

## RESEARCH ARTICLE

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2025, 9, 2900Temperature-induced helix inversion in  
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Achieving precise control over macroscopic chirality in self-organized systems is a key challenge in the development of advanced supramolecular functional materials. Here, we report a novel class of liquid crystalline compounds bearing a single chiral center, which exhibit reversible, thermally-induced helix inversion in the cholesteric phase. The (S)-naphthyl-3-hydroxypropanoic moiety is identified as the critical structural fragment responsible for this rare behavior. Remarkably, the helix inversion can be transferred from the pure chiral compound to an achiral nematic host, at guest concentrations as low as 6%, preserving the characteristic transition from a high-temperature left-handed helix to a low-temperature right-handed one. This also enables precise tuning of the helix inversion temperature across an exceptionally broad range – from below room temperature up to 114 °C. Importantly, structural modifications to the alkyl ester moiety do not suppress helix inversion, allowing for targeted tuning of inversion temperature, host compatibility, and potential incorporation of additional stimuli-responsive functions. The combination of thermally-induced helix inversion, the ability to transfer this unique feature to an achiral host, and the wide temperature range over which this inversion can be adjusted makes these new chiral mesogens a versatile molecular platform for designing thermoresponsive chiral materials.

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## Introduction

The hierarchical nanostructures found in nature have inspired the development of numerous supramolecular chiral materials in recent years, enabling applications in fields ranging from asymmetric synthesis<sup>1</sup> and chiral separation<sup>2</sup> to optics<sup>3</sup> and electronics.<sup>4</sup> However, achieving precise control over chirality in self-organized superstructures with tailored properties remains a major challenge in designing and developing advanced functional materials.

Cholesteric liquid crystals (CLCs), also known as chiral nematic liquid crystals, exhibit helical structures characterized by periodicity (pitch, P) and handedness.<sup>5</sup> This unique organization gives rise to the selective reflection of circularly polarized light with wavelengths comparable to the helical pitch. The helical structure is highly sensitive to external stimuli such as heat, electric fields, and light,<sup>6,7</sup> making CLCs promising

materials for a wide range of applications, including advanced reflective displays,<sup>8</sup> reflectors,<sup>9</sup> diffraction gratings,<sup>10</sup> anti-counterfeiting,<sup>11,12</sup> and smart windows.<sup>13</sup>

An intriguing feature observed in certain CLCs is helix inversion. This phenomenon, triggered by external stimuli, occurs through helix unwinding and subsequent rewinding with opposite handedness, driven by shifts in the balance of various competing interactions.<sup>14</sup> Over the past decade, significant progress has been made in developing photoisomerizable chiral dopants,<sup>8,15–21</sup> which enable helix inversion upon irradiation with light of an appropriate wavelength. In contrast, temperature-induced helix inversion remains relatively rare and less explored.

To date, thermally-induced helix inversion in CLCs has been achieved through several distinct strategies. In the early '90s, Goodby *et al.* reported thermally-induced inversion in pure CLCs containing a single chiral center in the terminal chain.<sup>22,23</sup> Helix inversion was attributed to the competition between populations of conformers with opposite twist senses, which can interconvert due to a low energy barrier. Another approach involves temperature-dependent chiral conflicts between multiple chiral centers—either intramolecular within a single-component CLC,<sup>24–26</sup> or intermolecular in a mixture of two CLCs with opposite helical senses.<sup>27</sup> A third method

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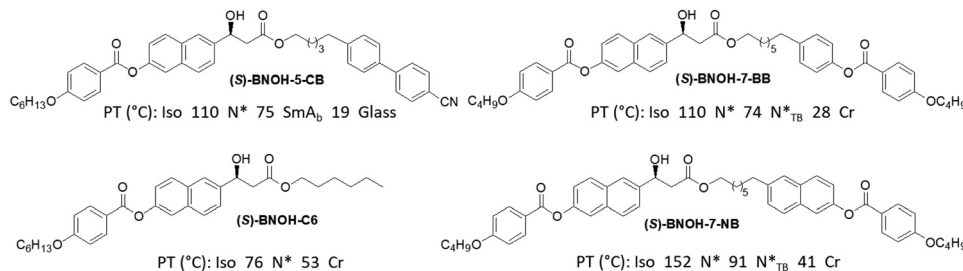


