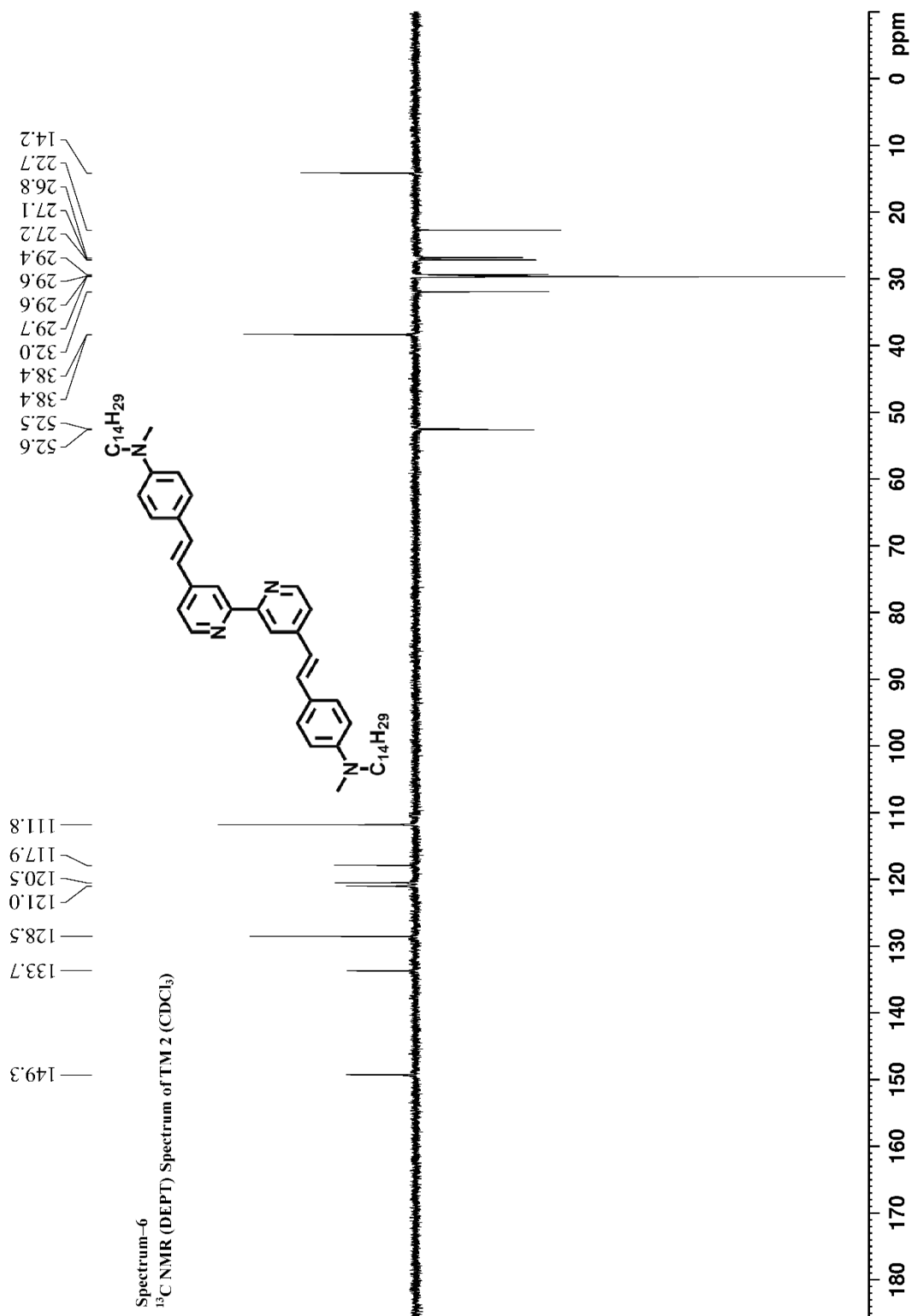


Figure S5. <sup>13</sup>C NMR Spectrum of TM2 (CDCl<sub>3</sub>, 100 MHz)



