Supporting Information

Probing the Dynamic Environment-Associated Conformational Conversion from Secondary to Supersecondary Structures in Oligo(Phenanthroline Dicarboxamide)s

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Contents

1. General Methods

Melting points, taken on an electrothermal melting point apparatus, are uncorrected. ^{1}H and ^{13}C NMR spectra were obtained in $CDCl_3$ solution (chemical shifts in ppm relative to internal TMS, *J* in Hertz). Mass spectra were obtained by MALDI-TOF technique. The CD spectra were obtained with a Jasco J-815 spectropolarimeter. The $CDCl_3$ solvent used in NMR experiment was dealt with basic aluminum oxide (for chromatographic use) and the other materials obtained commercially were used without further purification.

2. ^{1}H NMR and ^{13}C NMR Spectra of New Compounds

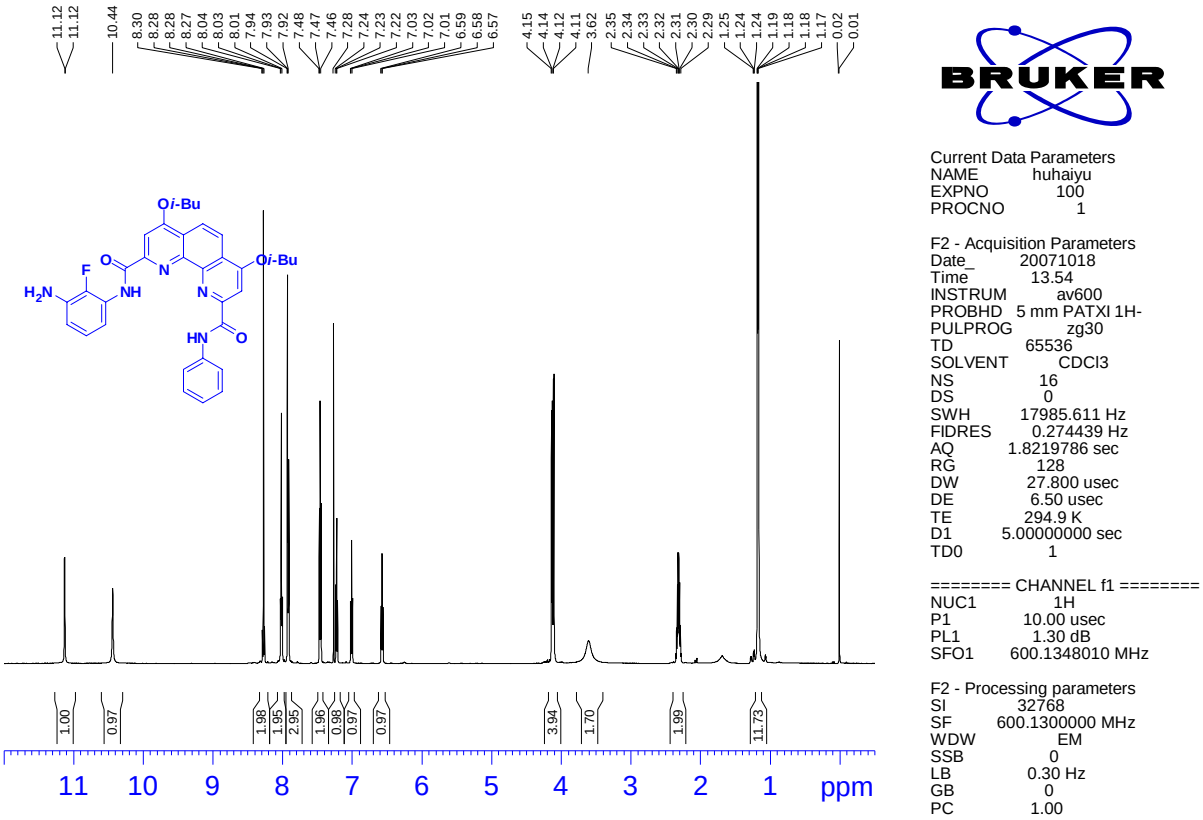


Figure S1. The ^{1}H NMR spectrum of compound **5**.

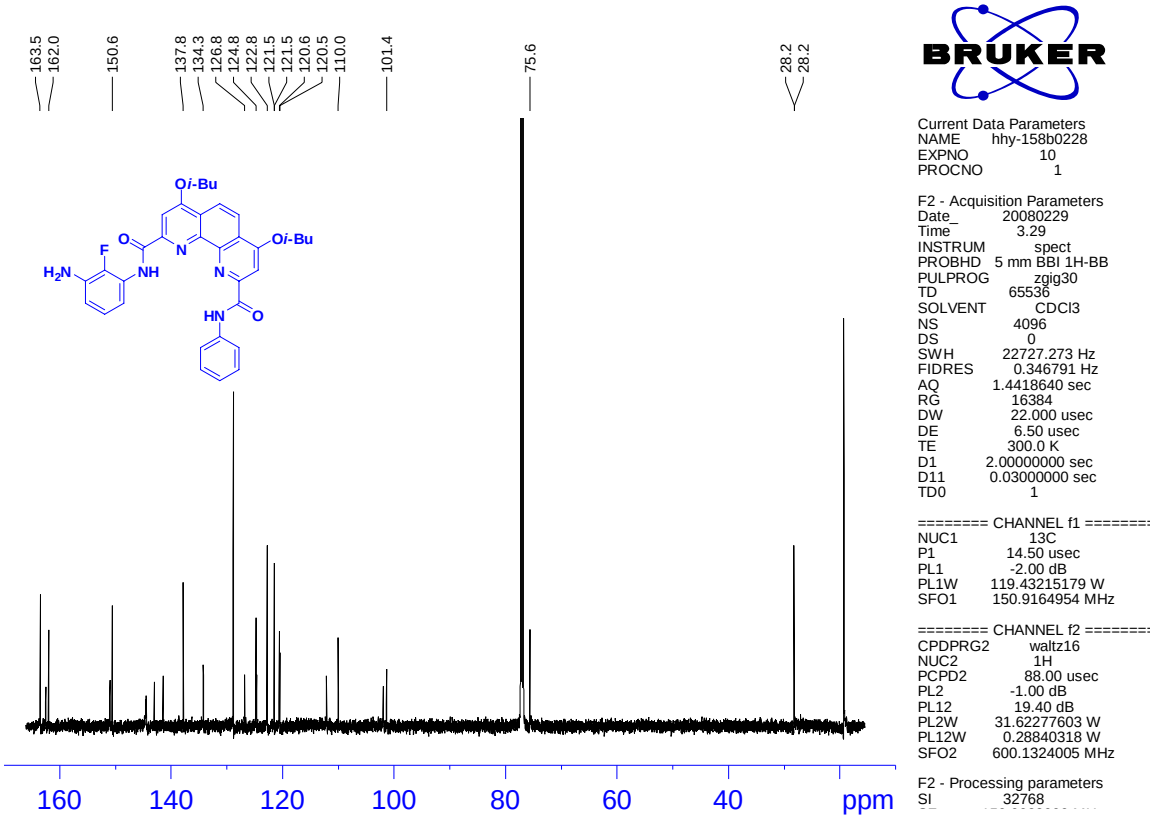
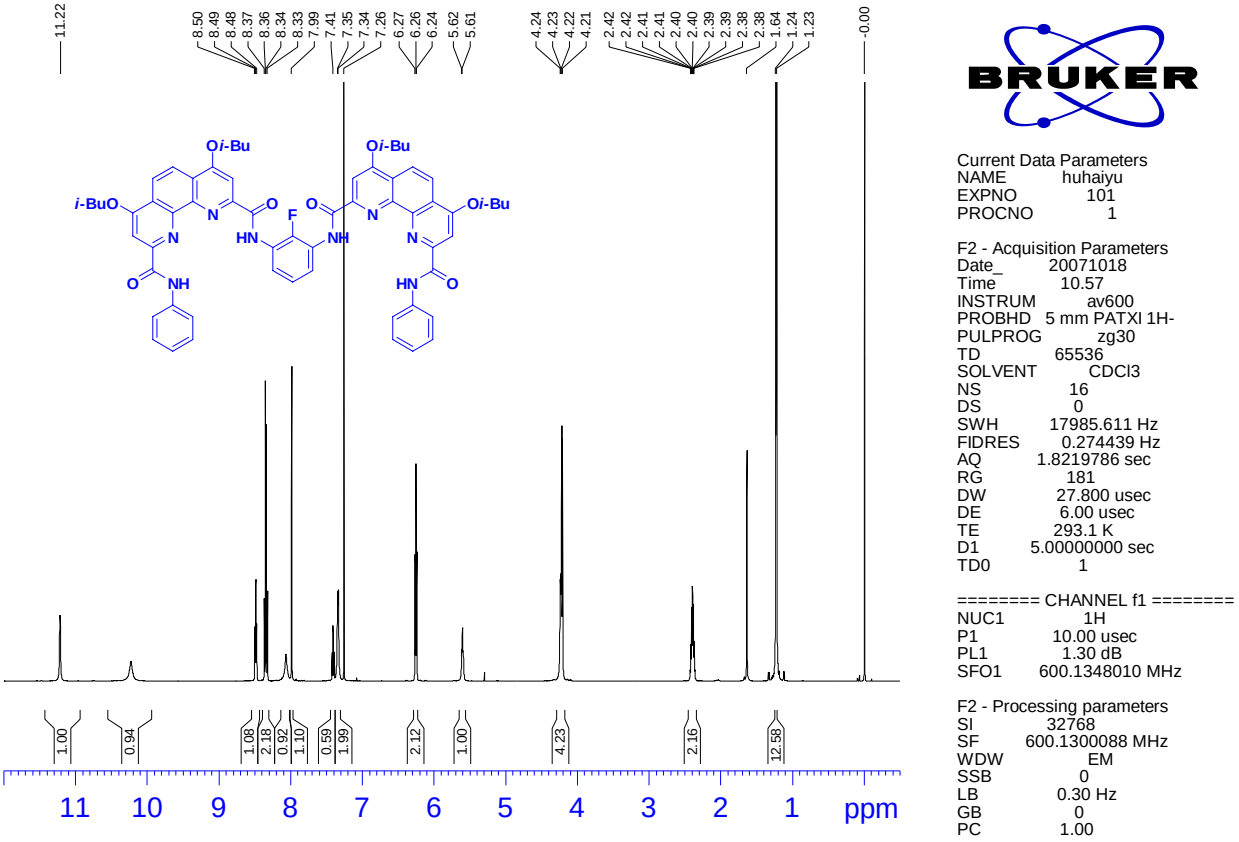


Figure S2. The ^{13}C NMR spectrum of compound **5**.



BRUKER

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PROCNO 1

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SOLVENT CDCl3
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SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219786 sec
RG 181
DW 27.800 usec
DE 6.00 usec
TE 293.1 K
D1 5.00000000 sec
TD0 1

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P1 10.00 usec
PL1 1.30 dB
SFO1 600.1348010 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
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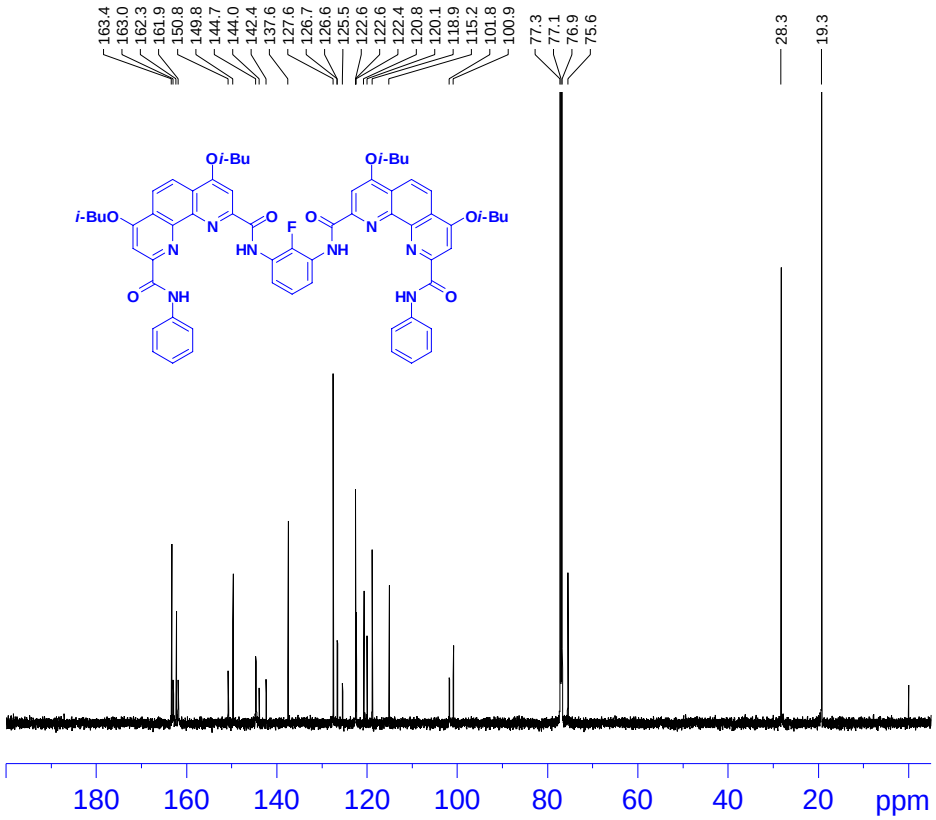
Figure S3. The ^{1}H NMR spectrum of compound **6**.



BRUKER

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D11 0.03000000 sec
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SFO1 150.9178988 MHz

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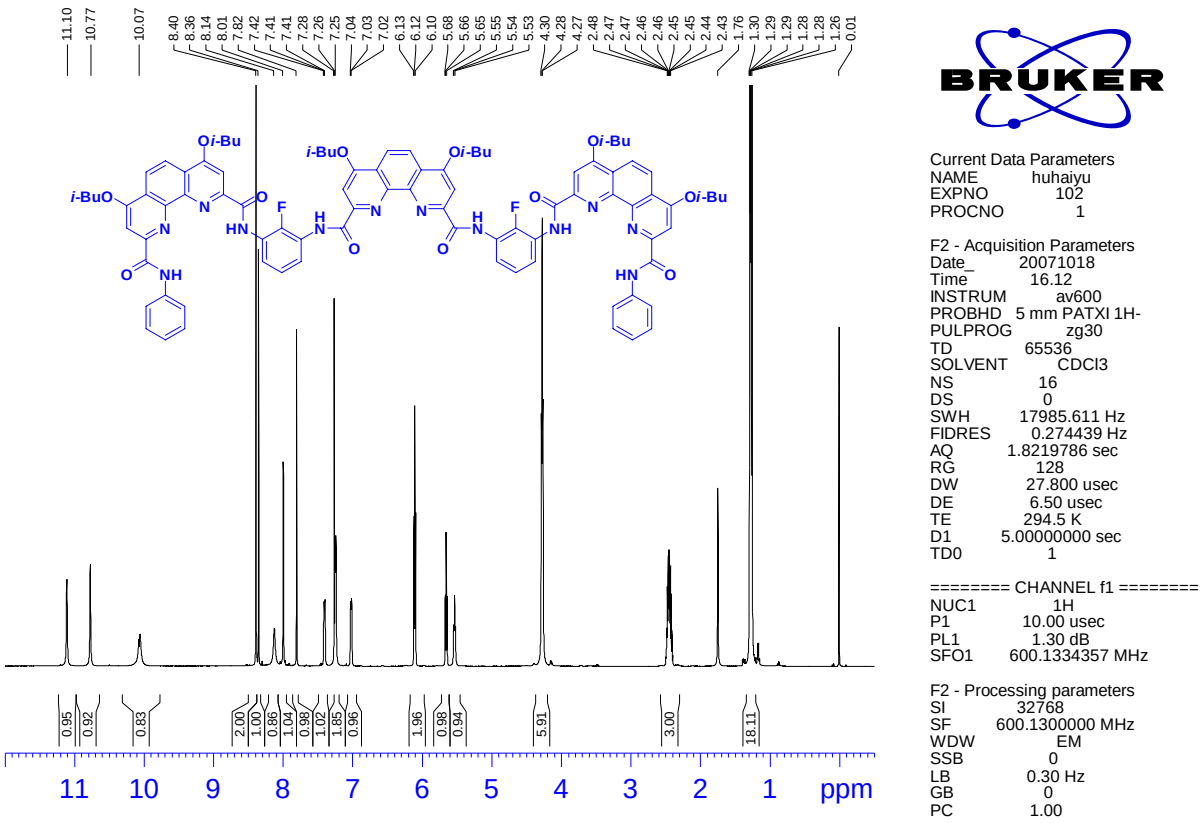
NUC2 1H
PCPD2 88.00 usec
PL2 -1.00 dB
PL12 19.40 dB
PL2W 31.62277603 W
PL12W 0.28840318 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768

Figure S4. The ^{13}C NMR spectrum of compound **6**.