Fig. 1 Chemical structures and phase transition temperatures obtained on cooling of the studied chiral materials.

involves transfer of invertible chirality to the LC phase, as seen with (*S*)-1,2-propanediol esters, which induce temperature-dependent inversion in the CLC phase when mixed with a nematic host.<sup>28,29</sup> These mixtures can be used to design materials that surpass the typical 50% reflectance limit observed in CLCs.<sup>9,30</sup>

Recently, while studying bent-shaped dimers with a single chiral center positioned in the spacer, we discovered that those containing the (*S*)-naphthyl-3-hydroxypropanoic moiety undergo thermally-induced helix inversion in the cholesteric phase (Fig. 1, (*S*)-BNOH-7-BB and (*S*)-BNOH-7-NB).<sup>31</sup> This finding prompted us to further investigate the influence of molecular structure on helix inversion. We examined structurally related compounds that differ in their alkyl ester moieties and overall molecular shapes: chiral (*S*)-naphthyl-3-hydroxypropanoic dimer ((*S*)-BNOH-5-CB) and corresponding monomer ((*S*)-BNOH-C6) (Fig. 1). Our objectives were to identify the structural factors responsible for this intriguing phenomenon, explore the possibility of tuning the temperature at which helix inversion occurs, and assess the ability of these chiral compounds to impart this unique property to an achiral nematic host.

## Results and discussion

The synthesis and characterization of (*S*)-BNOH-7-BB and (*S*)-BNOH-7-NB have been previously reported.<sup>31</sup> The chiral materials (*S*)-BNOH-5-CB and (*S*)-BNOH-C6 have been prepared following the analogous synthetic route reported for (*S*)-BNOH-7-BB. Complete chemical characterization and phase transition properties are provided in the SI.

Both new compounds, (*S*)-BNOH-C6 and (*S*)-BNOH-5-CB, exhibit an enantiotropic cholesteric phase (N\*) characterized by fan-like (Fig. S1a) and oily streak textures (Fig. S1b). Additionally, (*S*)-BNOH-5-CB undergoes a transition from the cholesteric phase to the smectic phase, displaying a typical fan-shaped texture (Fig. S1c). Using X-ray scattering (see SI, Fig. S2), the smectic phase was identified as an intercalated smectic A<sub>b</sub> phase (SmA<sub>b</sub>), which is consistent with the behavior of both symmetric and non-symmetric bent-shaped dimers.<sup>32,33</sup> A careful examination of the optical textures of the CLC phase of (*S*)-BNOH-C6 and (*S*)-BNOH-5-CB upon cooling revealed significant changes with temperature. The textures transformed from the fan-like and fingerprint textures (Fig. S3a), which are characteristic of the CLC phase, to a schlieren-like texture

typical of the racemic nematic phase (Fig. S3b). Further cooling led to the oily-streak texture (Fig. S3c). This observed change in the texture indicates helix inversion, which was previously noted for (*S*)-BNOH-7-BB and (*S*)-BNOH-7-NB.<sup>31</sup>

To confirm the occurrence of helix inversion definitively, the contact preparation of (*S*)-BNOH-5-CB and (*S*)-BNOH-7-NB, which has only a right-handed helix,<sup>31</sup> was performed. Upon cooling to 107 °C, two distinct regions with opposite helical senses appeared. These regions had a sharp boundary where the pitch became infinite (P<sub>∞</sub>) due to the formation of a mixture of left- and right-handed helices (Fig. 2a). As the temperature decreased, this boundary disappeared, resulting in a uniform texture, and confirming that the helices in the CLC phases of both compounds have the same twist sense (Fig. 2b). Thus, upon cooling, the handedness of the helix of the CLC phase of (*S*)-BNOH-5-CB changes from left-handed to