**Figure S6.** <sup>13</sup>C NMR Spectrum (DEPT) of TM2 (CDCl<sub>3</sub>, 100 MHz)

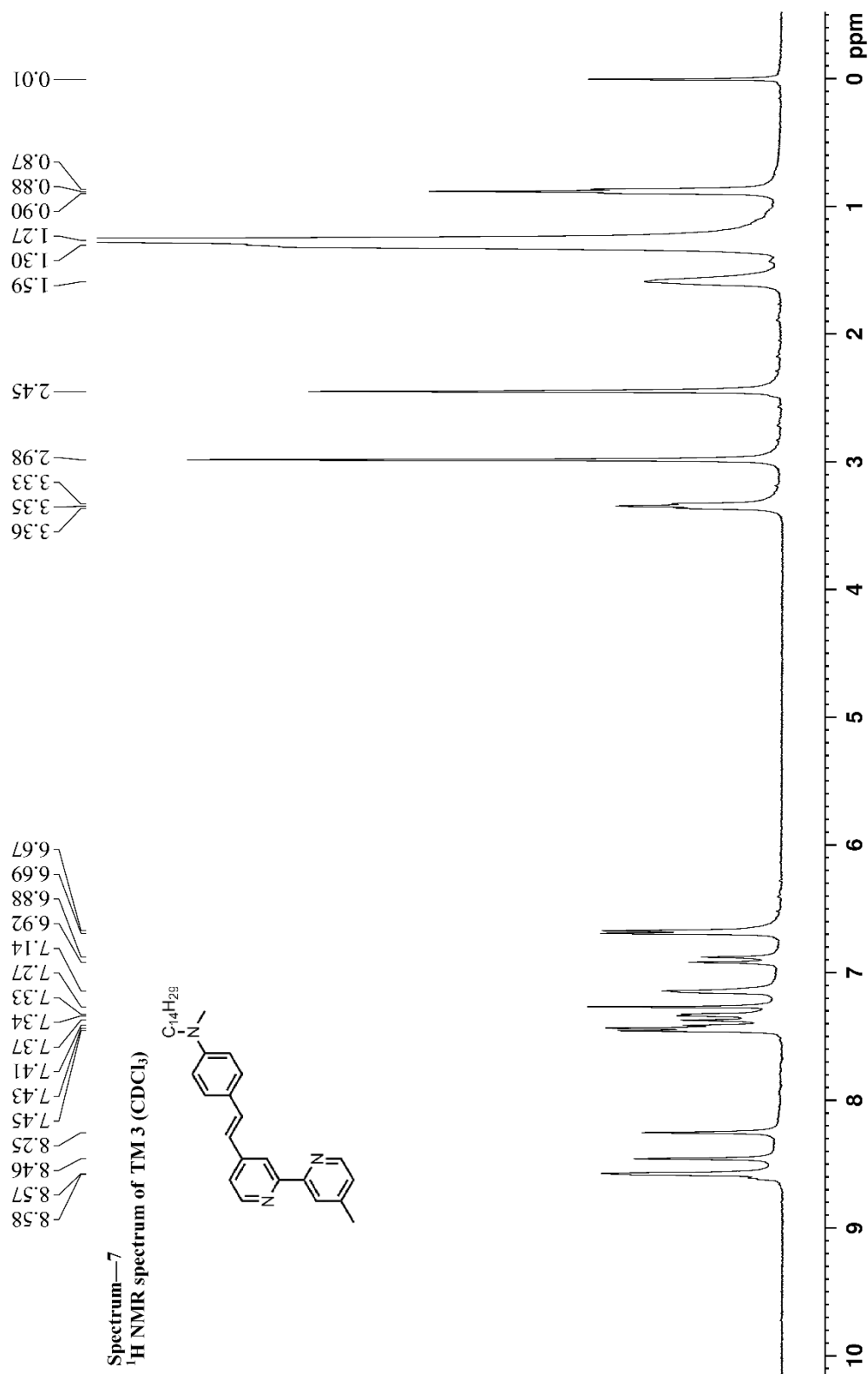