BRUKER

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PROCNO 1

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DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219786 sec
RG 128
DW 27.800 usec
DE 6.50 usec
TE 294.5 K
D1 5.00000000 sec
TD0 1

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PL1 1.30 dB
SFO1 600.1334357 MHz

F2 - Processing parameters
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LB 0.30 Hz
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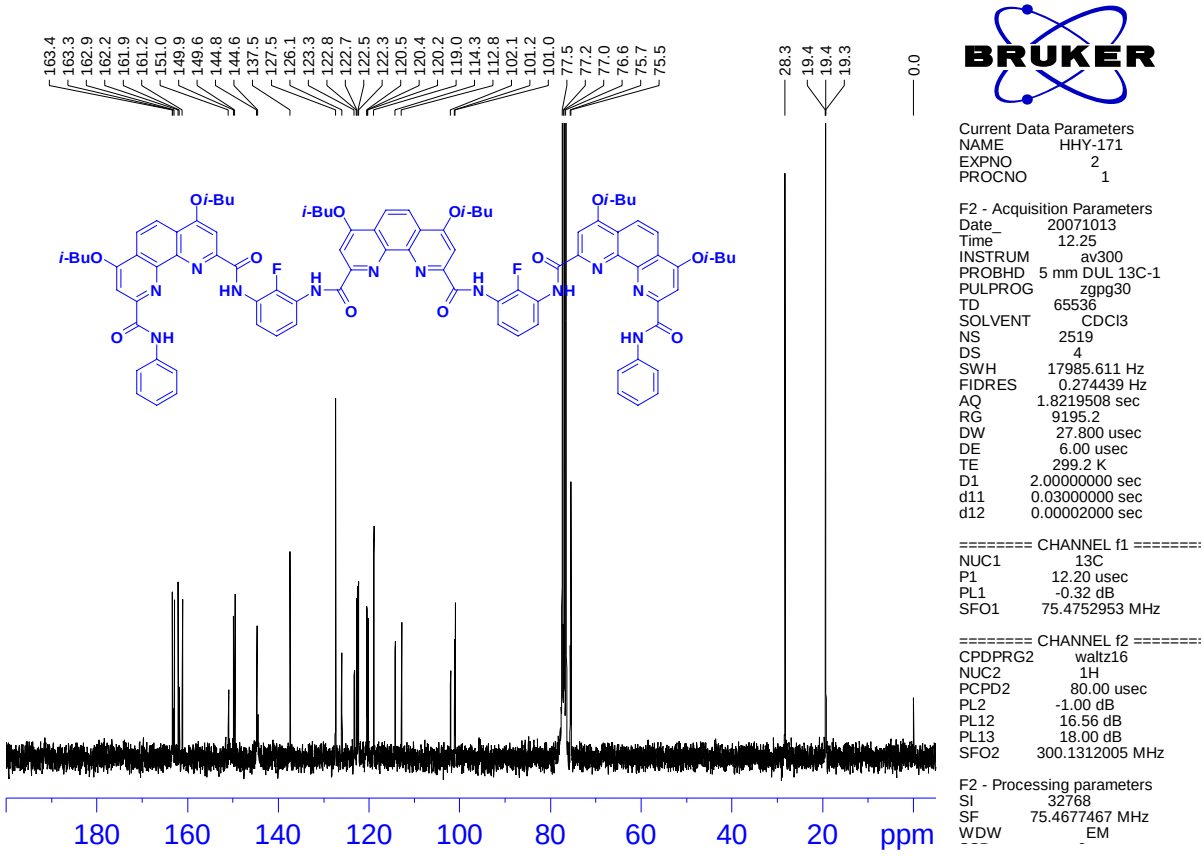
PC 1.00

Figure S5. The ^{1}H NMR spectrum of compound **7**.



BRUKER

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PROCNO 1

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FIDRES 0.274439 Hz
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RG 9195.2
DW 27.800 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.20 usec
PL1 -0.32 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.56 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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SF 75.4677467 MHz
WDW EM

Figure S6. The ^{13}C NMR spectrum of compound **7**.

3. TOCSY and NOESY Spectra of Compounds 5~7

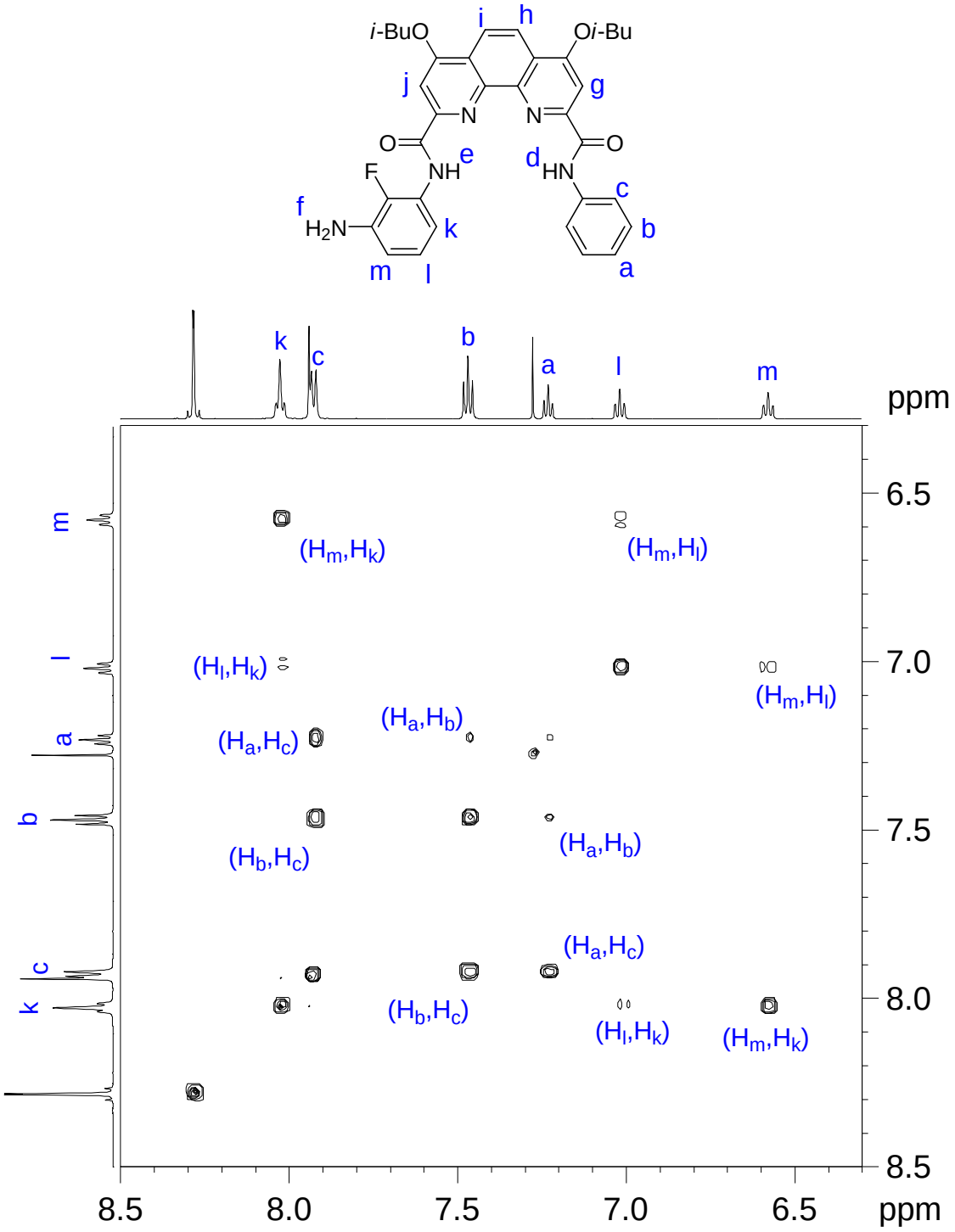


Figure S7. The TOCSY spectrum (600 MHz, $CDCl_3$) of compound **5**.

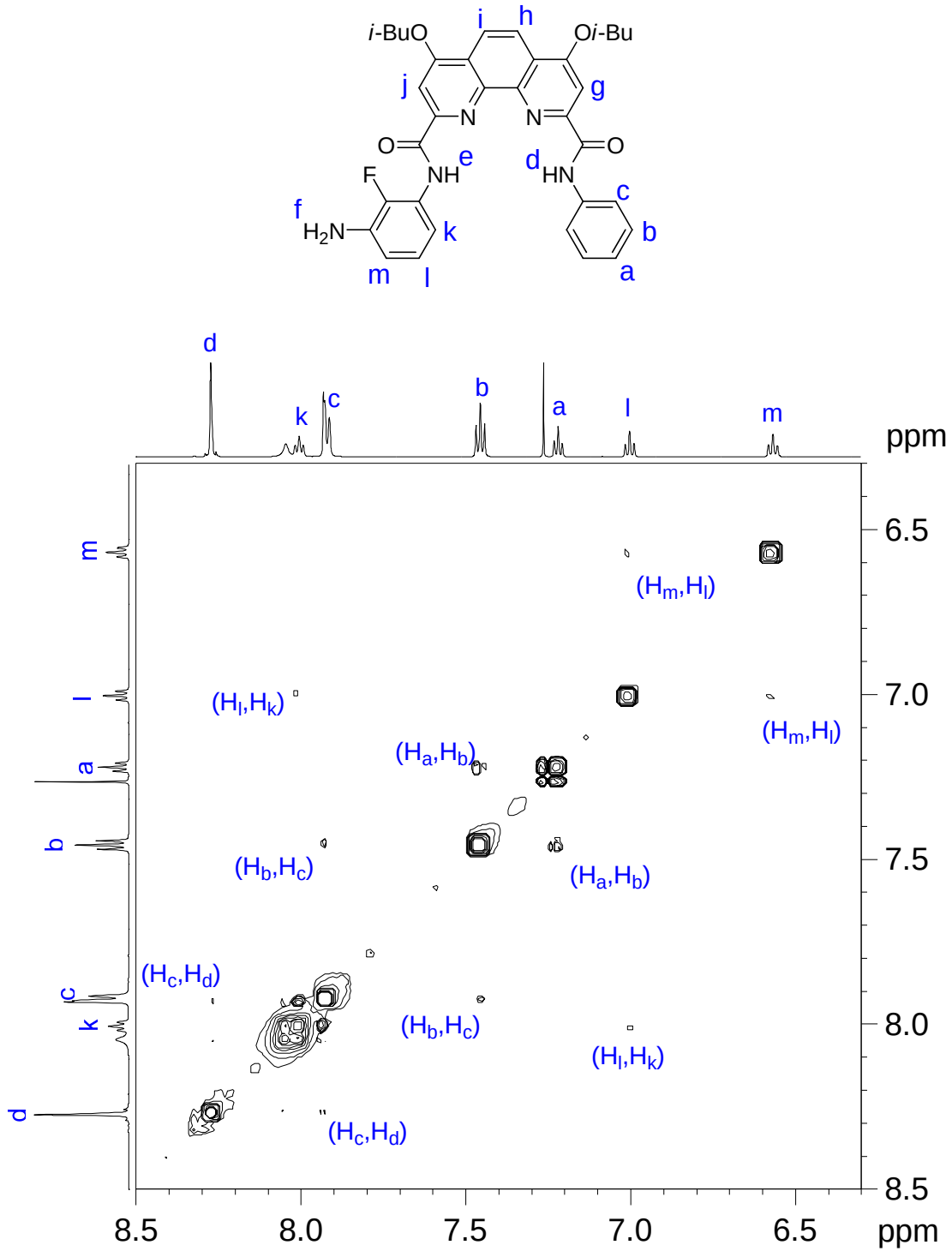


Figure S8. The NOESY spectrum (600 MHz, $CDCl_3$) of compound **5**.

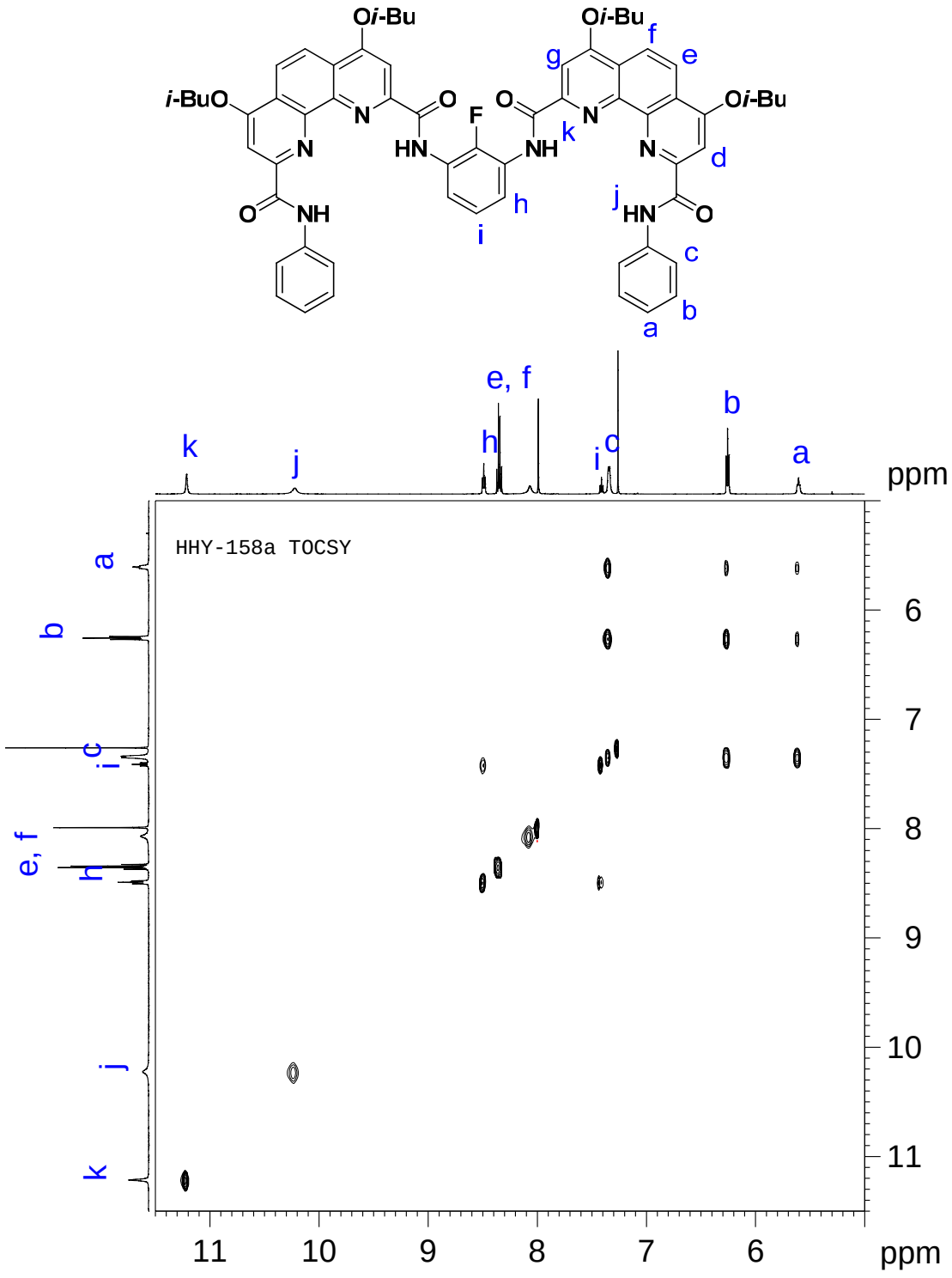


Figure S9. The TOCSY spectrum (600 MHz, $CDCl_3$) of compound **6**.