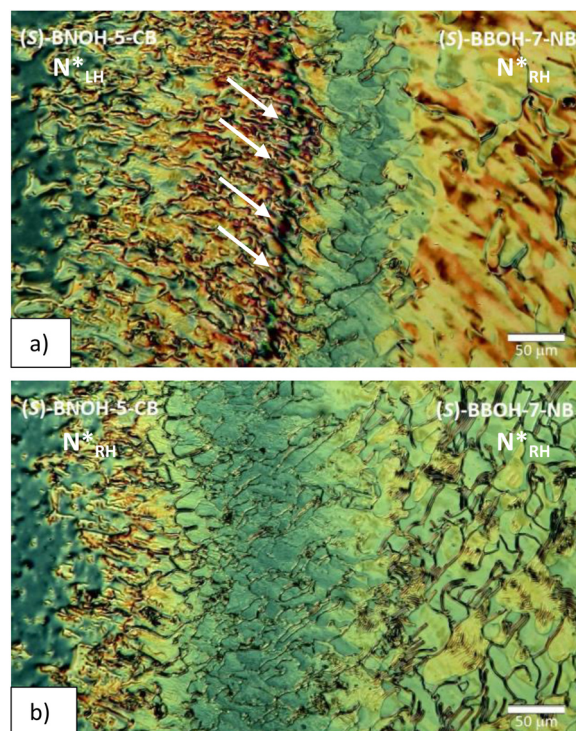


Fig. 2 Contact preparation of compounds (*S*)-BNOH-5-CB and (*S*)-BNOH-7-NB in the CLC phase with (a) opposite helical senses at 107 °C, the arrows point at the boundary between N\*<sub>LH</sub> and N\*<sub>RH</sub> (b) the same helical sense at 103 °C.



right-handed. This helix inversion from left-handed at high-temperature to right-handed at low-temperature was also confirmed for the monomer (*S*)-BNOH-C6 (Fig. S4). The change in the helical sense is thermally reversible, as previously observed for (*S*)-BNOH-7-BB and (*S*)-BNOH-7-NB.<sup>31</sup>

The process of helical twist inversion is further illustrated by the observation of tiny droplets deposited on untreated glass slides (Fig. 3 and Video S1). In the chiral form, the droplets appear blurred and bluish. Upon cooling, a schlieren-like texture develops, with four brushes distorted in a spiral-like pattern due to the chirality of the phase. As the temperature approaches the point of helix inversion, the four brushes start rotating, which reveals a rotation of the molecular director because of the chirality variation. At the temperature of left-to-right-handed inversion, the spiral of the brushes strikingly changes its sign, revealing chirality inversion.

The temperature-dependent pitch behavior of (*S*)-BNOH-5-CB was investigated more quantitatively using the Cano-wedge method<sup>34</sup> upon cooling from the isotropic melt (Fig. 4). The pitch of the  $N_L^*$  phase was measured just below the Iso- $N^*$  phase transition at 109 °C, but, as the helix inversion temperature was approached, the distance between the lines became too large to allow for accurate measurements.

Nevertheless, the pitch measurements revealed that the helix inversion occurs at around 103–104 °C. Upon further cooling from 101 °C to 80 °C, the pitch changed significantly, decreasing from 2.9 μm to 0.7 μm. Below 80 °C, the stripe and grid-like textures, which spontaneously form in bent-shaped LC dimers due to their low bend elastic constant,<sup>35</sup> appeared, preventing further measurements. These temperature-dependent pitch measurements confirm that the cholesteric pitch of (*S*)-BNOH-5-CB varies strongly with temperature. Similar temperature-dependent pitch behavior was observed for (*S*)-BNOH-7-NB (Fig. S5) and (*S*)-BNOH-7-BB (Fig. S6a), in good agreement with the previously reported behavior of other CLCs that exhibit helix inversion.<sup>25,27,28</sup> The monomer (*S*)-BNOH-C6 also showed helix inversion upon supercooling at 58–59 °C, just a few degrees above crystallization, which hindered the pitch measurements as a function of temperature.