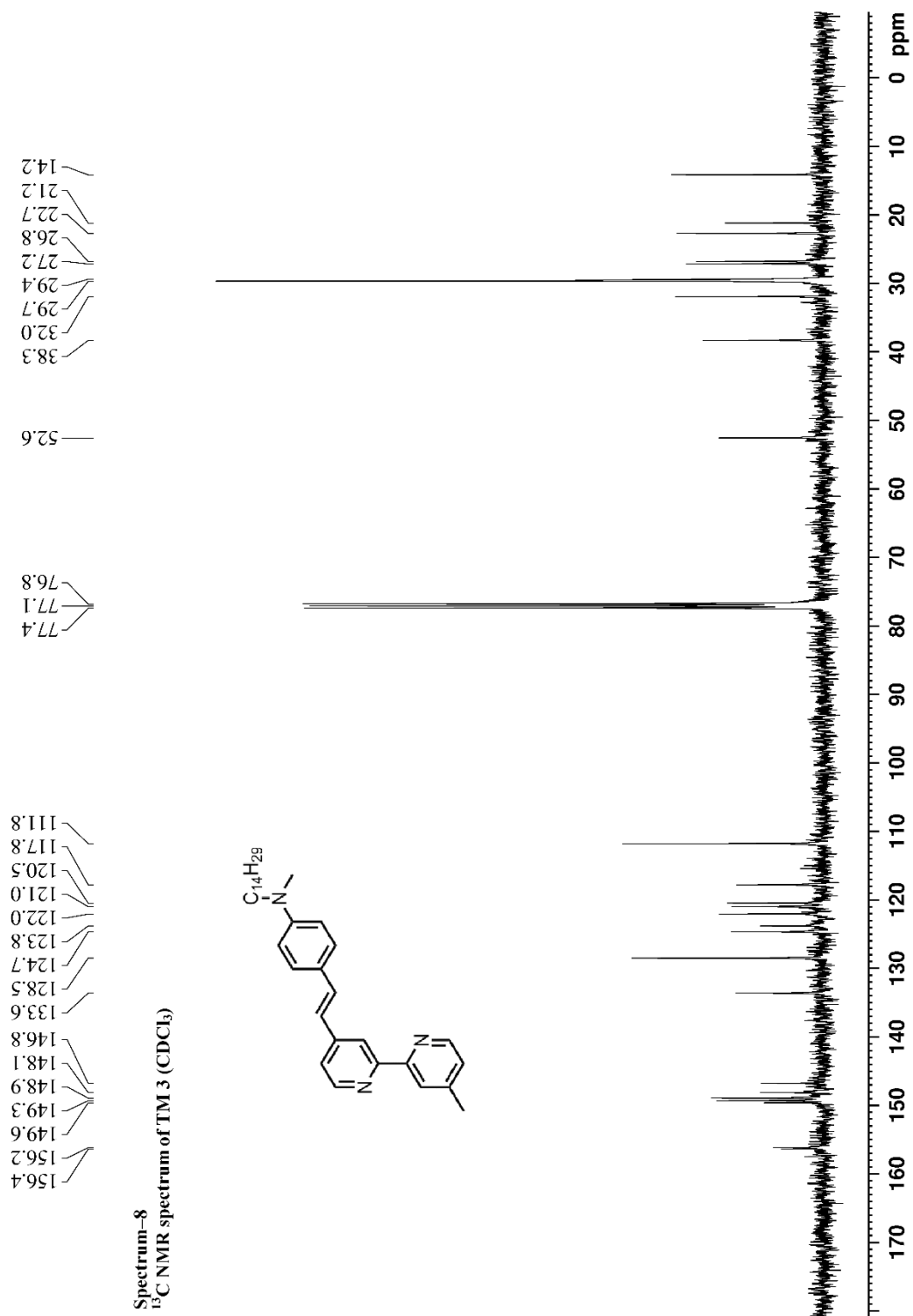
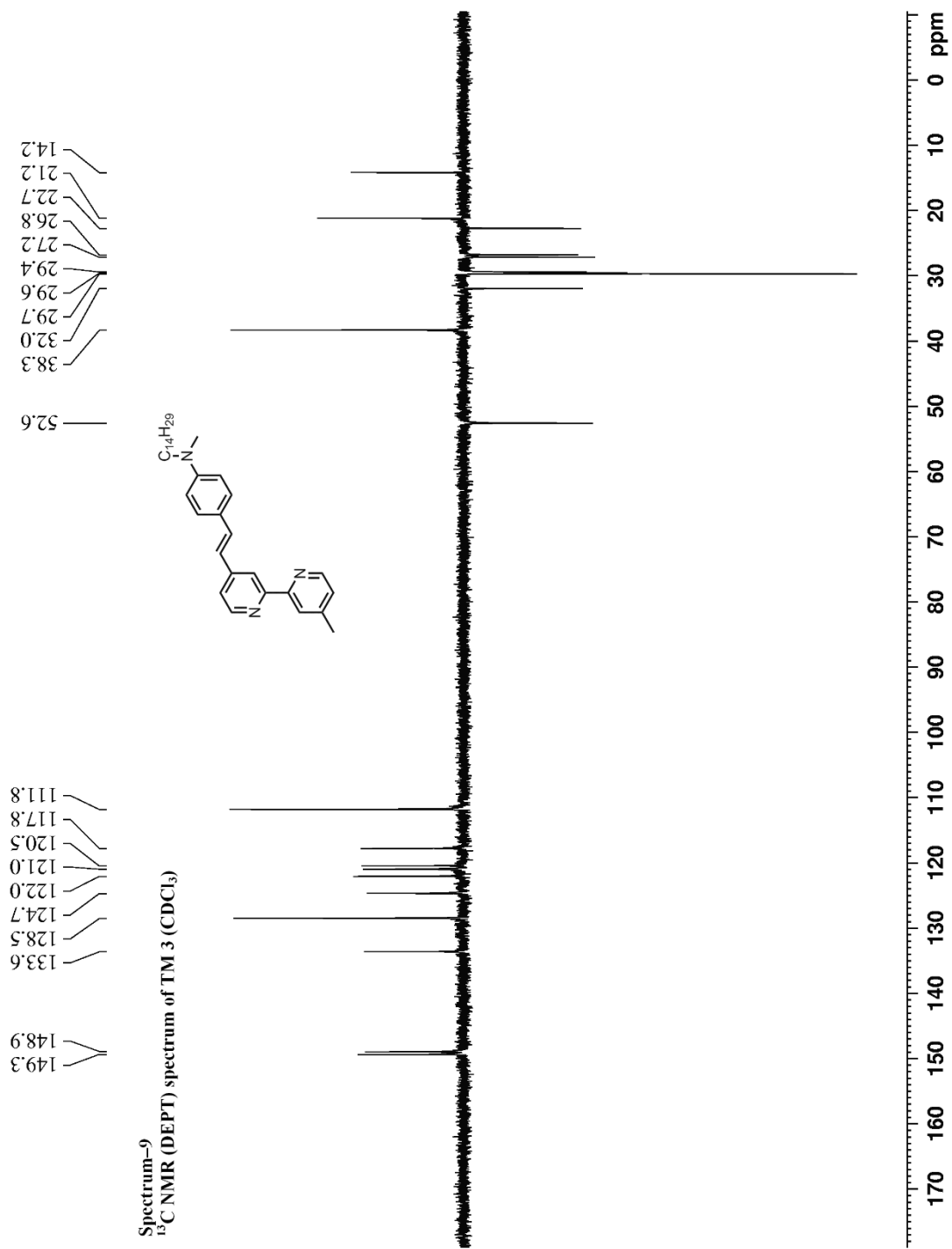