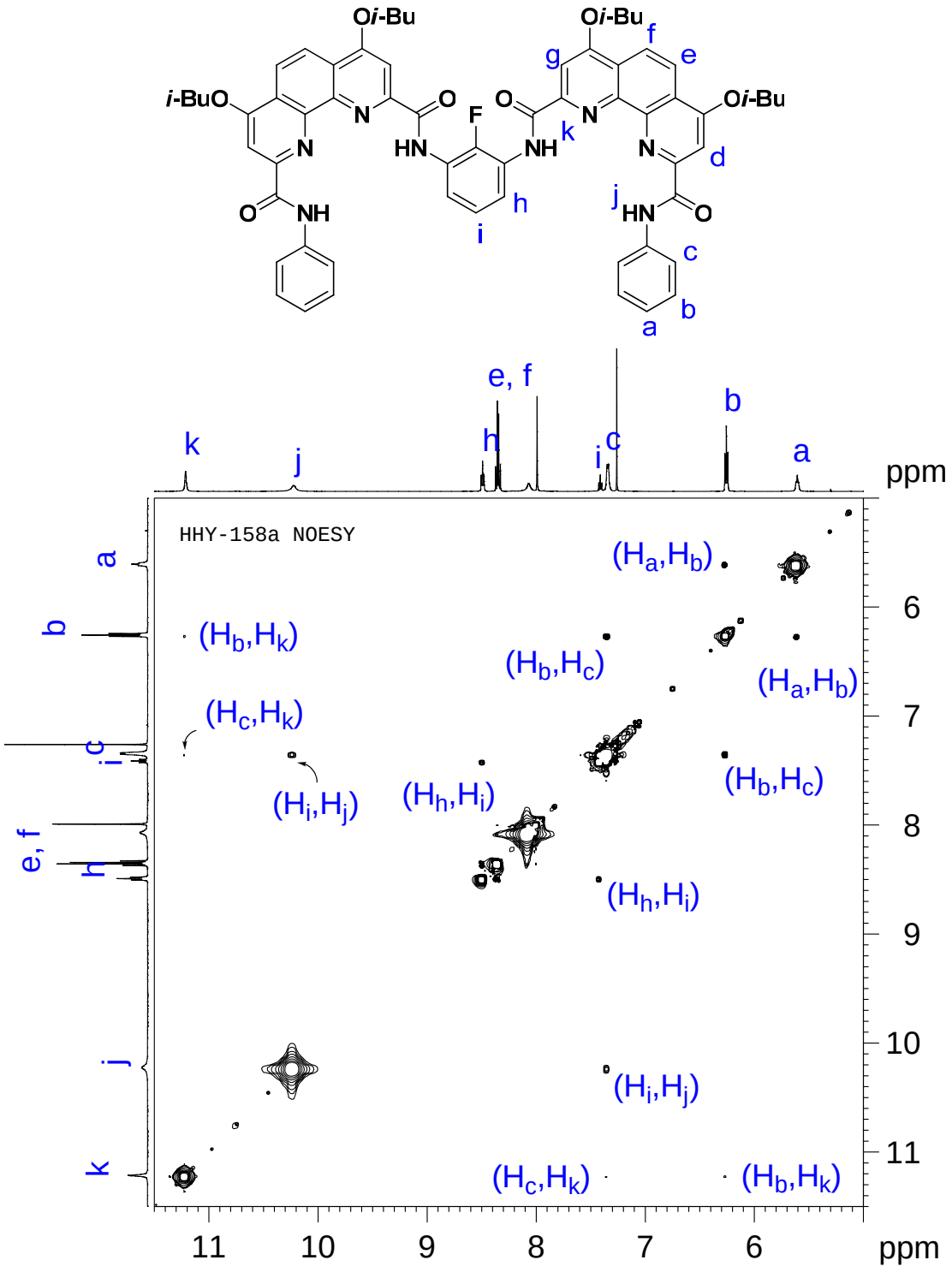


Figure S10. The NOESY spectrum (600 MHz, $CDCl_3$) of compound **6**.

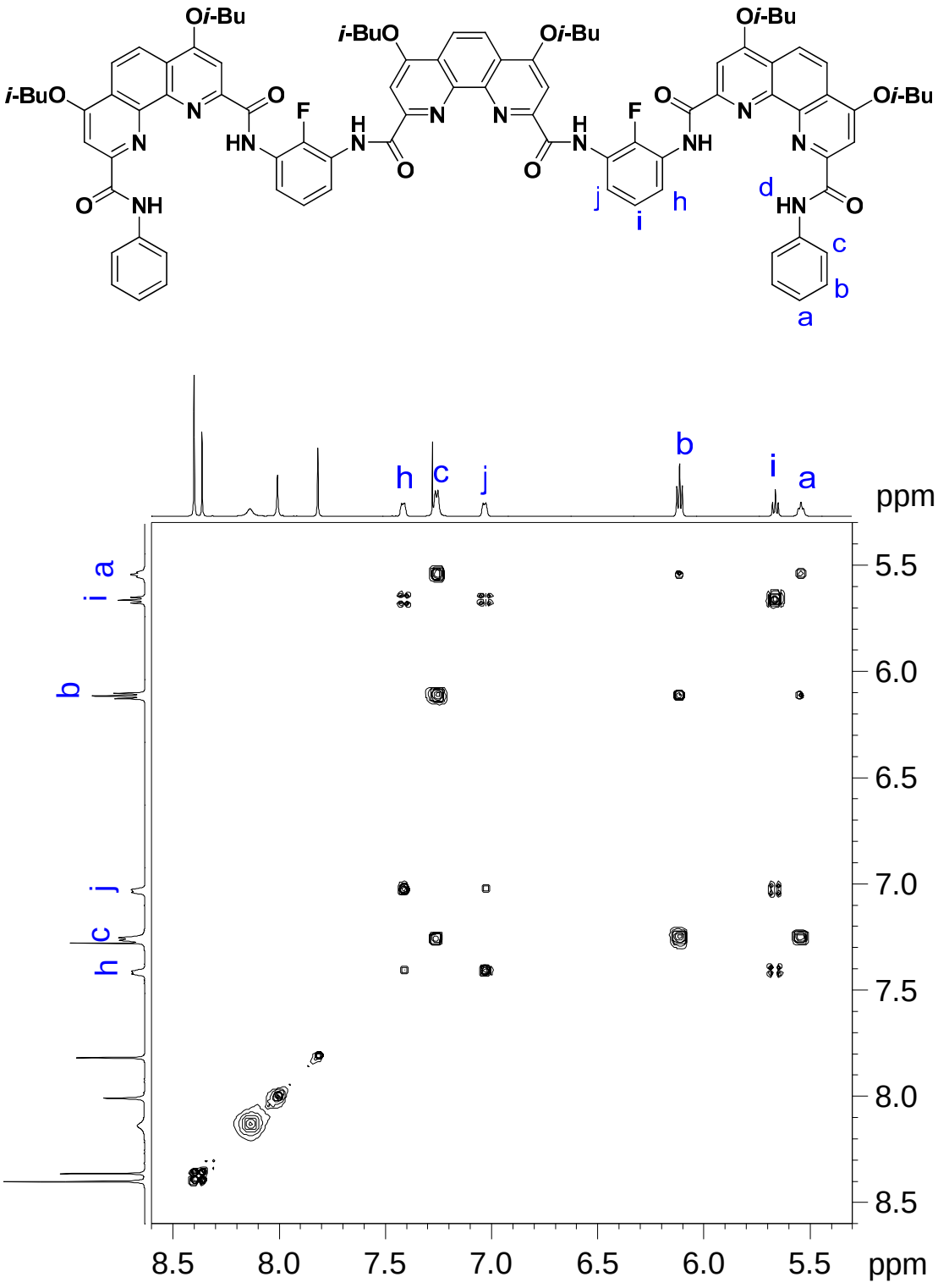


Figure S11. The TOCSY spectrum (600 MHz, $CDCl_3$) of compound **7**.

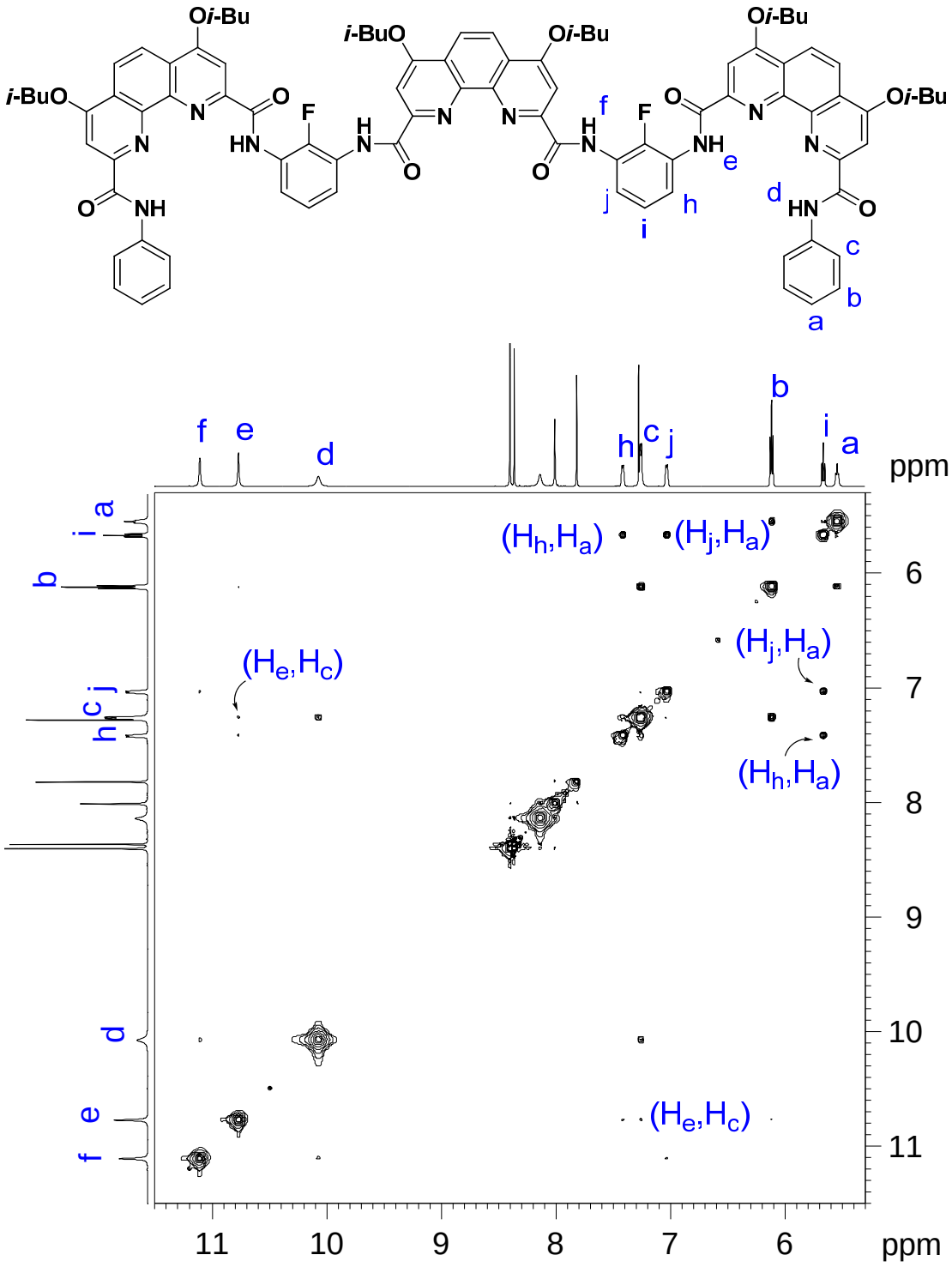
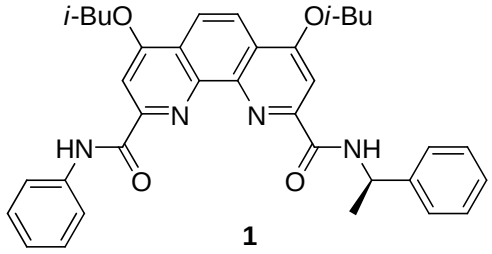


Figure S12. The NOESY spectrum (600 MHz, $CDCl_3$) of compound **7**.

4. Variable-Temperature ^{1}H NMR Studies on Oligomers 1~4 and 1a~4a



1

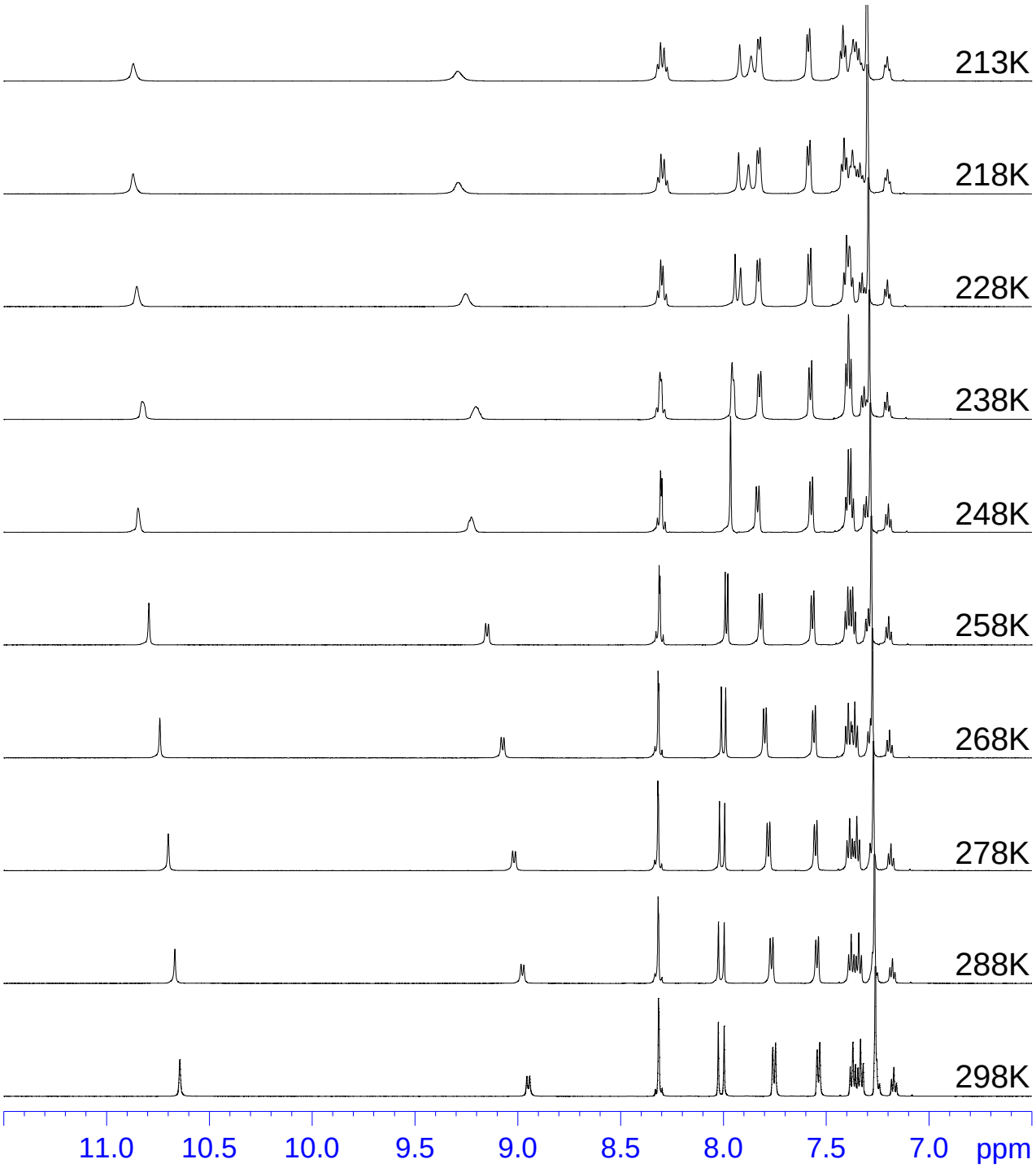


Figure S13. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **1**.