The helix inversion temperatures observed in the CLC phase of the chiral compounds presented in Fig. 1 are summarized in Table 1. These results show that helix inversion is not related to the dimeric structure or bent shape of the molecule.

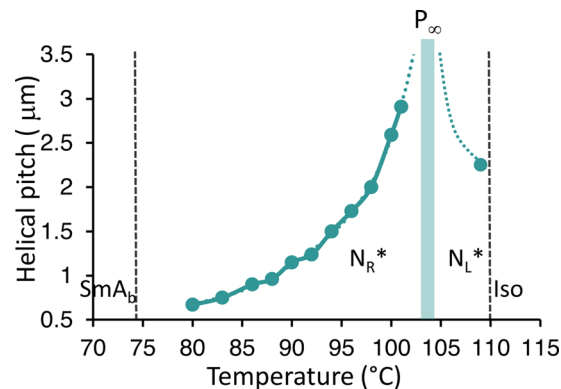


Fig. 4 Temperature dependence of the helical pitch of the CLC phase of (*S*)-BNOH-5-CB. The solid dots represent the measured pitch values. The dotted line depicts the pitch trend. (Iso, isotropic phase;  $N_L^*$ , left-handed cholesteric phase;  $N_R^*$ , right-handed cholesteric phase;  $SmA_b$ , biaxial smectic A phase;  $P_\infty$ , infinite pitch).

Table 1 Helix inversion temperatures in the CLC phase of (*S*)-naphthyl-3-hydroxypropanoic mesogens

Chiral compound	$T_{P_\infty}$ (°C)
( <i>S</i> )-BNOH-5-CB	$N_R^* \Leftrightarrow 103 - 104 \Leftrightarrow N_L^*$
( <i>S</i> )-BNOH-C6	$N_R^* \Leftrightarrow 58 - 59 \Leftrightarrow N_L^*$
( <i>S</i> )-BNOH-7-BB <sup>31</sup>	$N_R^* \Leftrightarrow 83 - 84 \Leftrightarrow N_L^*$
( <i>S</i> )-BNOH-7-NB <sup>31</sup>	$N_R^* \Leftrightarrow 95 - 96 \Leftrightarrow N_L^*$

The naphthyl-3-hydroxypropanoic moiety is a common structural motif among the compounds presented in Fig. 1 that undergo helix inversion. In contrast, compounds with a phenyl<sup>31,36</sup> or cyanobiphenyl-3-hydroxypropanoic group<sup>37</sup> do not exhibit this phenomenon. It is worth noting that helix inversion was not observed for the compound (*S*)-NNOH-C6 (Fig. S7).<sup>38</sup> Compared to (*S*)-BNOH-C6, (*S*)-NNOH-C6 has two naphthyl groups in its mesogenic unit. This structural modification raises the Iso- $N^*$  transition temperature to 131 °C, higher than that observed for (*S*)-BNOH-C6. It also leads to a TGBA-SmA-Cr phase sequence starting at 110 °C. The absence of helix inversion in (*S*)-NNOH-C6 can be attributed to stronger  $\pi$ - $\pi$  interactions, which stabilize the smectic organization and facilitate crystallization,<sup>39</sup> thereby preventing the complete unwinding of the cholesteric helical structure.