Figure S7. <sup>1</sup>H NMR Spectrum of TM 3 (CDCl<sub>3</sub>, 400 MHz)



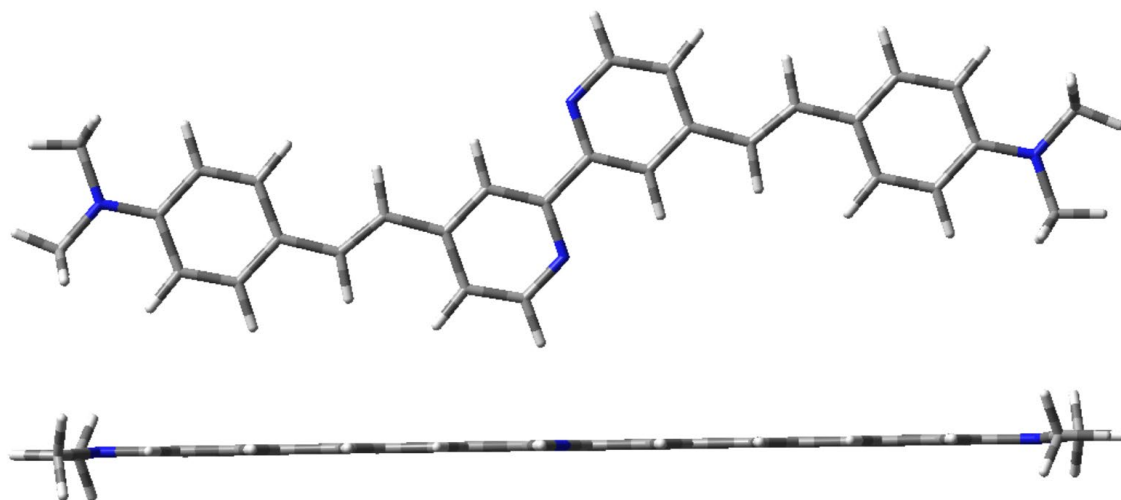


**Figure S8.** <sup>13</sup>C NMR Spectrum of TM3 (CDCl<sub>3</sub>, 100 MHz)

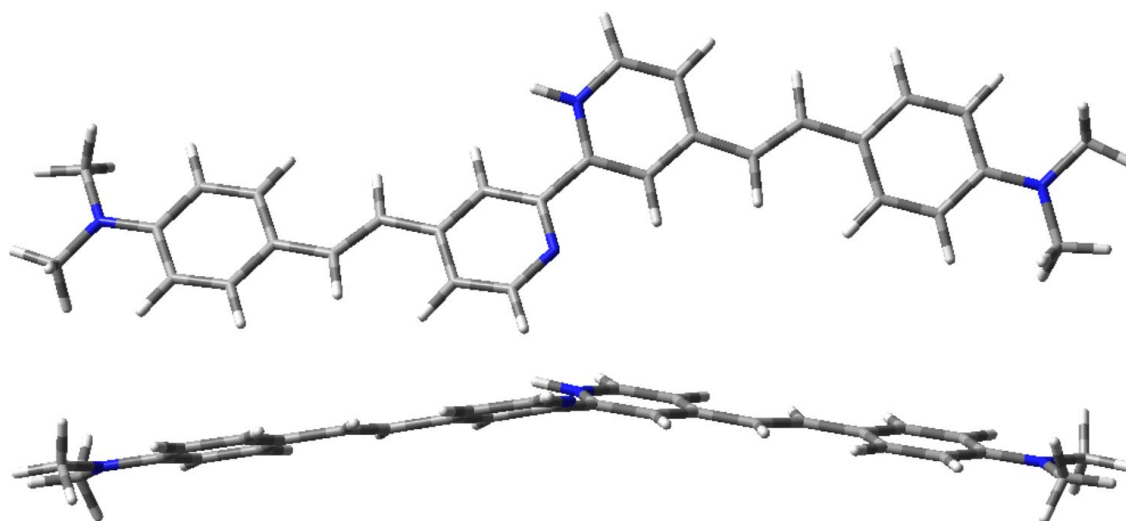


**Figure S9.** <sup>13</sup>C NMR Spectrum (DEPT) of TM3 (CDCl<sub>3</sub>, 100 MHz)

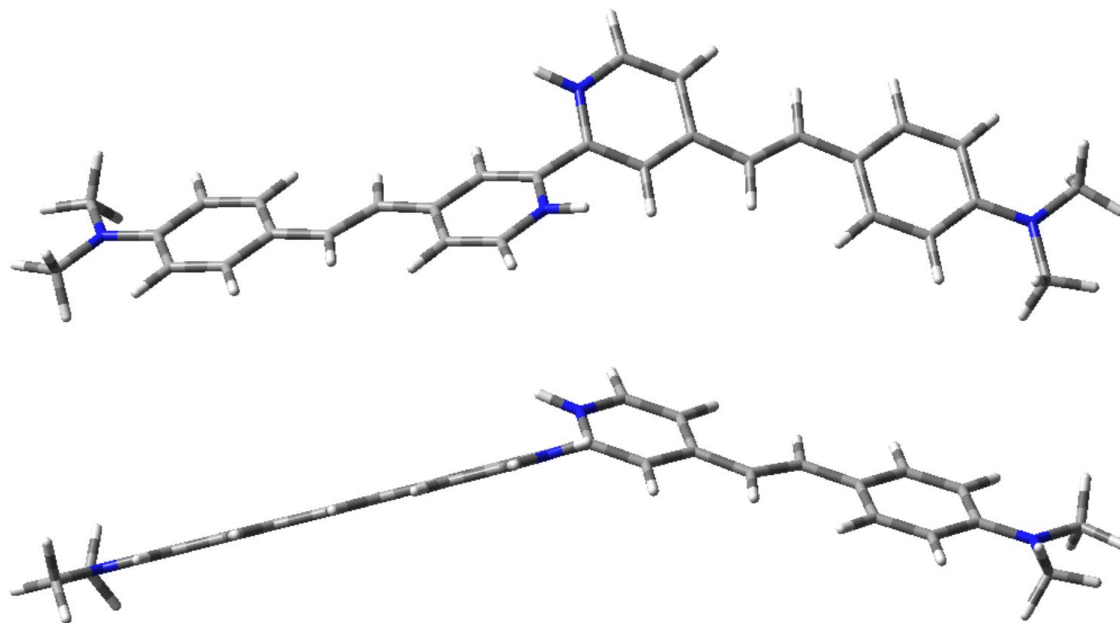
### Computational data



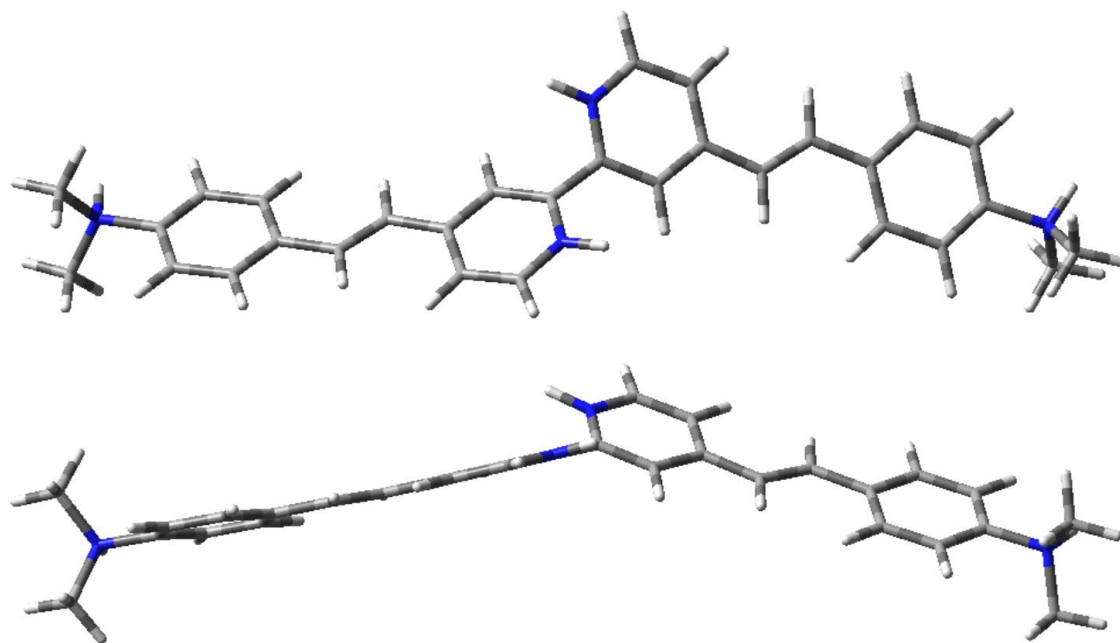
**Figure S10.** Ground state optimized structure of the neutral species in dichloromethane.



**Figure S11.** Ground state optimized structure of the mono protonated species in dichloromethane.



**Figure S12.** Ground state optimized structure of the di-protonated species in dichloromethane.



**Figure S13.** Ground state optimized structure of the tetra-protonated species in dichloromethane.

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