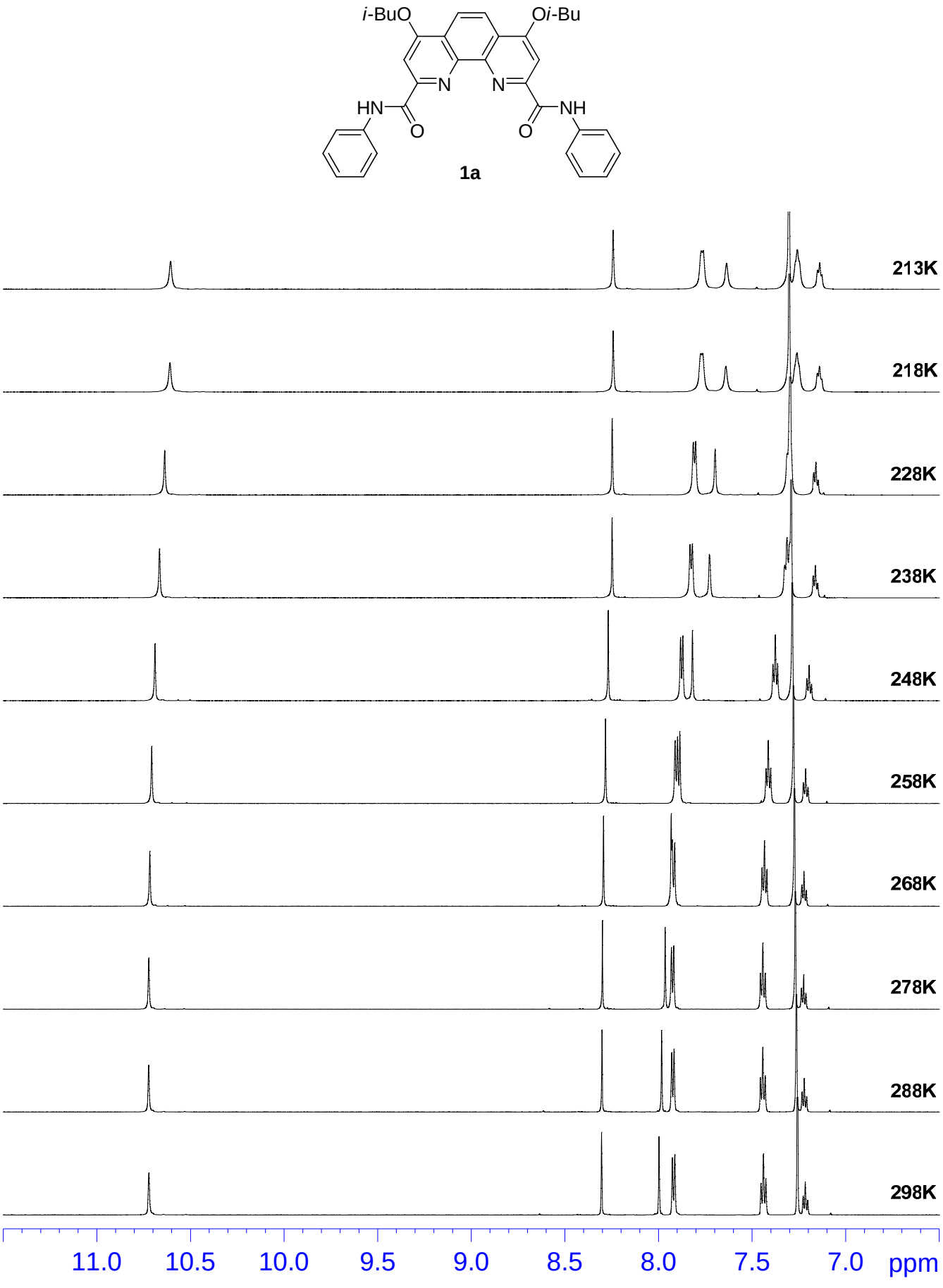


Figure S14. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **1a**.

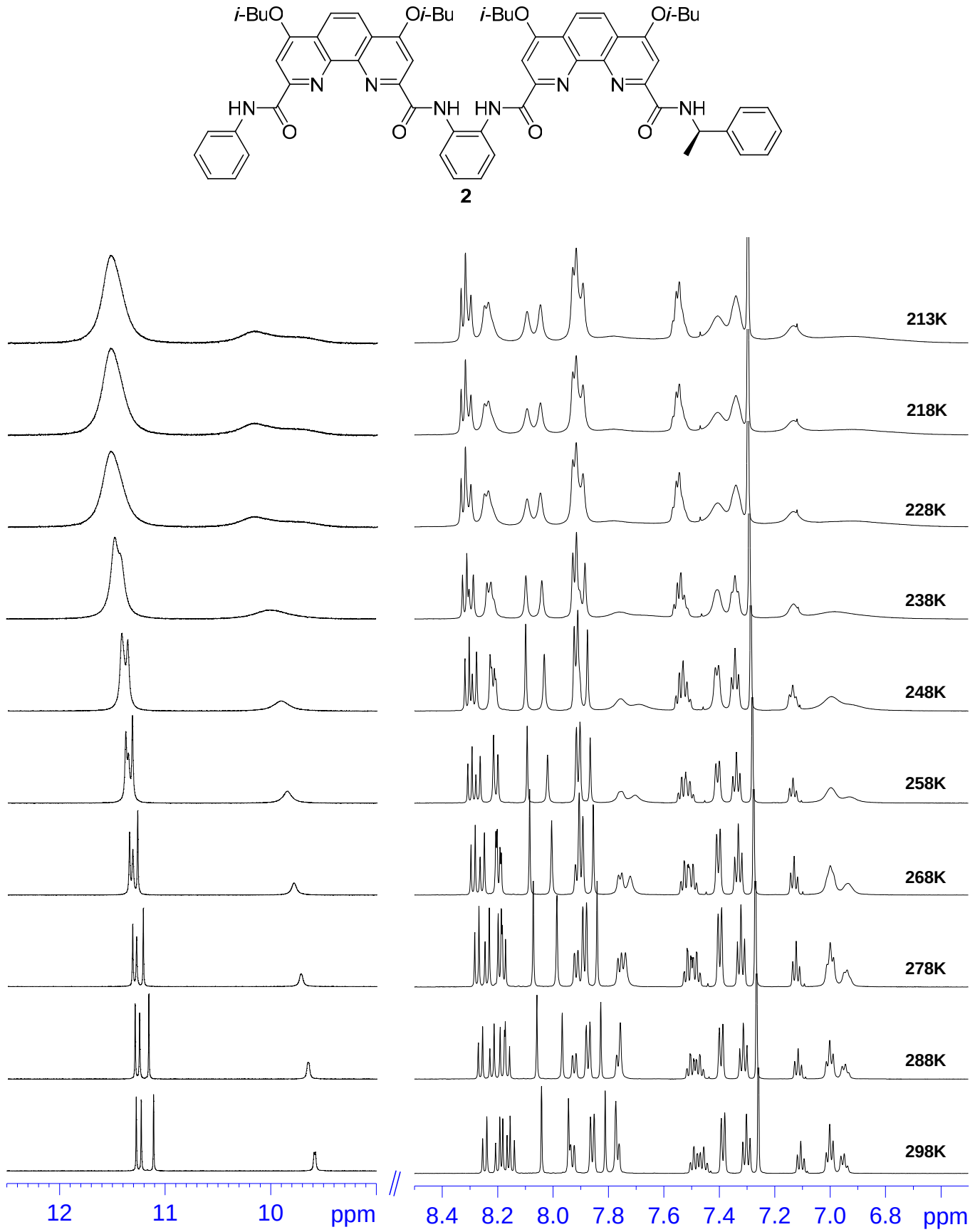


Figure S15. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **2**.

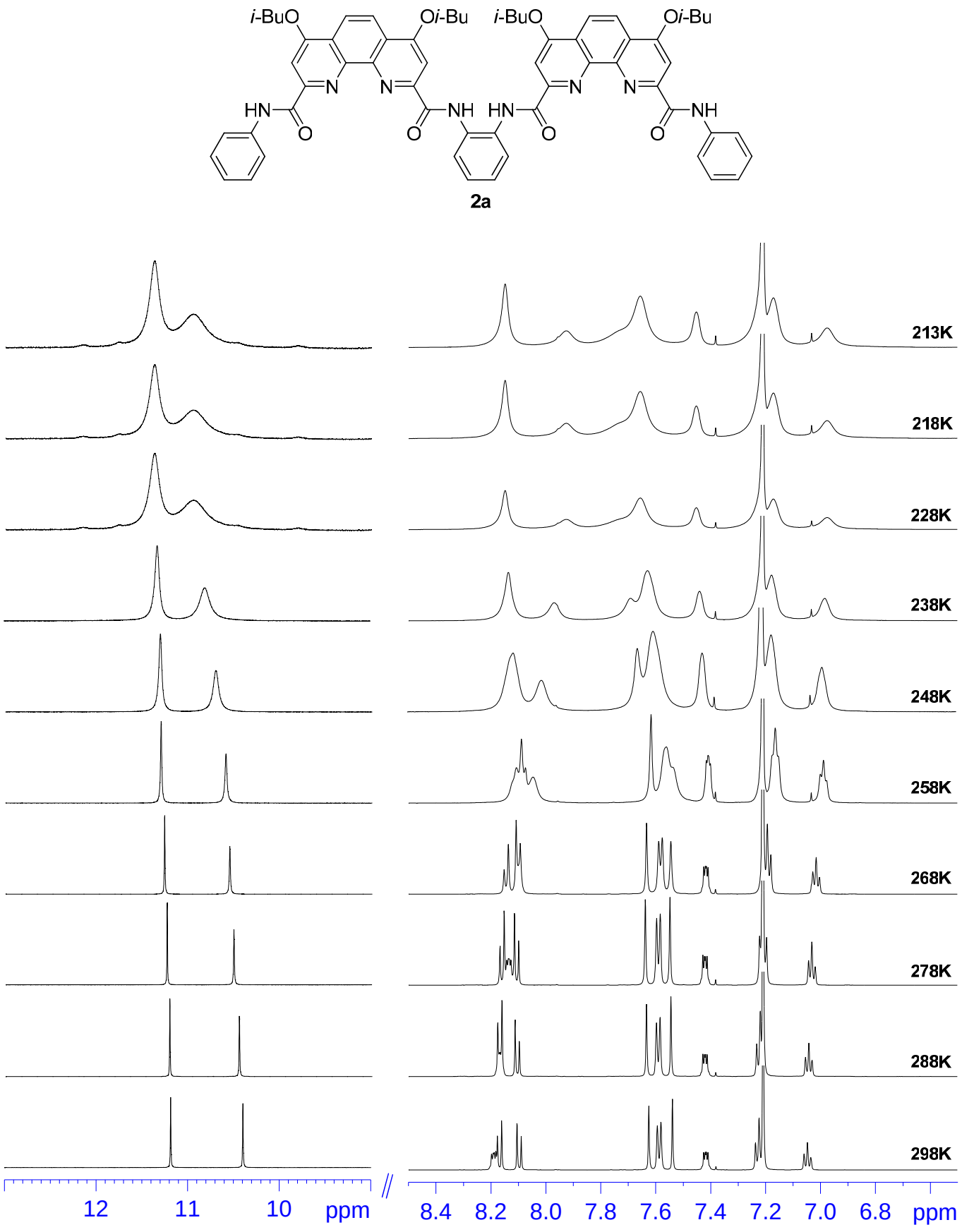


Figure S16. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **2a**.

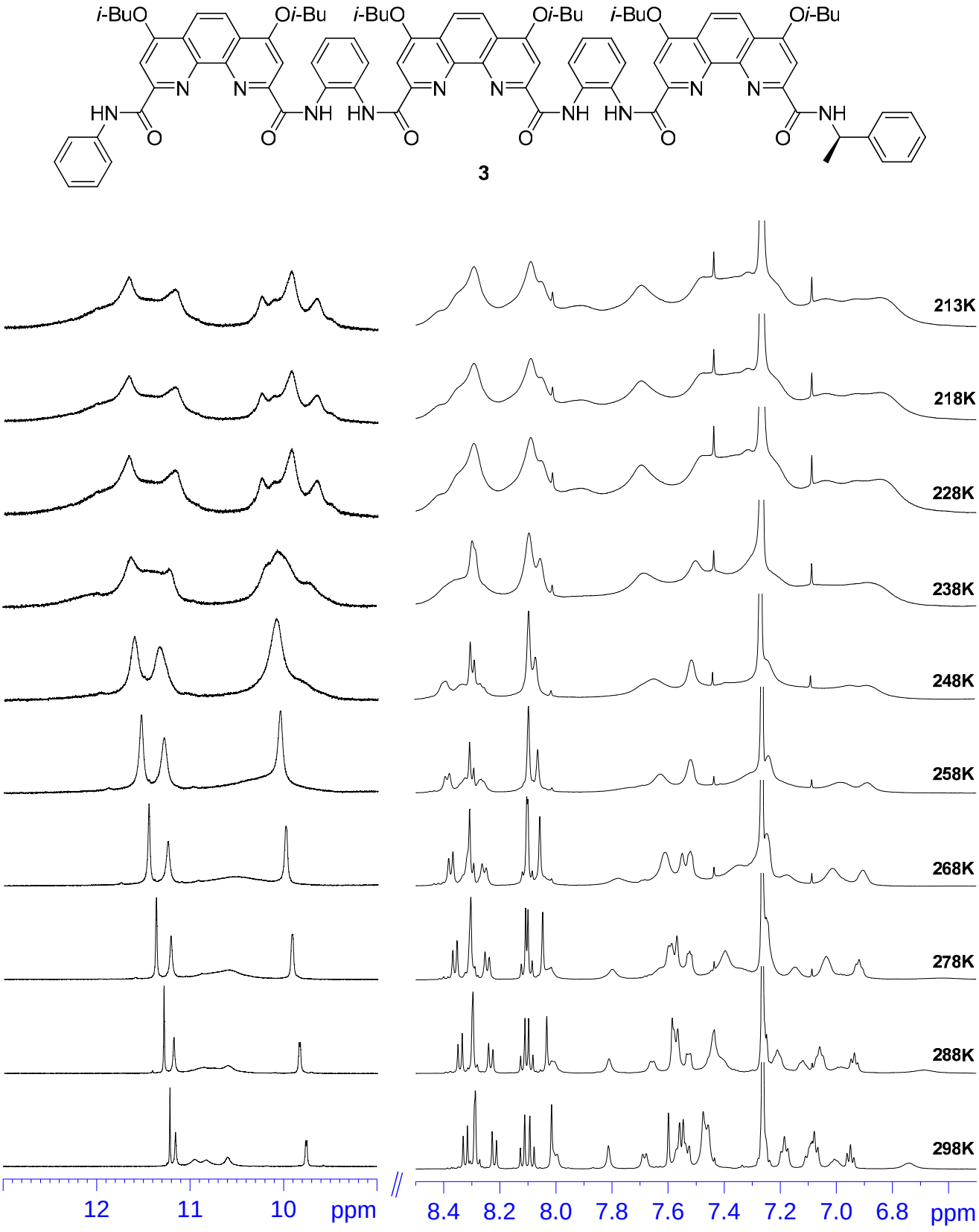


Figure S17. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **3**.

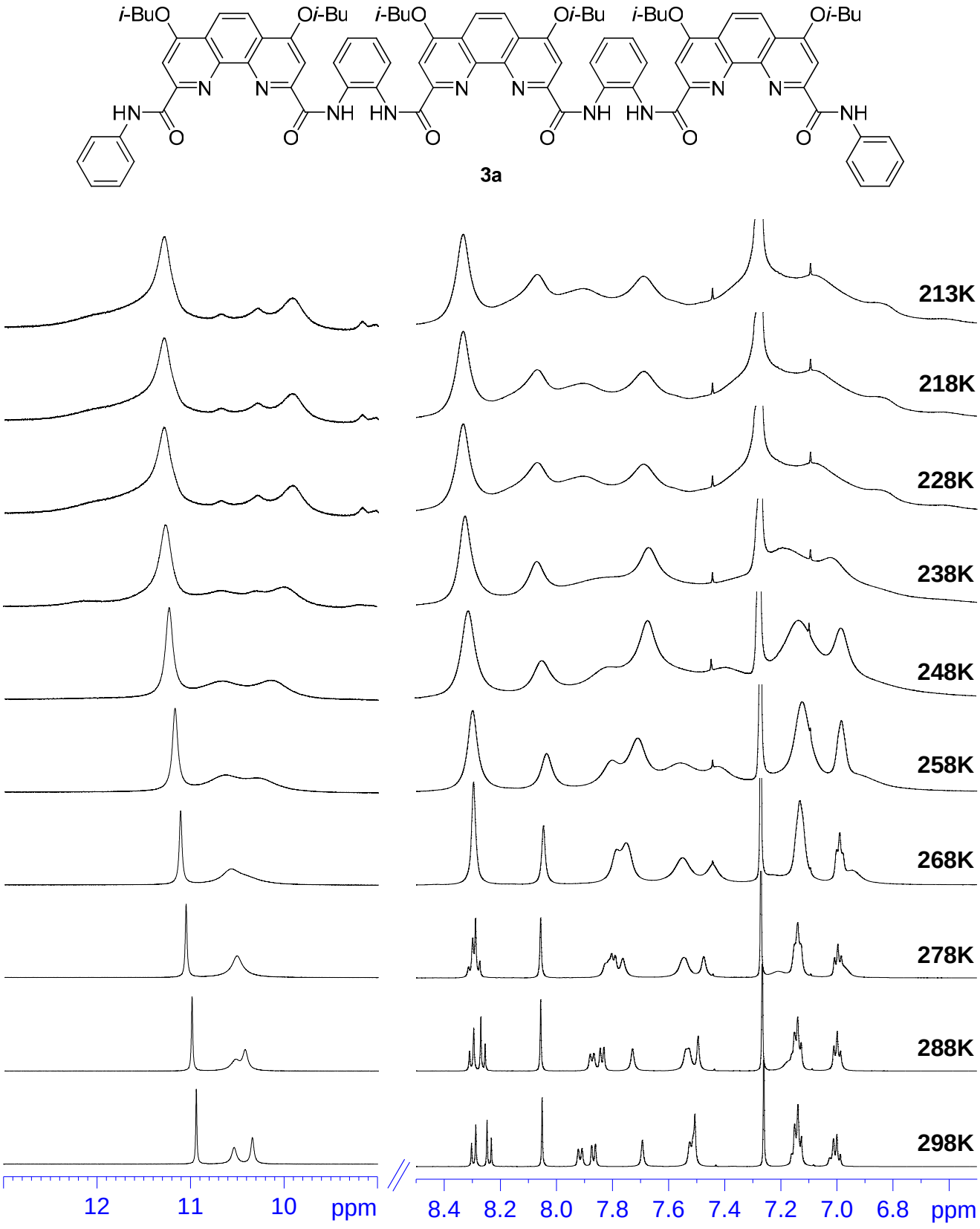


Figure S18. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **3a**.

