

Supporting Information

An indolocarbazole dimer as a new stereodynamic probe for chiral 1,2-diamines

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General: Dichloromethane was purified by drying over CaH_2 , followed by distillation. NMR spectra were recorded on Bruker (Avance II) 400 MHz spectrometer. The chemical shifts of NMR spectra were reported using the solvent signal as an internal reference DMSO- d_6 (2.50 ppm for ^1H NMR, 39.5 ppm for ^{13}C NMR) and dichloromethane- d_2 (5.32 ppm for ^1H NMR). FT-IR spectrum was recorded on Bruker (Vertex70). MALDI-TOF mass spectrum was recorded on a Bruker (LRF20). Melting point was determined with a Barnsted Electrochemical (IA9100). Circular dichroism (CD) spectra were conducted on a JASCO (J-815). The elemental analysis data were obtained from *Center for research facilities* at Yonsei University

1. ^1H NMR spectra of cyclic diimines **3b-h**

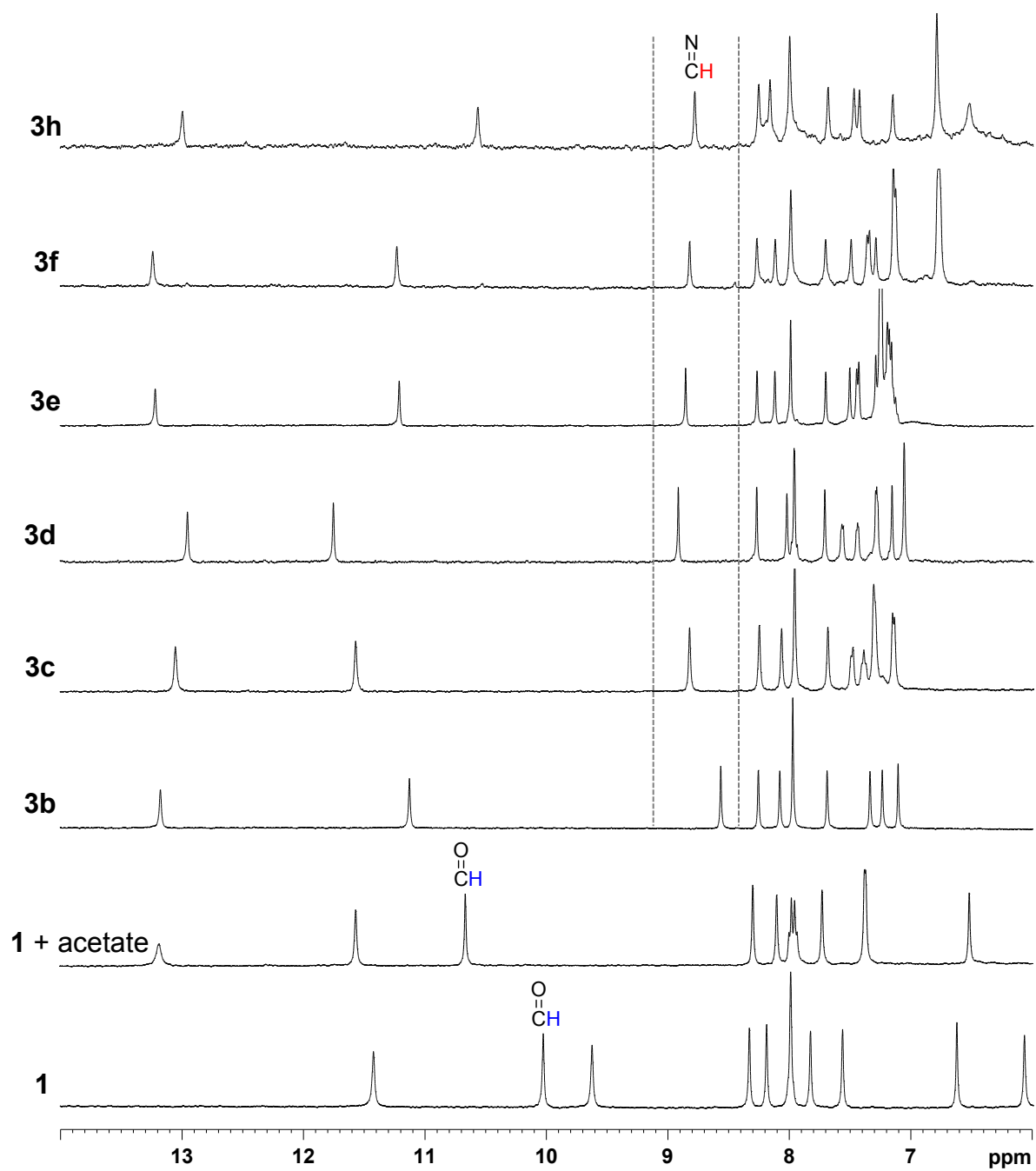


Fig. S1 Partial ^1H NMR (400 MHz, CD_2Cl_2 , r.t.) spectra of **1**, **1** with acetate, and cyclic diimines **3b-h**.