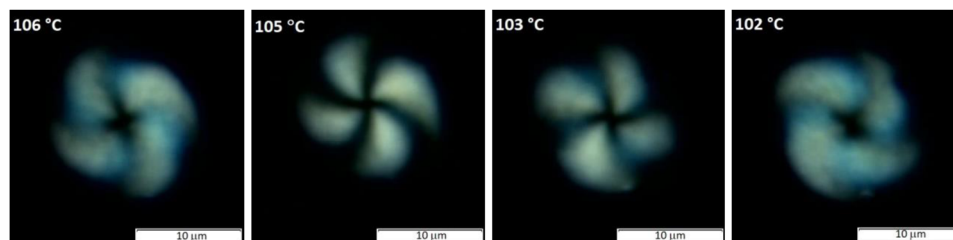


Fig. 3 The change of optical textures of a droplet of (*S*)-BNOH-5-CB on untreated glass slides before and after the helix inversion at  $T_{P_\infty} = 104$  °C. (Sample viewed between crossed polarizers parallel to the photograph edges).



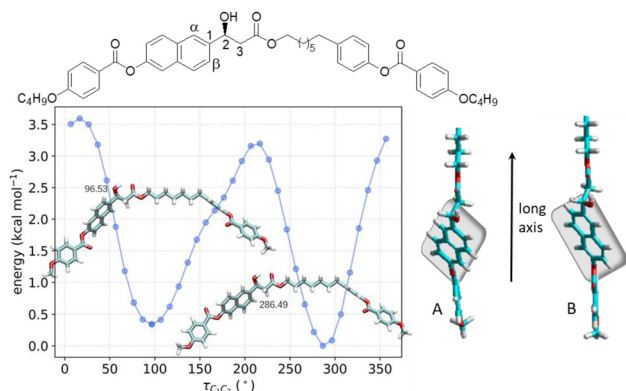


Fig. 5 (a) Relaxed potential energy scan along the  $C_1$ - $C_2$  bond of **(S)-BNOH-7-BB**, performed at the B3LYP/cc-pVDZ level of theory.<sup>41</sup> The energy profile is shown as a function of the  $C_\beta$ - $C_1$ - $C_2$ - $C_3$  dihedral angle. The optimized geometries of the two conformers corresponding to the energy minima are shown with their respective dihedral angle values. (b) Section of optimized models of the two conformers aligned along the long molecular axis.

The rarely observed helix inversion in the CLC phase of a liquid crystal with a single chiral center was attributed to a competition between the populations of various conformers with opposite twist senses.<sup>22,23,40</sup> Therefore, we conducted a conformational analysis focusing on the conformational space around the bond between the chiral center and the naphthyl group. Using density functional theory (DFT) at the B3LYP level with a cc-pVDZ basis set,<sup>41,42</sup> the calculations were performed on the most extended conformer of **(S)-BNOH-7-BB** as an example. Unlike the phenyl ring, the  $\alpha$  and  $\beta$  positions on the naphthyl ring are not equivalent, resulting in two stable conformers (Fig. 5a). Full optimization of these conformers revealed that conformer B is more stable than conformer A by  $1.5 \text{ kcal mol}^{-1}$ . From this optimized structure, a relaxed scan was then performed by systematically rotating the  $C_1$ - $C_2$  bond over a range of  $\pm 180^\circ$  in  $10^\circ$  increments. The  $3.2 \text{ kcal mol}^{-1}$  rotational barrier around the  $C_1$ - $C_2$  bond indicates that the two conformers are interconvertible. The theoretical model suggests that a variation in the orientation of the “chiral area” with respect to the orientation axis could cause a change in the sense of the helical twist.<sup>43</sup> The conformers A and B, aligned along the long molecular axis, exhibit different orientations of the naphthyl group planes relative to this axis (Fig. 5b). Assuming that the direction of the helix is influenced by these orientations, the relative populations of conformers A and B will likely have the most significant impact on the helical twist. According to the experimental data, the helix inversion temperature varies with the structure of the alkyl ester moiety. This suggests that the different conformations of the alkyl ester moiety contribute to balancing the species with opposing helical twists, thus affecting the temperature of helix inversion. Although this phenomenological approach is a simplified model, it provides a reasonable explanation for the thermally induced helix inversion observed in liquid crystal materials with a single chiral center.