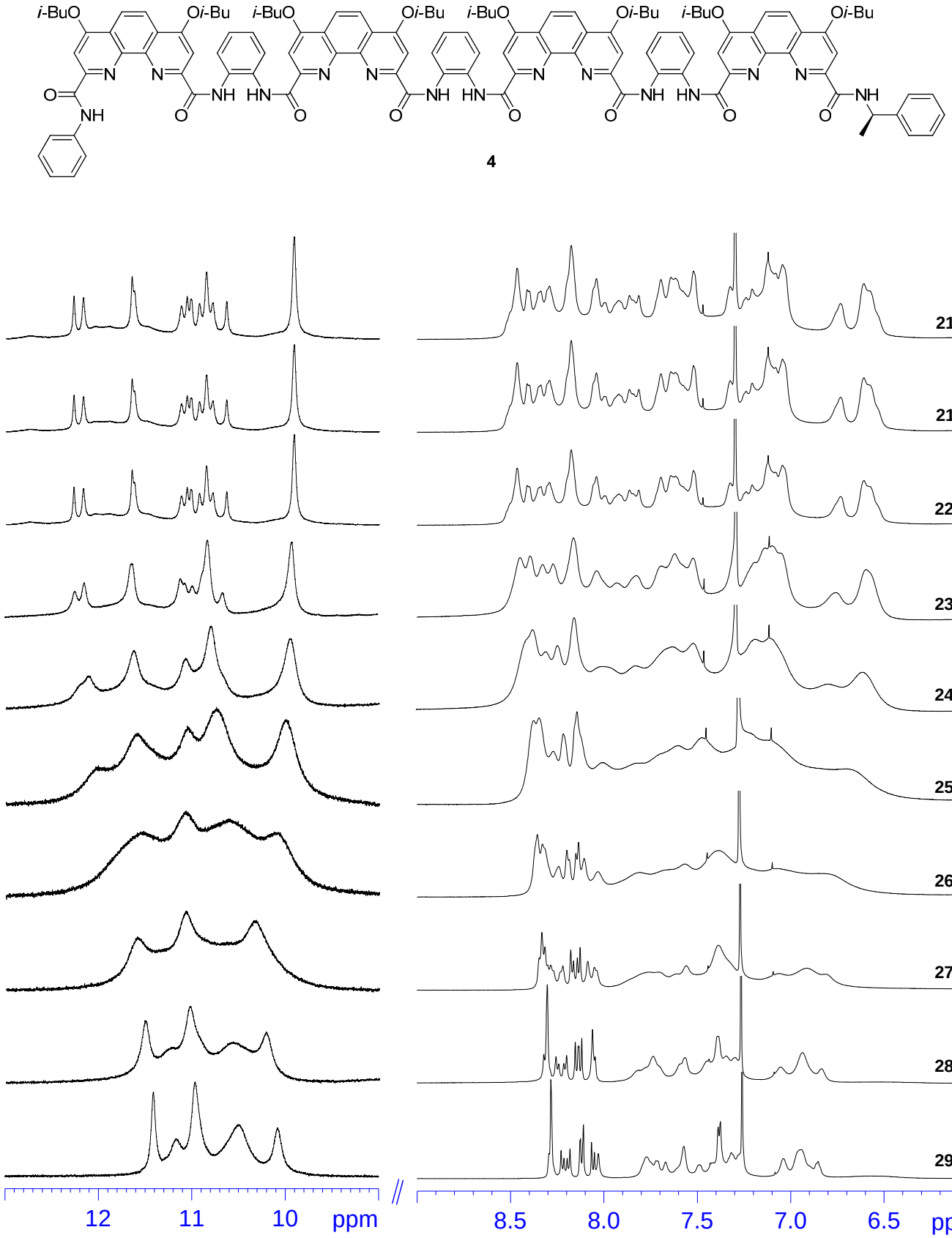


Figure S19. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **4**.

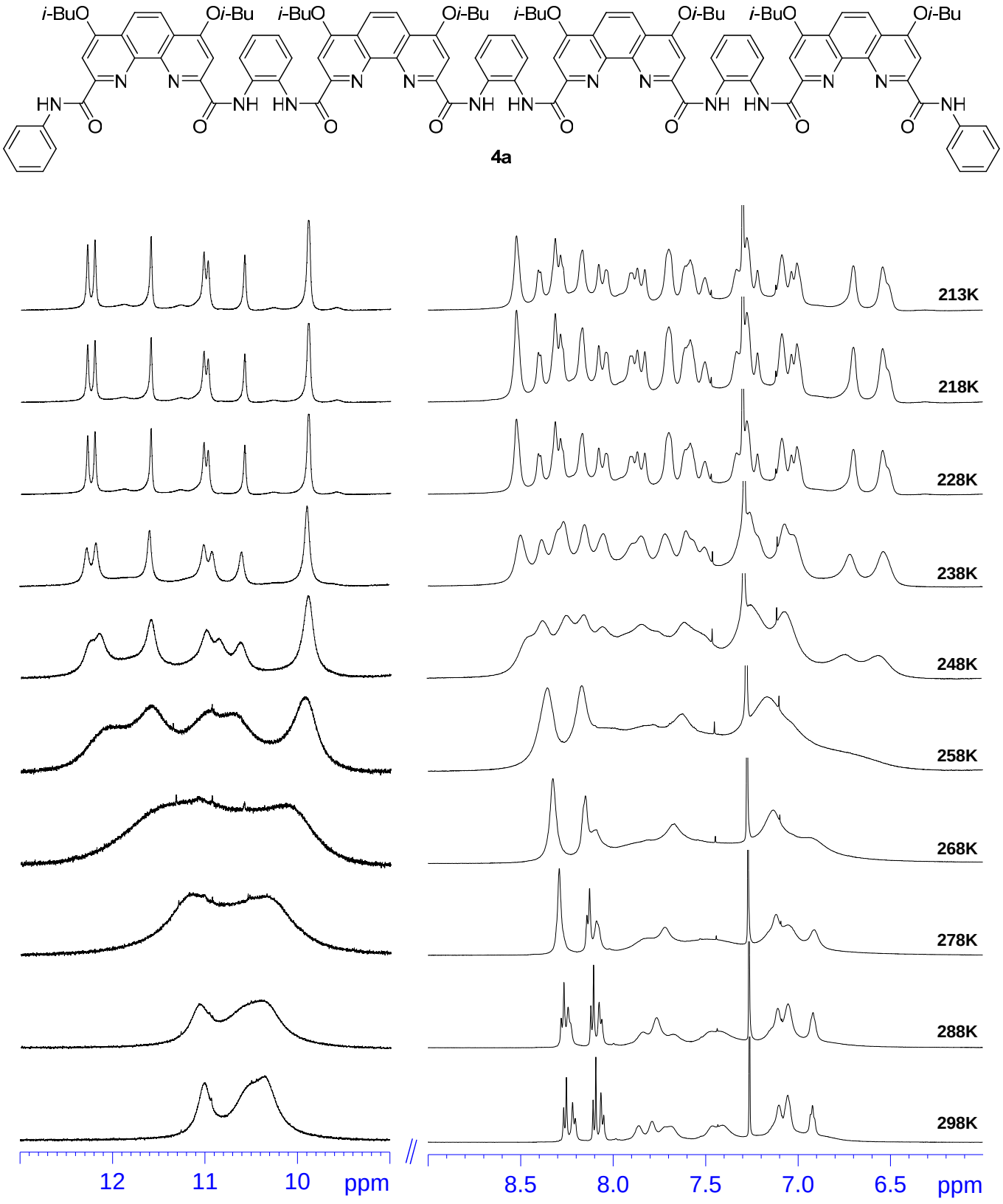


Figure S20. Temperature dependent ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **4a**.

5. CD Spectra of Oligomers 1~4 at Various Concentrations in Various Solvents

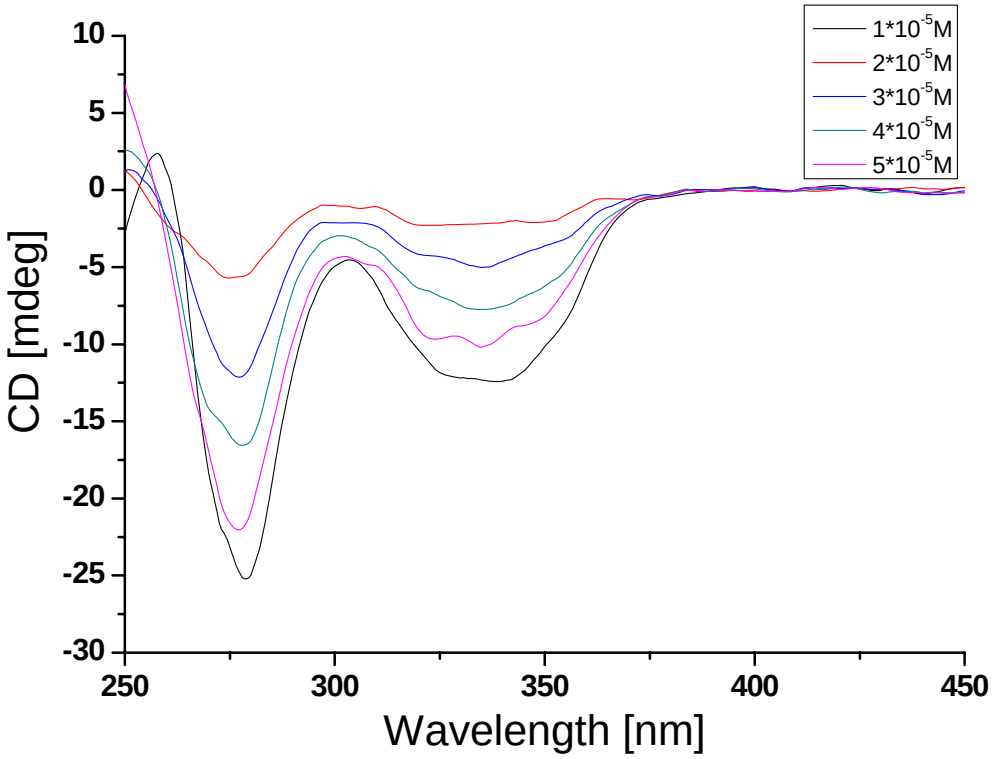


Figure S21. CD spectra of **1** in CH_3OH at various concentrations.

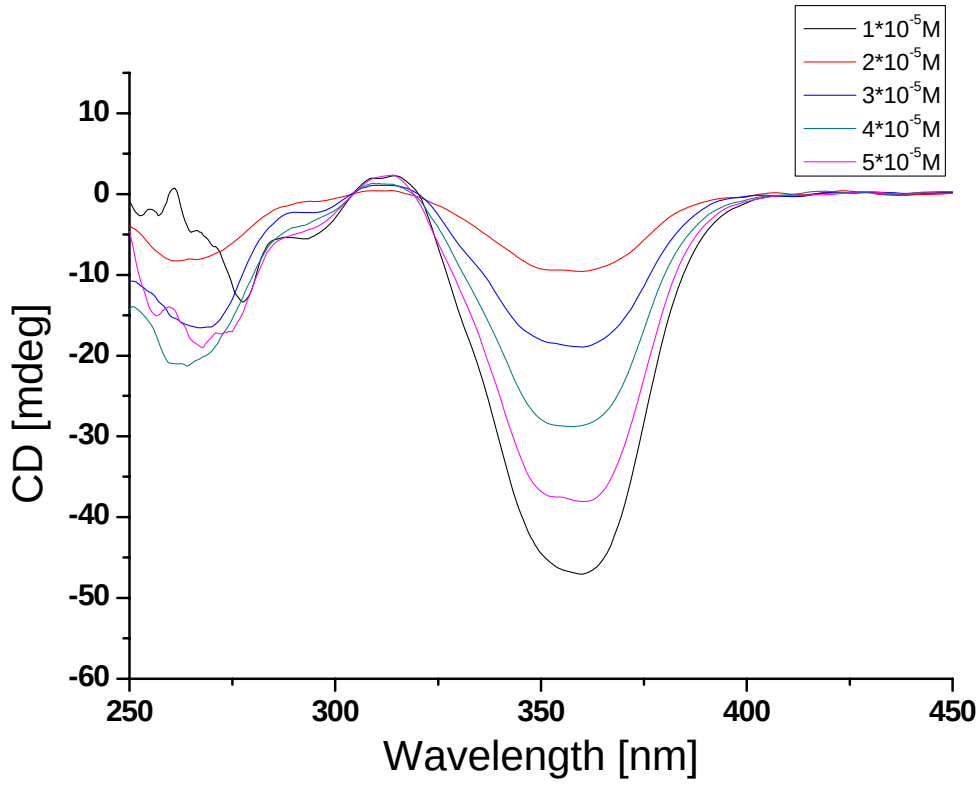


Figure S22. CD spectra of **2** in CH_3OH at various concentrations.

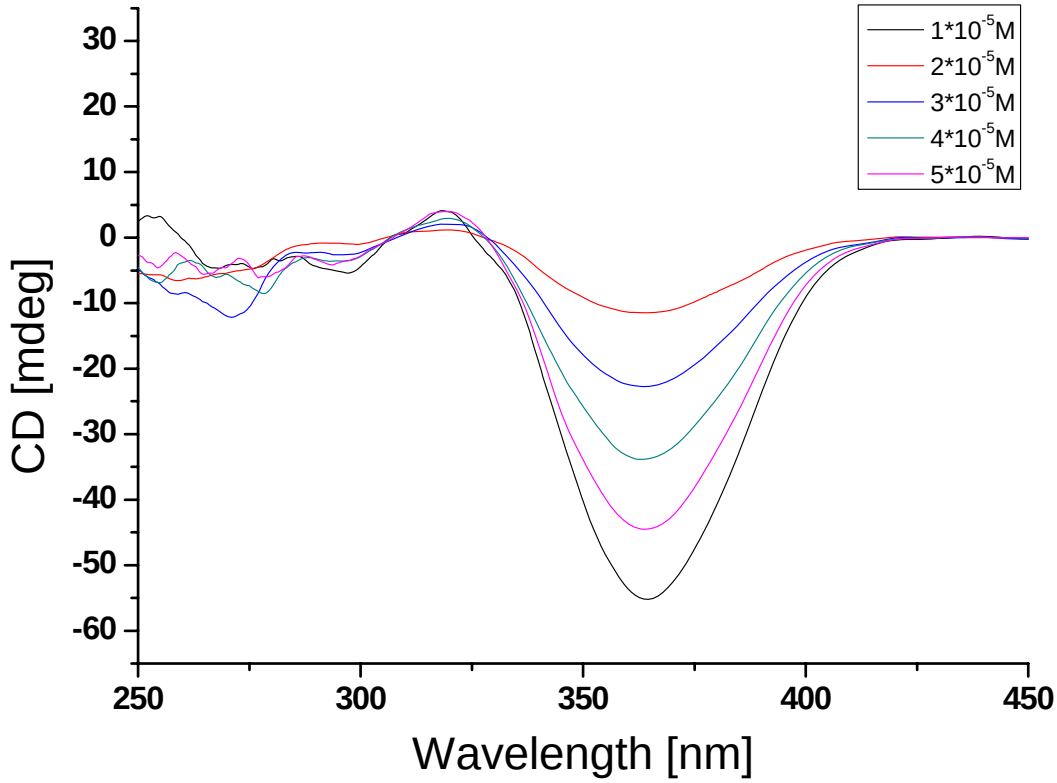


Figure S23. CD spectra of **3** in CH_3OH at various concentrations.