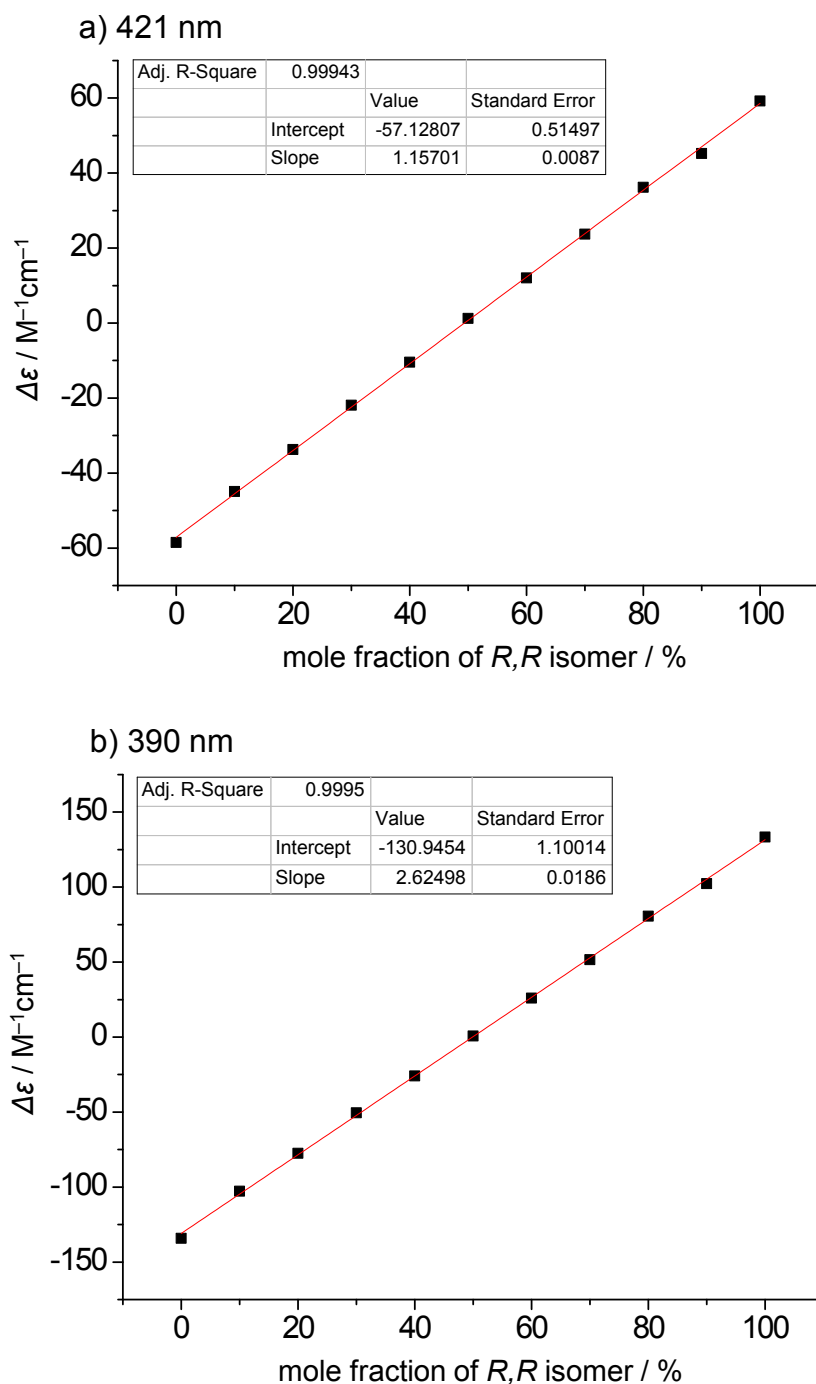
2. CD values of cyclic diimines **3b-h**

Table S1 CD values at first and second Cotton effects of cyclic didimines **3b-h**

Diamine	$\Delta\epsilon$ (421 nm) / $M^{-1}cm^{-1}$	$\Delta\epsilon$ (390 nm) / $M^{-1}cm^{-1}$
<i>(R,R)</i> - 3b	+61	+137
<i>(S,S)</i> - 3b	-60	-138
<i>(R,R)</i> - 3c	+45	+98
<i>(S,S)</i> - 3c	-46	-96
<i>(R,R)</i> - 3d	+55	+120
<i>(S,S)</i> - 3d	-54	-119
<i>(R,R)</i> - 3e	+51	+100
<i>(S,S)</i> - 3e	-50	-100
<i>(R,R)</i> - 3f	+51	+91
<i>(S,S)</i> - 3f	-50	-93
<i>(R,R)</i> - 3g	+29	+58
<i>(S,S)</i> - 3g	-31	-56
<i>(R,R)</i> - 3h	+44	+82
<i>(S,S)</i> - 3h	-44	-84

