Electronic Supplementary Information

Bio-based chiral dopants having an isohexide skeleton for cholesteric liquid crystal materials

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1. Analysis data of isohexide-based chiral dopants

Chemical structures of synthetic isohexide-based chiral dopants (IH-*n*, n= 1-4) were identified by NMR and mass spectrometers. The ¹H-NMR and ¹³C-NMR spectra were measured using Bruker-600 (MHz) spectrometer with trimethylsilane (TMS) peak as reference. Mass spectra were recorded by using JEOL, JMS-600W spectrometer.

1) 1,4:3,6-Dianhydro-d-sorbitol-2,5-bis(4-acetoxybenzoate) (IH-1)



¹H-NMR (600 MHz, CDCl₃): δ = 8.12 (d, *J* = 8.6 Hz, 2H), 8.06 (d, *J* = 8.6 Hz, 2H), 7.19 (dd, *J_I* = 11.8 Hz, *J₂* = 8.6 Hz, 4H), 5.49 (s, 1H), 5.43 (q, *J* = 5.3 Hz, 1H), 5.06 (t, *J* = 5.0 Hz, 1H), 4.67 (d, *J* = 4.7 Hz, 1H), 4.10-4.03 (m, 4H), 2.33 (d, *J* = 16.6 Hz, 6H) ppm; ¹³C-NMR (150 MHz, CDCl₃): a calculated mass for C₂₄H₂₂O₁₀: 470.1, found: ESI-MS, m/z, positive [M+H]⁺: 471.1294

¹N-NMR



¹³C-NMR

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2) 1,4:3,6-Dianhydro-d-mannitol-2,5-bis(4-acetoxybenzoate) (IH-2)



¹H-NMR (600 MHz, CDCl₃): δ = 8.14 (d, *J* = 8.6 Hz, 4H), 7.20 (d, *J* = 8.6 Hz, 4H), 5.34 (d, *J* = 5.8 Hz, 2H), 4.89 (d, *J* = 7.7 Hz, 2H), 4.14 (dd, *J*₁ = 9.4 Hz, *J*₂ = 6.3 Hz, 2H), 4.00 (dd, *J*₁ = 9.4 Hz, *J*₂ = 6.7 Hz, 2H), 2.33 (s, 6H) ppm; ¹³C-NMR (150 MHz, CDCl₃): δ = 168.7, 165.3, 154.5, 131.1, 126.9, 121.5, 80.6, 73.9, 70.6, 21.0 ppm; a calculated mass for C₂₄H₂₂O₁₀: 470.1, found: ESI-MS, m/z, positive [M+H]⁺: 471.1288.

¹N-NMR







3) 1,4:3,6-Dianhydro-d-sorbitol-2,5-bis(4-hexyloxybenzoate) (IH-3)



¹H-NMR (600 MHz, CDCl₃): δ = 8.03 (d, *J* = 8.8 Hz, 2H), 7.96 (d, *J* = 8.8 Hz, 2H), 6.91 (dd, *J*₁ = 13.4 Hz, *J*₂ = 8.8 Hz, 4H), 5.46 (d, *J* = 3.0 Hz, 1H), 5.40 (q, *J* = 5.3 Hz, 1H), 5.04 (t, *J* = 5.0 Hz, 1H), 4.68 (d, *J* = 4.6 Hz, 1H), 4.14-4.07 (m, 3H), 4.03-4.00 (m, 5H), 1.83-1.78 (m, 4H), 1.47-1.46 (m, 4H), 1.36-1.35 (m, 8H), 0.93-0.91 (m, 6H) ppm; ¹³C-NMR (150 MHz, CDCl₃): δ = 165.8, 165.4, 163.3, 131.8, 121.6, 114.1, 86.2, 81.2, 78.2, 74.2, 73.6, 70.7, 68.2, 31.5, 29.0, 25.7, 22.6, 14.0 ppm; a calculated mass for C₃₂H₄₂O₈: 554.3, found: ESI-MS, m/z, positive [M+H]⁺: 555.2953.

¹H-NMR



¹³C-NMR



4) 1,4:3,6-Dianhydro-d-mannitol-2,5-bis(4-hexyloxybenzoate) (IH-4)



¹H-NMR (600 MHz, CDCl₃): δ = 8.04 (d, *J* = 8.8 Hz, 4H), 6.92 (d, *J* = 8.8 Hz, 4H), 5.34 (q, *J* = 5.1 Hz, 2H), 4.87 (d, *J* = 4.3 Hz, 2H), 4.16-4.13 (m, 3H), 4.03-3.99 (m, 5H), 1.83-1.79 (m, 4H), 1.50-1.45 (m, 4H), 1.36-1.35 (m, 8H), 0.93-0.91 (m, 6H) ppm; ¹³C-NMR (150 MHz, CDCl₃): 165.8, 163.3, 131.9, 121.6, 114.1, 80.8, 74.0, 70.8, 68.3, 31.5, 29.1, 25.7, 22.6, 14.0 ppm; a calculated mass for C₃₂H₄₂O₈: 554.3, found: ESI-MS, m/z, positive [M+H]⁺: 555.2962.

¹H-NMR





2. DSC thermogram of IH-2 with super slow cooling rate



Fig. S9 DSC first cooling and second heating scans of IH-2; cooling rate was 0.1 K min⁻¹ and heating rate was 5.0 K min⁻¹.



3. DSC thermograms of IH-4 and IH-3 with different cooling rates

Fig. S10 DSC first cooling and second heating scans of IH-4 with different first cooling rates $(2.5, 5.0, 10.0 \text{ K min}^{-1})$ and second heating rate was fixed at 5 K min⁻¹.



Fig. S11 DSC first cooling and second heating scans of IH-3 with different first cooling rates $(2.5, 5.0, 10.0 \text{ K min}^{-1})$ and second heating rate was fixed at 5 K min⁻¹.

4. POM microphotographs of IH-*n* (*n*= 1-4)

Optical textures of chiral dopants were studied with a Nikon 100POL polarized optical microscope (POM) equipped with a Mettler Toledo FP-82 hot stage. Small amount of chiral dopants were placed between cover slips. They were heated to isotropic phase with heating rate of 6 K min⁻¹ and slowly cooled. Textures formed during cooling from isotropic state were taken in this study (IH-3 and IH-4). However IH-1 and IH-2 didn't show crystal texture so their textures obtained during heating process were displayed instead.





Fig. S12 POM microphotographs of (a) IH-1 taken at 65 °C in the heating process, (b) IH-2 taken at 30 °C in the heating process, (c) IH-3 taken at 70 °C in the cooling process, (d) IH-4 taken at 36.5 °C in the cooling process. Magnification of all microphotographs is x100.

5. 1D WXRD patterns of IH-3 and IH-4

For the one-dimensional (1D) wide angle X-ray diffraction (WXRD) measurement, chiral dopant samples were mounted in glass capillary tubes. Prior to measurements, samples were heated to isotropic temperature and cooled down to room temperature. Chiral dopant was transferred to the chamber maintained at desired temperature and exposed for 300 s to obtain a XRD spectrum.



Fig. S13 1D WXRD spectra of (a) IH-3 and (b) IH-4 as a function of temperature.

6. UV-Vis spectra of CLC films prepared with IH-1



Fig. S14 UV-Vis spectra and polarized optical microscopy images of cholesteric films prepared with different amount of IH-1; (a) 10.0 mol%, (b) 9.0 mol%, (c) 8.0 mol%.