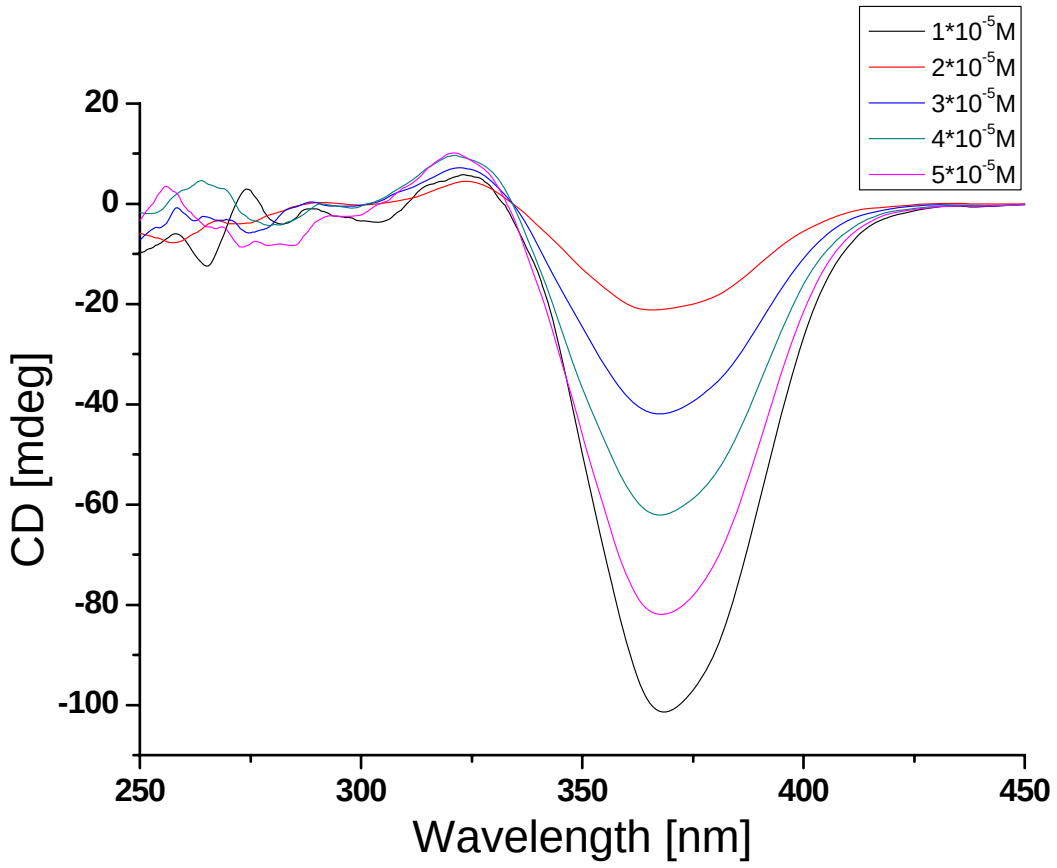


Figure S24. CD spectra of **4** in CH_3OH at various concentrations.

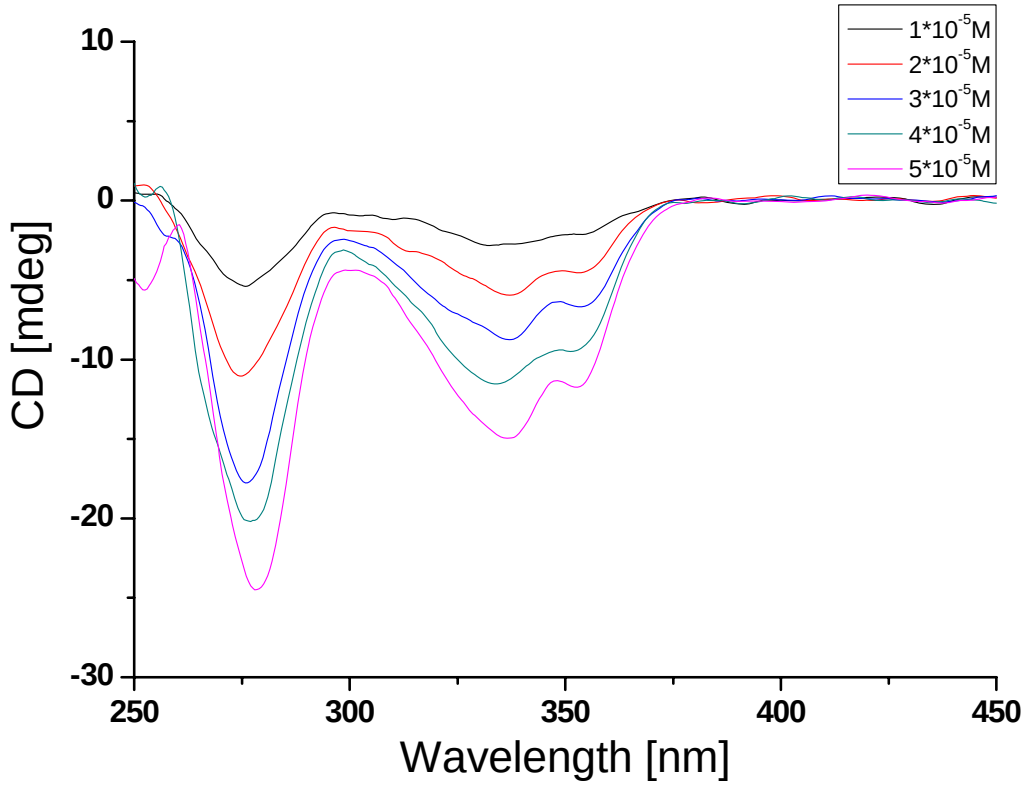


Figure S25. CD spectra of **1** in CH_2Cl_2 at various concentrations.

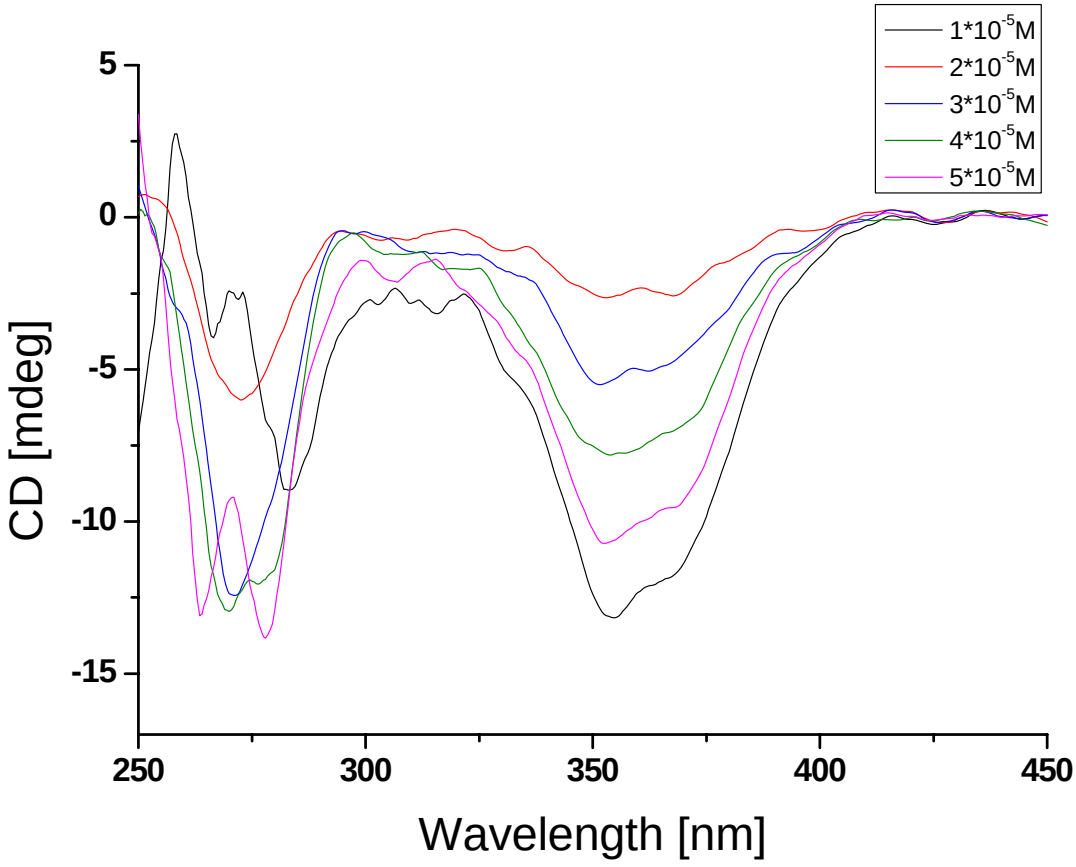


Figure S26. CD spectra of **2** in CH_2Cl_2 at various concentrations.

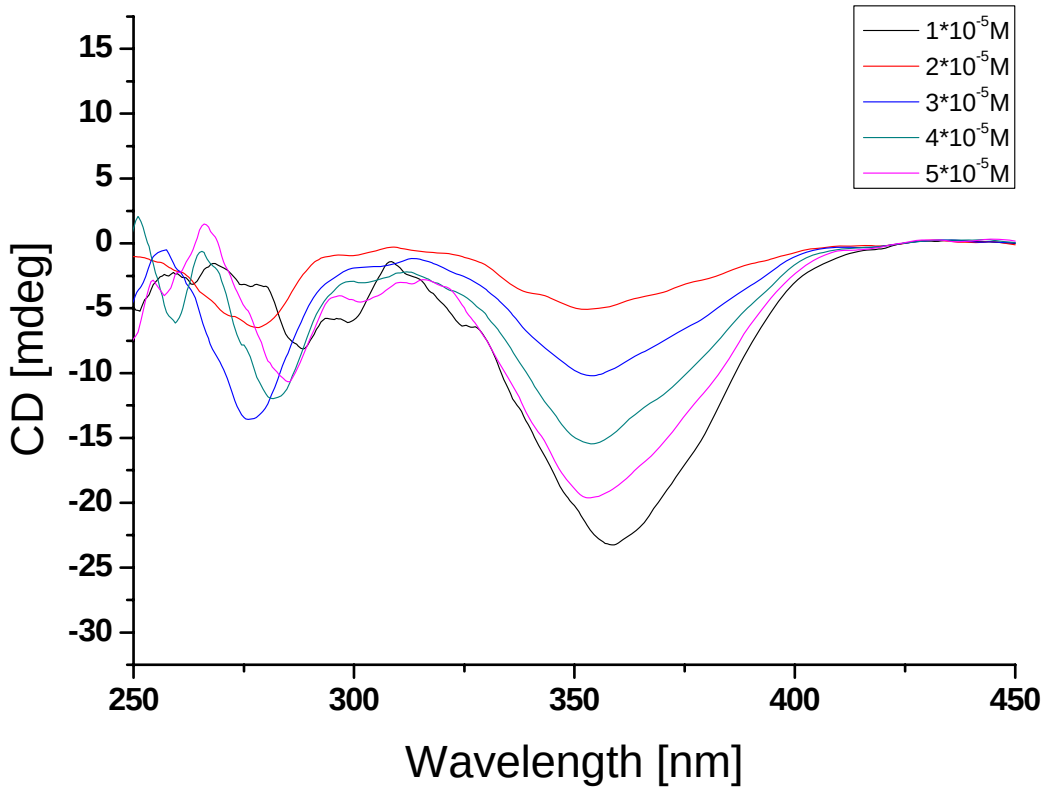


Figure S27. CD spectra of **3** in CH_2Cl_2 at various concentrations.

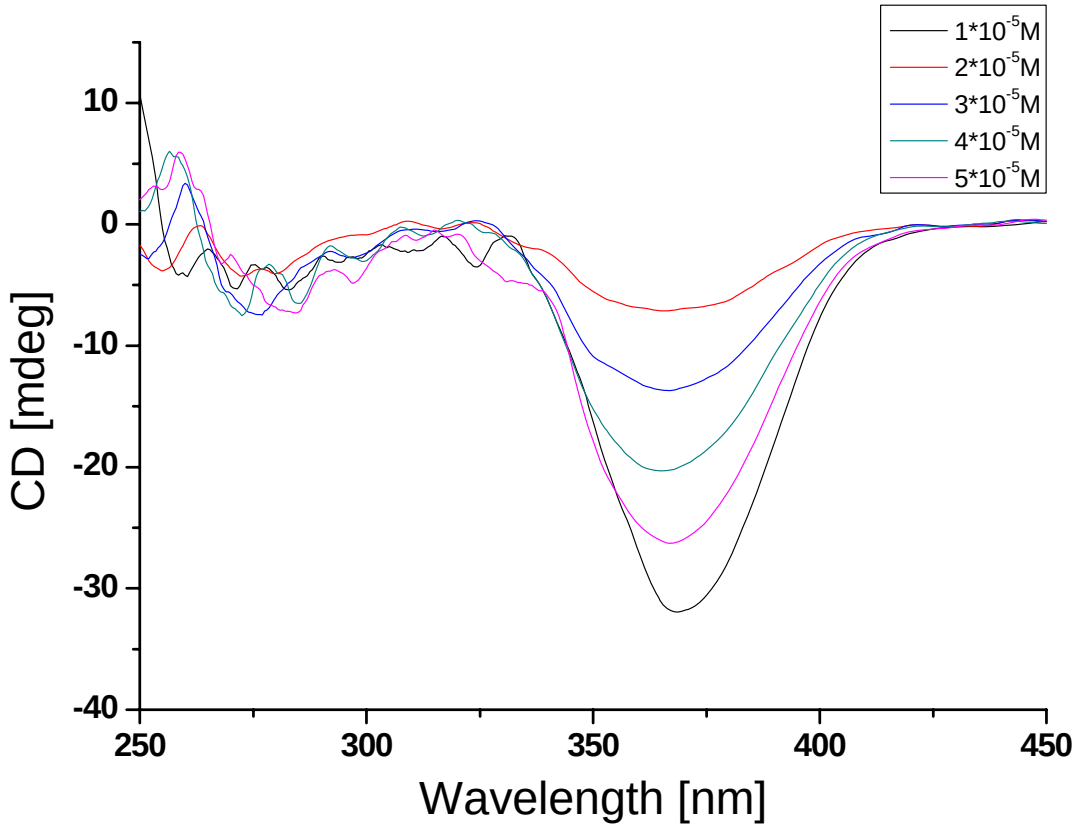


Figure S28. CD spectra of **4** in CH_2Cl_2 at various concentrations.

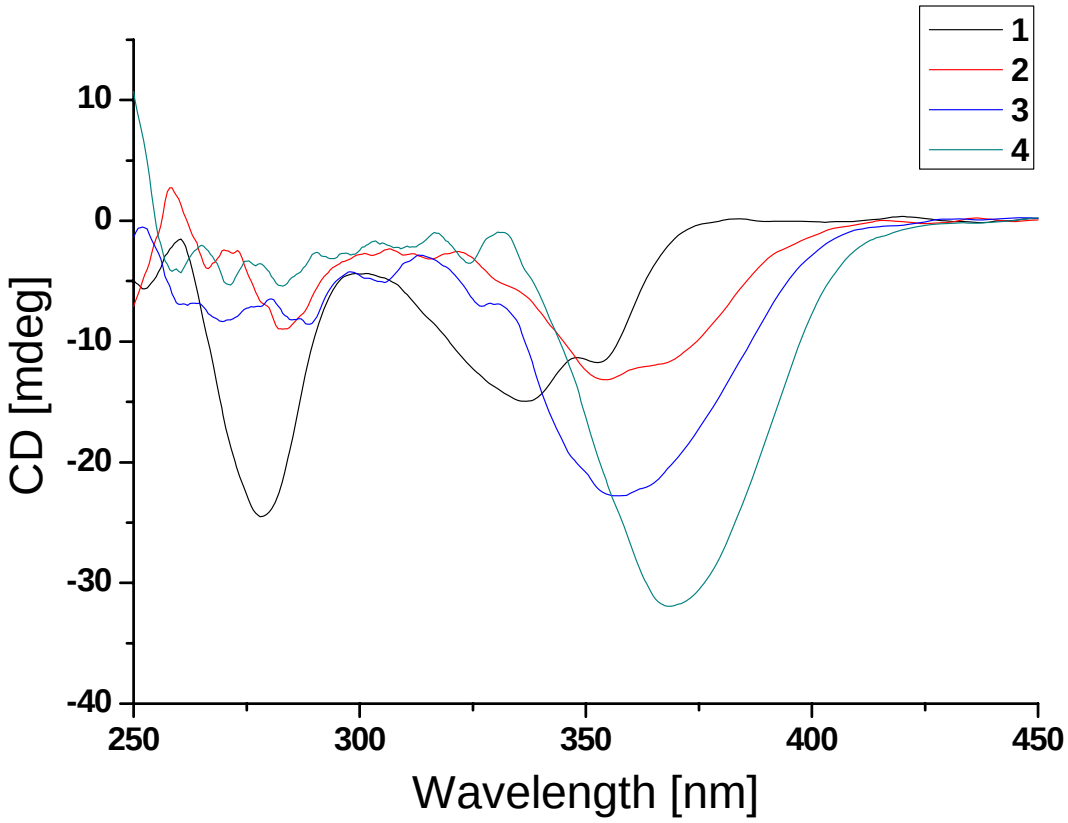


Figure S29. CD spectra of **1~4** (5 ×1 0^{-5} M) in CH_2Cl_2.

