Supporting Information

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

Hai-Yu Hu, a,b Wei Xue, a,b Zhi-Qiang Hu, a Jun-Feng Xiang, a Chuan-Feng Chen, a,* and Sheng-Gui He a,*

a Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China. b Graduate School, Chinese Academy of Sciences, Beijing 100049, China.

E-mail: cchen@iccas.ac.cn

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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. \textsuperscript{1}H NMR and \textsuperscript{13}C NMR Spectra of New Compounds

![Figure S1. The \textsuperscript{1}H NMR spectrum of compound 5.](image)

![Figure S2. The \textsuperscript{13}C NMR spectrum of compound 5.](image)
Figure S3. The $^1$H NMR spectrum of compound 6.

Figure S4. The $^{13}$C NMR spectrum of compound 6.
Figure S5. The $^1$H NMR spectrum of compound 7.

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, CDCl₃) of compound 5.
Figure S8. The NOESY spectrum (600 MHz, CDCl₃) of compound 5.
Figure S9. The TOCSY spectrum (600 MHz, CDCl$_3$) of compound 6.
Figure S10. The NOESY spectrum (600 MHz, CDCl₃) of compound 6.
Figure S11. The TOCSY spectrum (600 MHz, CDCl₃) of compound 7.
**Figure S12.** The NOESY spectrum (600 MHz, CDCl₃) of compound 7.
4. Variable-Temperature $^1$H NMR Studies on Oligomers 1~4 and 1a~4a

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$_3$OH at various concentrations.

Figure S22. CD spectra of 2 in CH$_3$OH at various concentrations.
Figure S23. CD spectra of 3 in CH$_3$OH at various concentrations.

Figure S24. CD spectra of 4 in CH$_3$OH at various concentrations.
**Figure S25.** CD spectra of 1 in CH$_2$Cl$_2$ at various concentrations.

**Figure S26.** CD spectra of 2 in CH$_2$Cl$_2$ at various concentrations.
**Figure S27.** CD spectra of 3 in CH$_2$Cl$_2$ at various concentrations.

**Figure S28.** CD spectra of 4 in CH$_2$Cl$_2$ at various concentrations.
Figure S29. CD spectra of 1~4 (5 \times 10^{-5} M) in CH$_2$Cl$_2$.

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 × 10⁻⁵ 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 ($5.0 \times 10^{-5}$ M) of oligomer 3 in methanol at various temperatures.

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