3. Calibration curves for the determination of enantiomeric excesses (ee's) (See Fig. 6)

CH_2Cl_2 solutions containing 10:0, 9:1, 8:2, 7:3, 6:4, 5:5, 4:6, 3:7, 2:8, 1:9 and 0:10 ratios of (*R,R*)- and (*S,S*)-**2b** were prepared and the concentrations of **2b** were 1 mM. The CD spectra were recorded and the CD intensities at four wavelengths (328 nm, 363 nm, 390 nm, and 421 nm) were plotted against the mole fraction of (*R,R*)-**2b**.



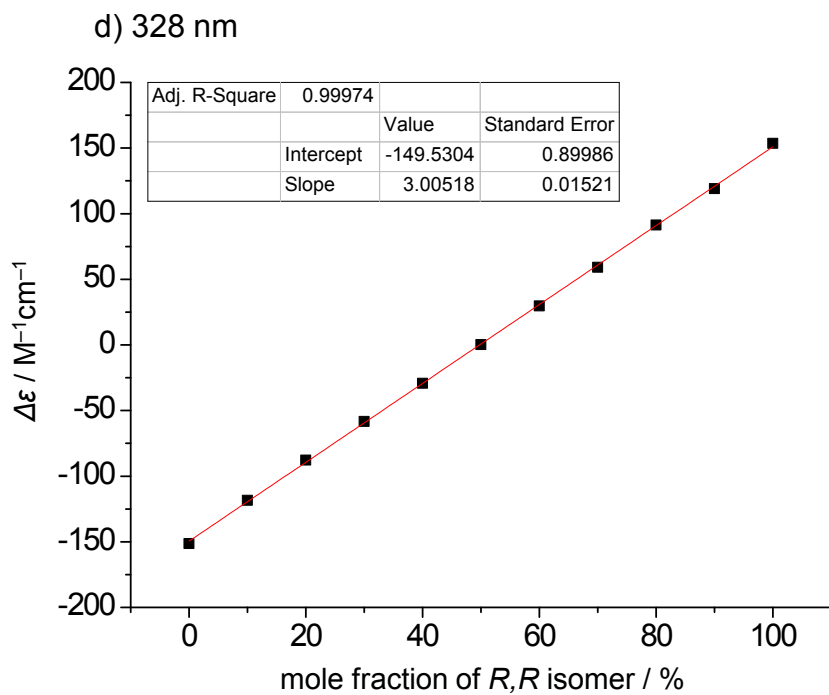
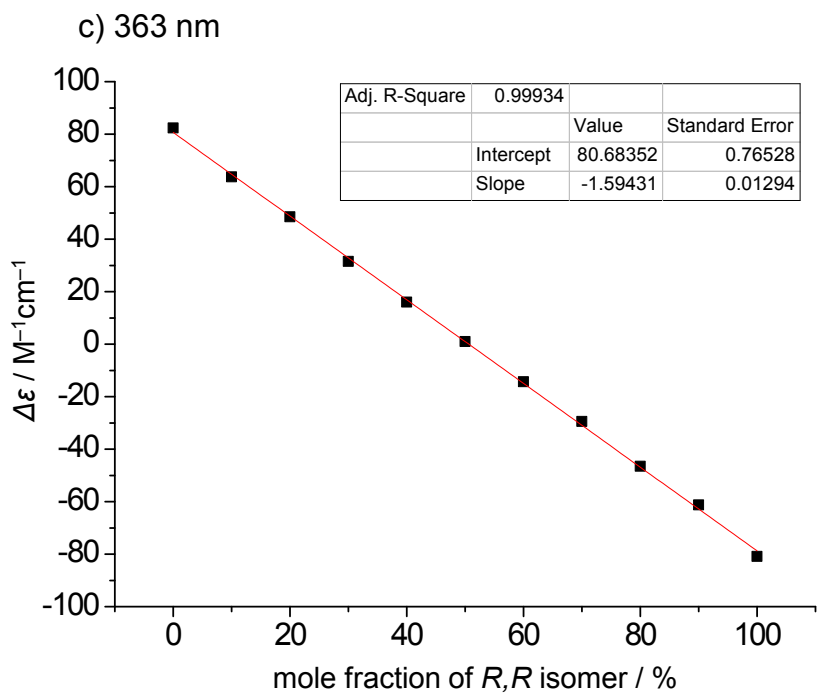


Fig. S2 Calibration curves of **3b** at four wavelengths (328 nm, 363 nm, 390 nm, 421 nm).