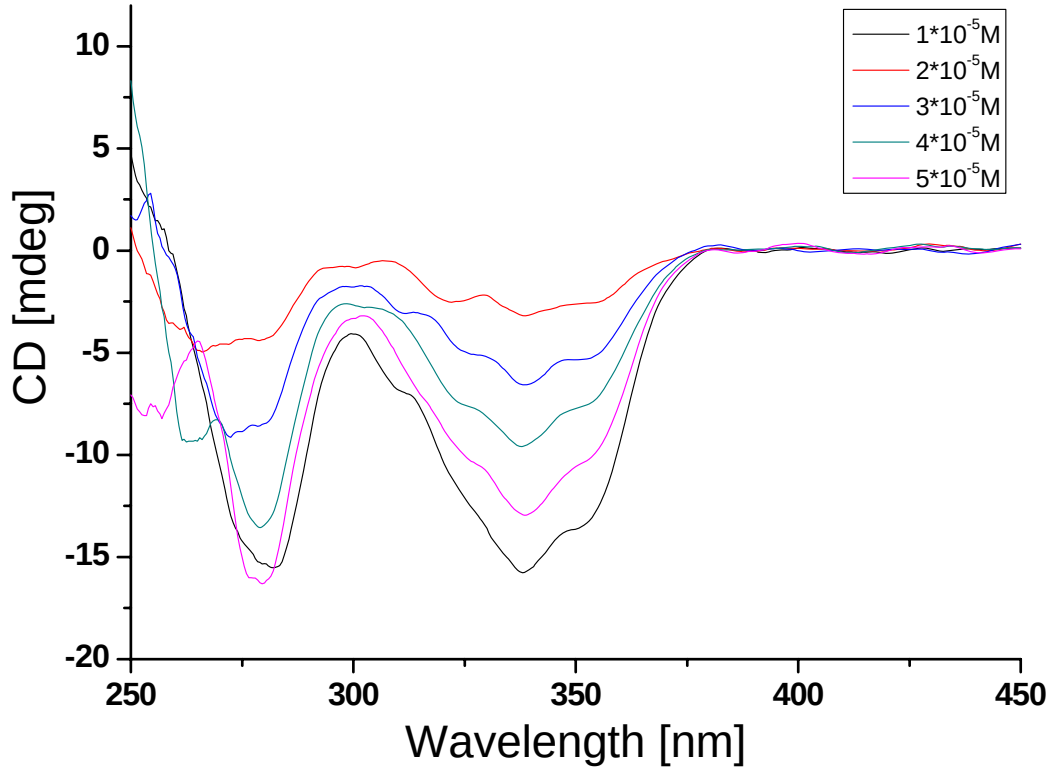


Figure S30. CD spectra of **1** in DMSO at various concentrations.

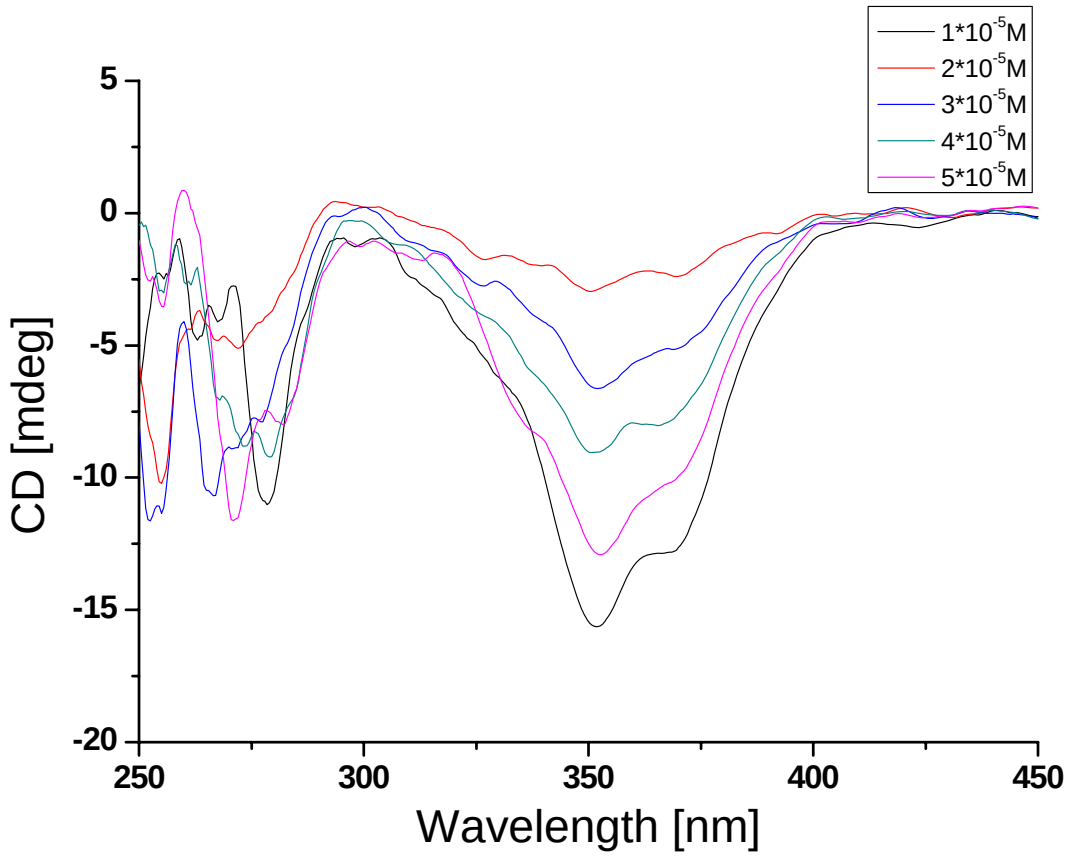


Figure S31. CD spectra of **2** in DMSO at various concentrations.

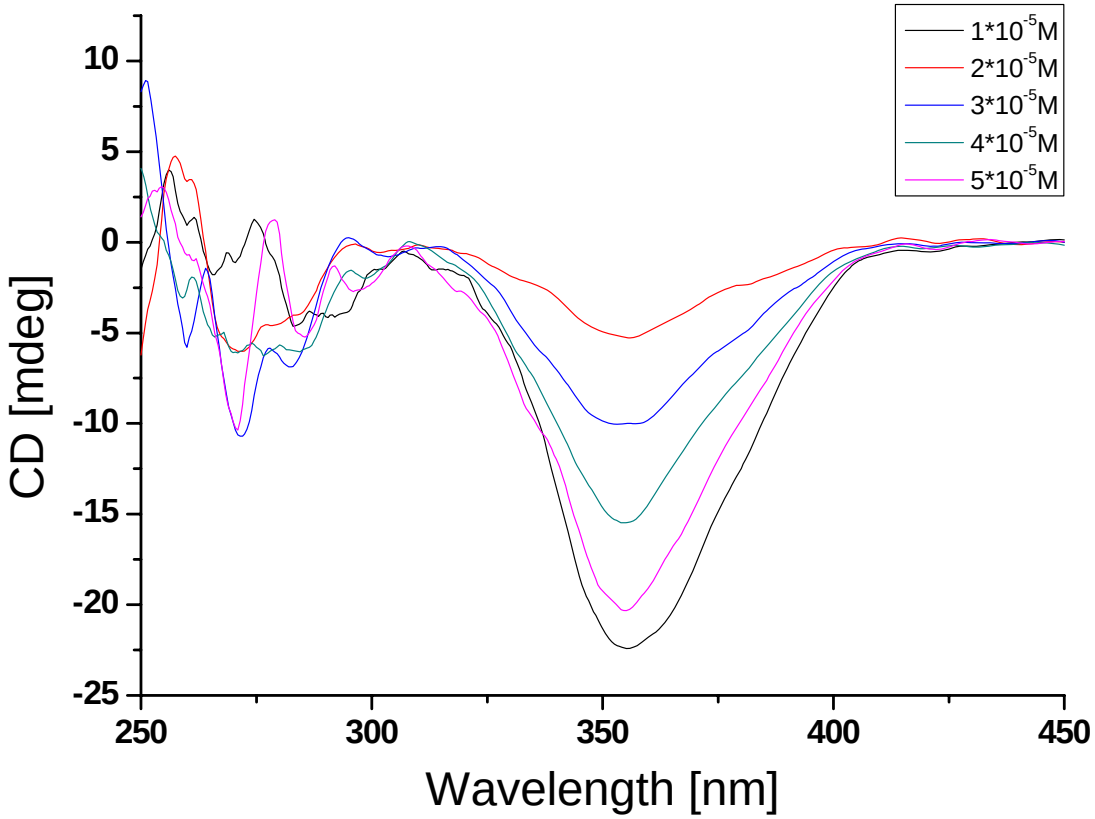


Figure S32. CD spectra of **3** in DMSO at various concentrations.

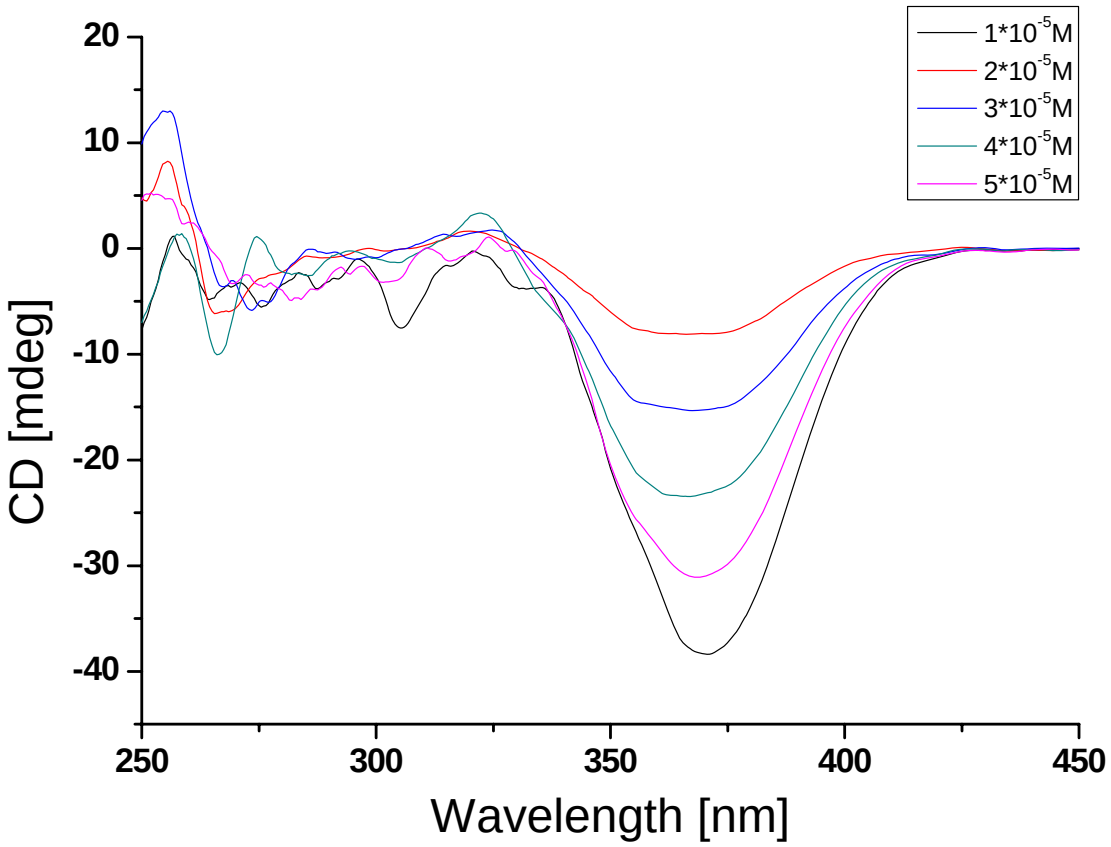


Figure S33. CD spectra of **4** in DMSO at various concentrations.

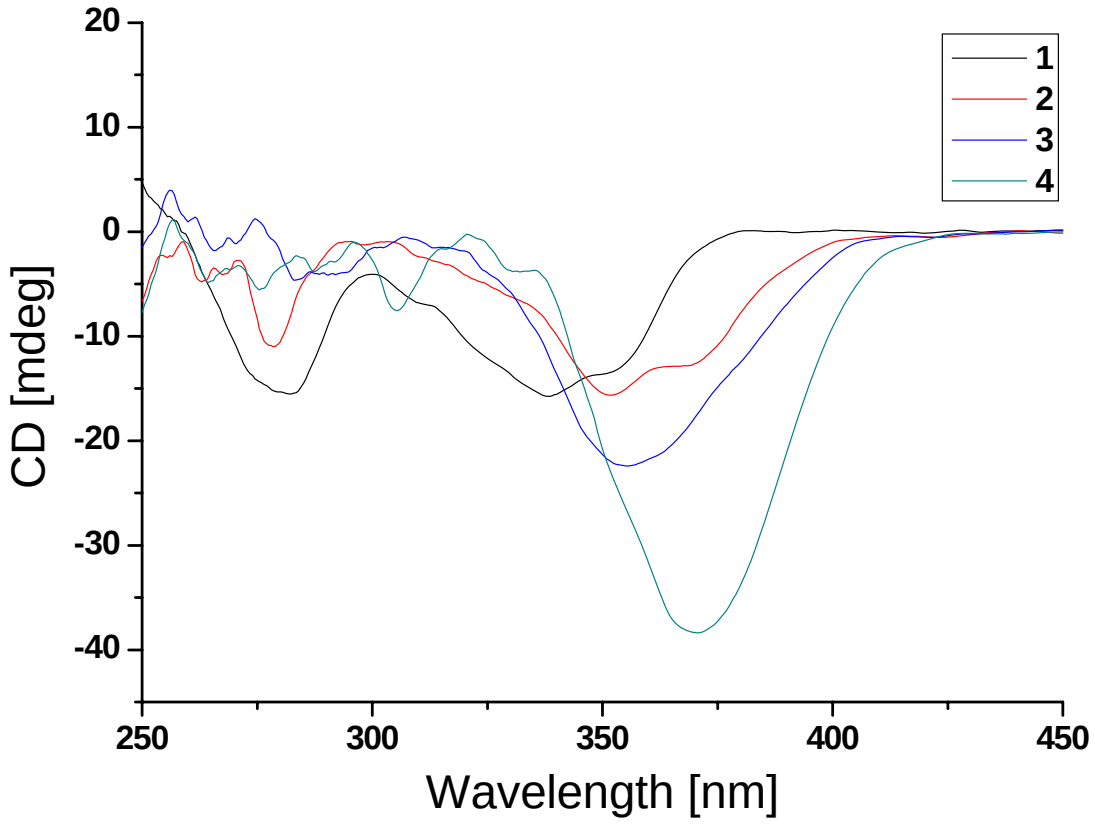


Figure S34. CD spectra of **1~4** (5 ×1 0^{-5} M) in DMSO.

6. CD and Absorption Spectra of Oligomers 1~4 at Various Temperatures

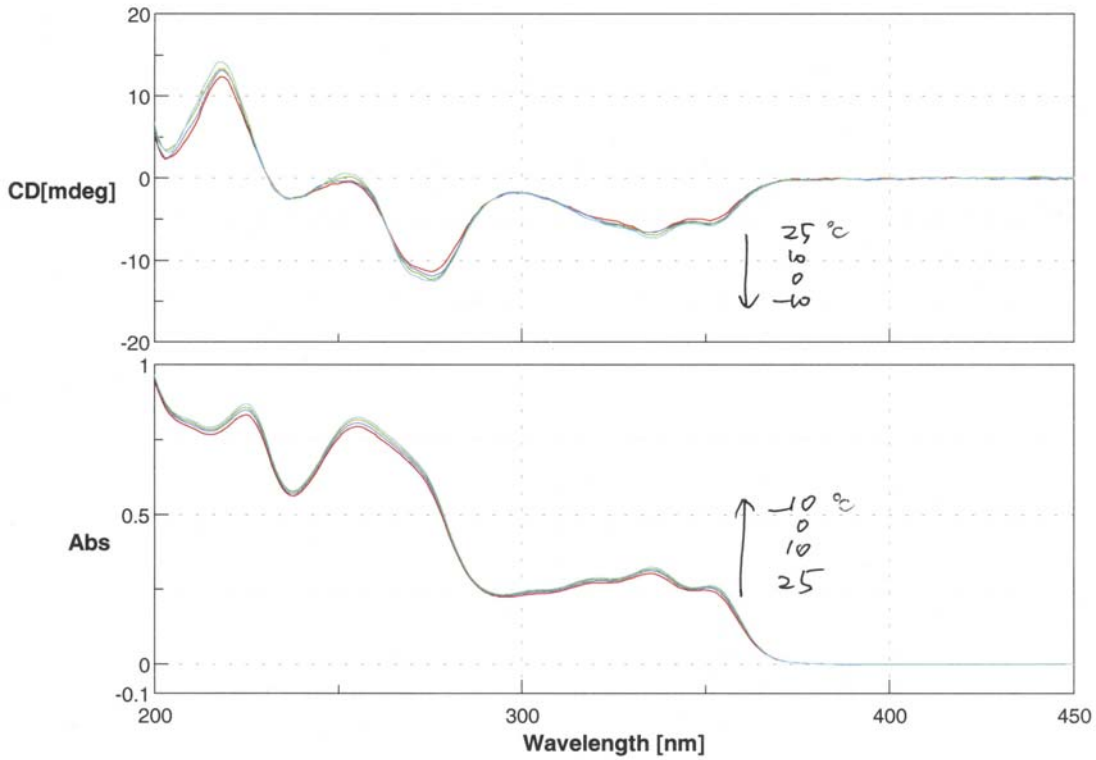


Figure S35. CD and absorption spectra (2.0×10^{-5}M) of oligomer **1** in acetonitrile at various temperatures.