4. Computer modeling

Energy-minimized structures of diimine **3b** complexed with acetate anion were generated using MacroModeling 9.1^[1] program. The structures were found with OPLS2005 force field^[2] in the gas phase via 3000 separated search steps in Monte Carlo conformation search.^[3] The generated structure is very similar to the crystal structure.

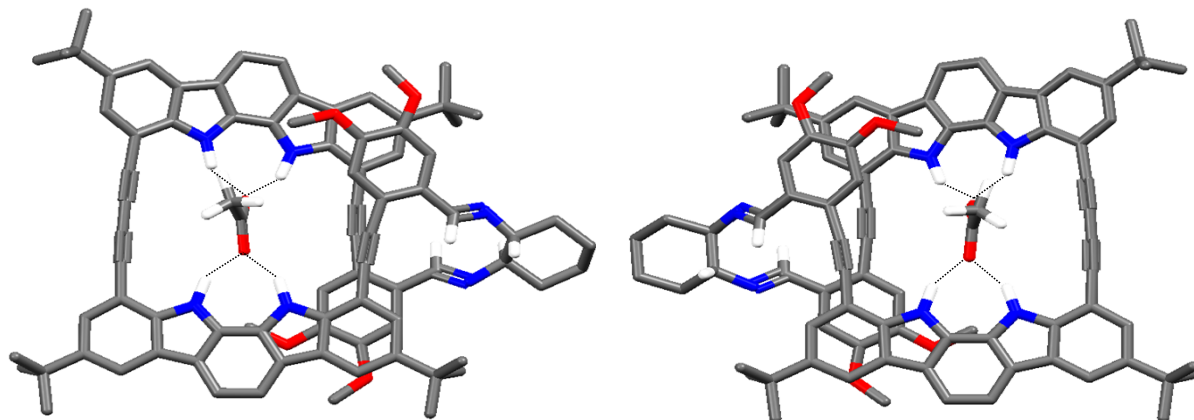


Fig. S3 Energy minimized structure of (*R,R*)-**3b** complexed with anionic acetate. *P*-helix (energy = 147.5 kJ/mol, left) and *M*-helix (energy = 188.6 kJ/mol, right).

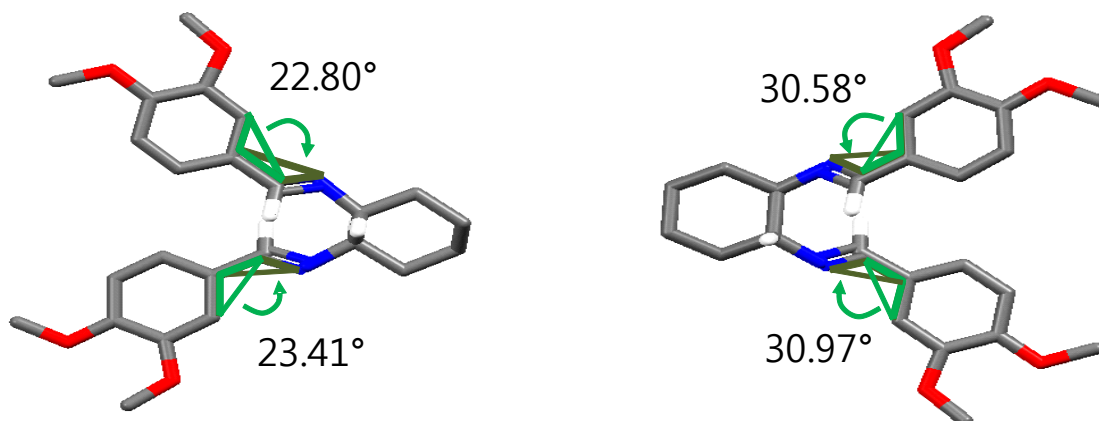


Fig. S4 Terminal aryls and diimine bridge structures of *P*-helix (left) and *M*-helix (right) of (*R,R*)-**3b**. *M*-helix has more distorted dihedral angles than *P*-helix.

^[1] F. Mohamedi, N. G. T. Richards, W. C. H. Liskamp, M. Lipton, C. Caufield, G. Chang, T. Hendrickson and W. C. Still, *J. Comp. Chem.* **1990**, *11*, 440-467.

^[2] G. A. Kaminski, R. A. Friesner, J. Tirado-Rives and W. J. Jorgensen, *J. Phys. Chem. B* **2001**, *105*, 6474-6487.

^[3] M. Saunders, K. N. Houk, Y. D. Wu, W. C. Still, M. Lipton, G. Chang and W. C. Guida, *J. Am. Chem. Soc.* **1990**, *112*, 1419-1427.