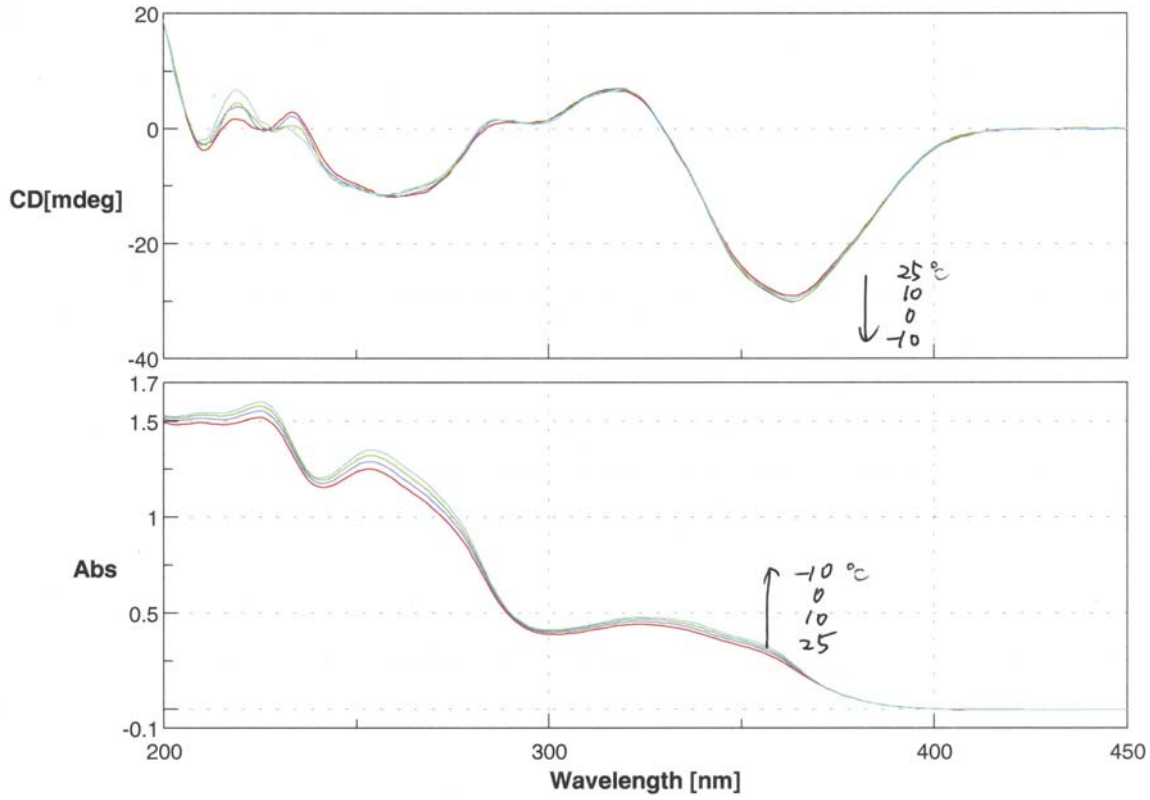


Figure S36. CD and absorption spectra (2.0×10^{-5} M) of oligomer **3** in acetonitrile at various temperatures.

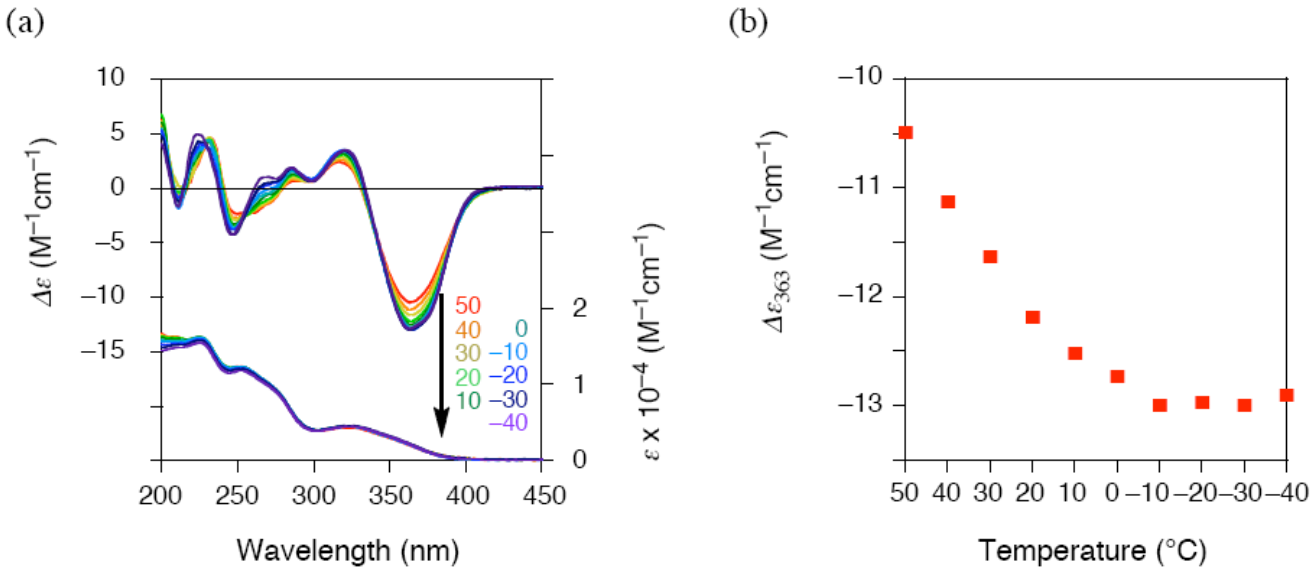


Figure S37. (a) CD and absorption spectra (2.0×10^{-5} M) of oligomer **4** in acetonitrile at various temperatures. (b) Plots of CD intensity at 363nm versus temperature.

In contrast, with lowering of the temperature, the molar CD values of oligomer **2** in methanol increased. Temperature-dependent CD measurements demonstrated that the helical conformation is stable for oligomer **2** in both of the acetonitrile and methanol solvents.

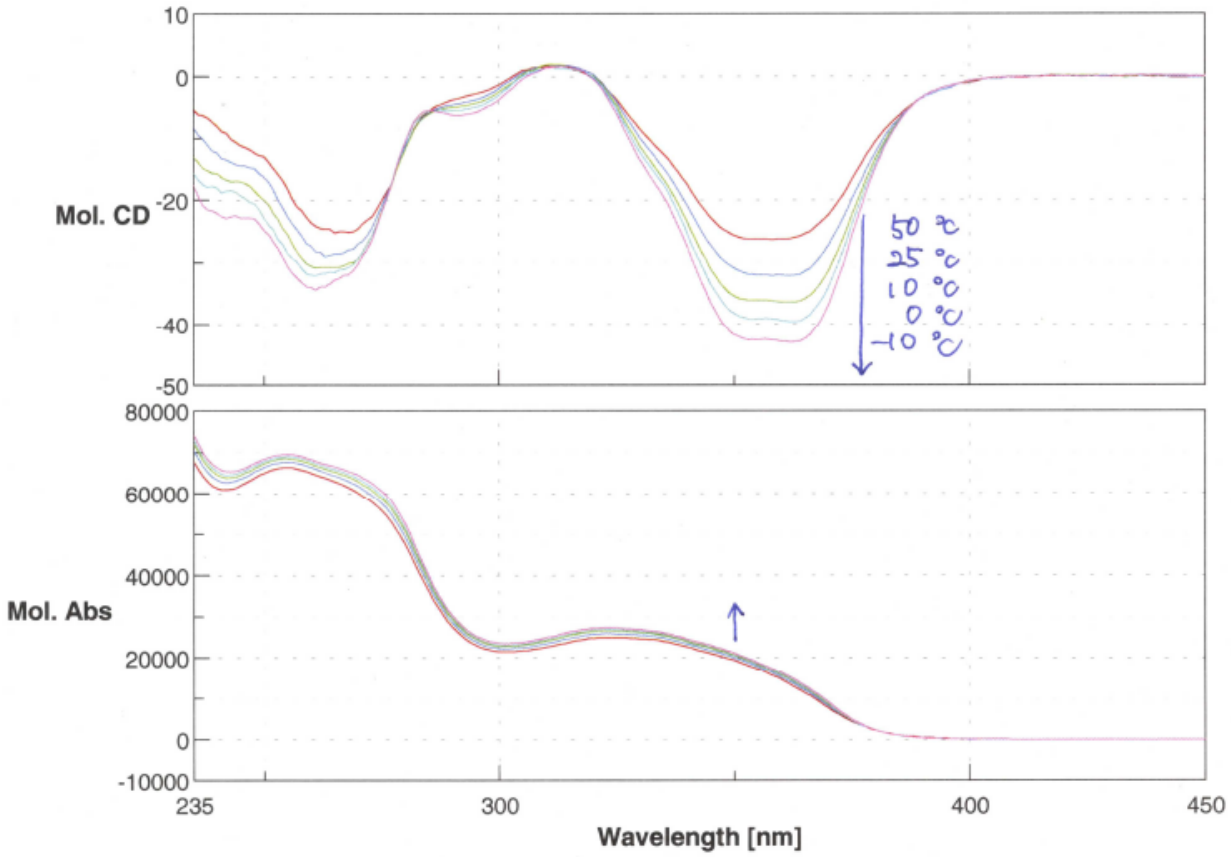


Figure S38. CD and absorption spectra (5.0×10^{-5} M) of oligomer **2** in methanol at various temperatures.

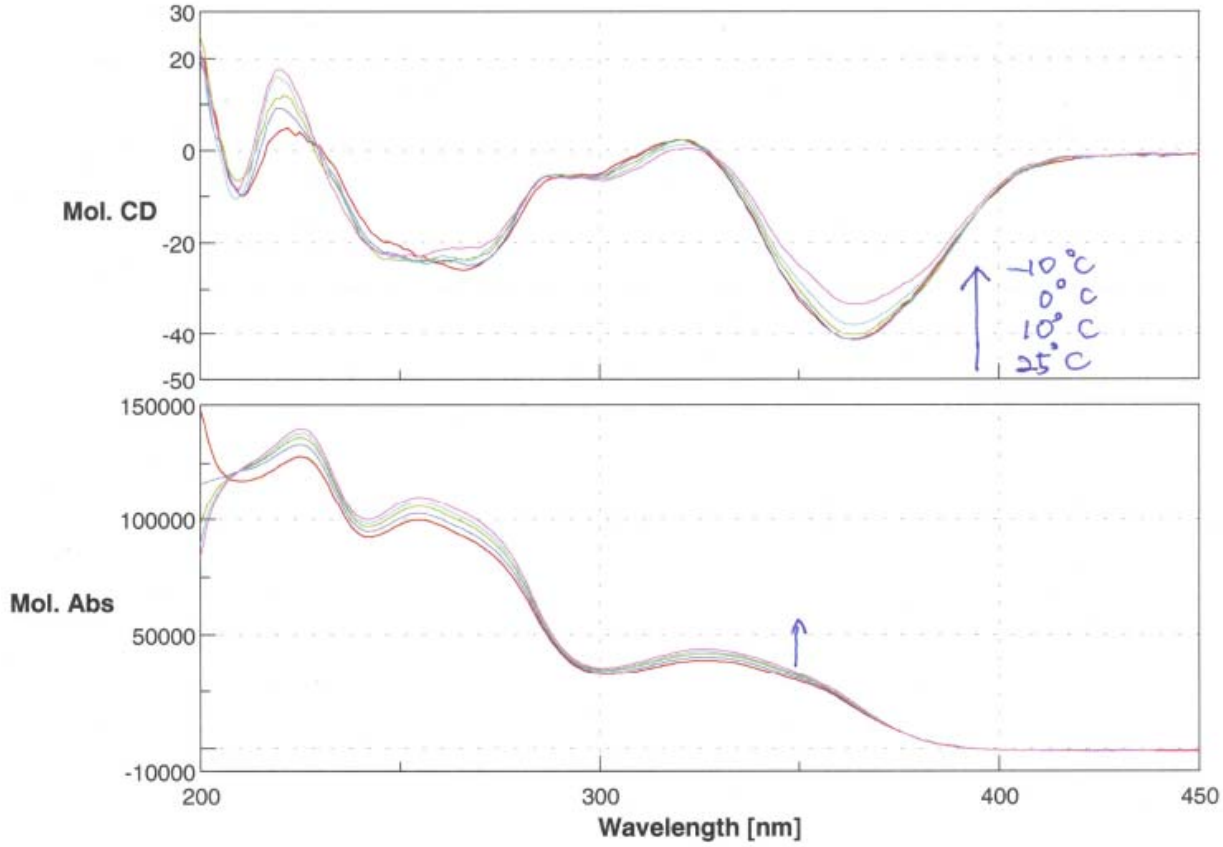


Figure S39. CD and absorption spectra (5.0×10^{-5} M) of oligomer **3** in methanol at various temperatures.

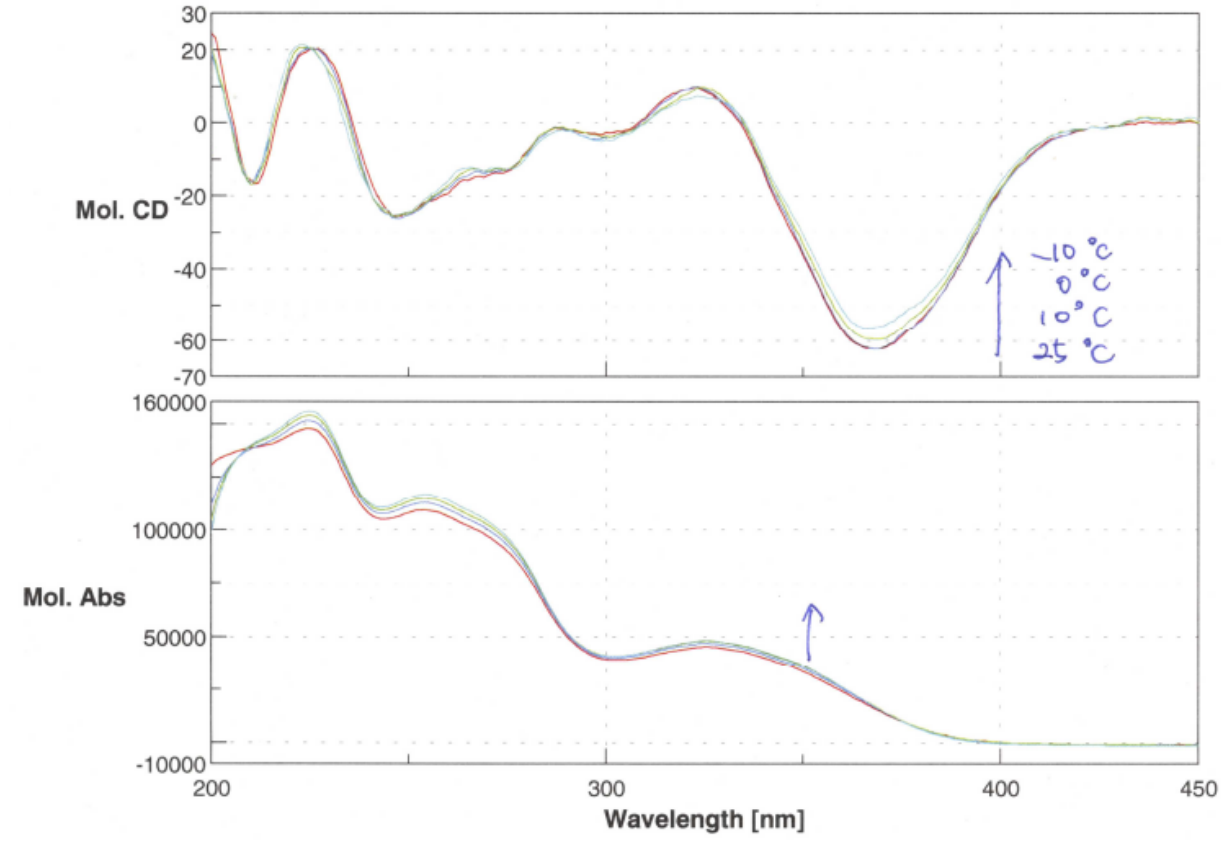


Figure S40. CD and absorption spectra (5.0×10^{-5} M) of oligomer **4** in methanol at various temperatures.