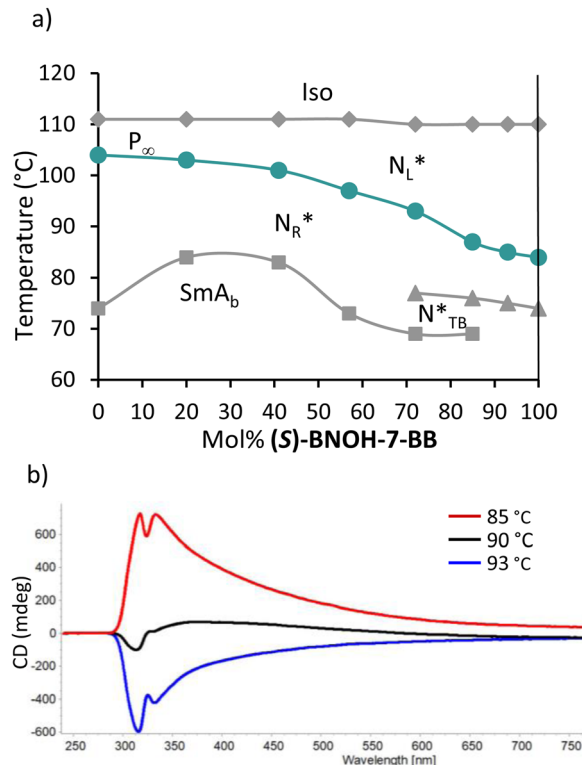


Fig. 6 (a) Helix inversion temperature and phase behavior of binary mixtures of **(S)-BNOH-7-BB** and **(S)-BNOH-5-CB**, represented versus mol percent of **(S)-BNOH-7-BB**. The symbol (●) depicts the helix inversion temperature. The other symbols represent phase transitions: Iso- $N_L^*$  (◆),  $N_L^*$ - $SmA_b$  (■),  $N_R^*$ - $N_{TB}^*$  (▲). The transition to the crystalline phase is omitted for clarity. (Iso, isotropic phase;  $N_L^*$ , left-handed cholesteric phase;  $N_R^*$ , right-handed cholesteric phase;  $N_{TB}^*$ , chiral twist-bend nematic phase;  $SmA_b$ , biaxial smectic A phase). (b) CD spectra of the mixture with 85 mol% of **(S)-BNOH-7-BB** in **(S)-BNOH-5-CB**, at 85 °C (red), 90 °C (black), and 93 °C (blue).

The limited number of single-component CLCs exhibiting thermally induced helix inversion prompted us to investigate mixtures that would display similar properties. Unlike other mixtures where two CLCs with opposite helical senses lead to helix inversion,<sup>27</sup> we explored mixtures of **(S)-BNOH-7-BB** and **(S)-BNOH-5-CB**, where both CLC components exhibit a transition from the high-temperature  $N_L^*$  to the low-temperature  $N_R^*$  phase. The two chiral compounds have similar clearing points, making mixing and manipulation easier, yet they exhibit significantly different helix inversion temperatures. The helix inversion temperature and phase behavior are represented as a function of the molar percentage (mol%) of **(S)-BNOH-7-BB** in Fig. 6a. The helix inversion temperature continuously decreases with increasing **(S)-BNOH-7-BB** concentration until it reaches that of the pure compound. However, the relationship is not linear, revealing the complex interplay between various conformations and their helical twist senses. The decrease in helix inversion temperature in mixtures with more than 80 mol% of **(S)-BNOH-7-BB**, along with the absence of rapid crystallization observed in the pure compound, allowed us to monitor helix inversion using circular dichroism (CD). The CD spectra of the



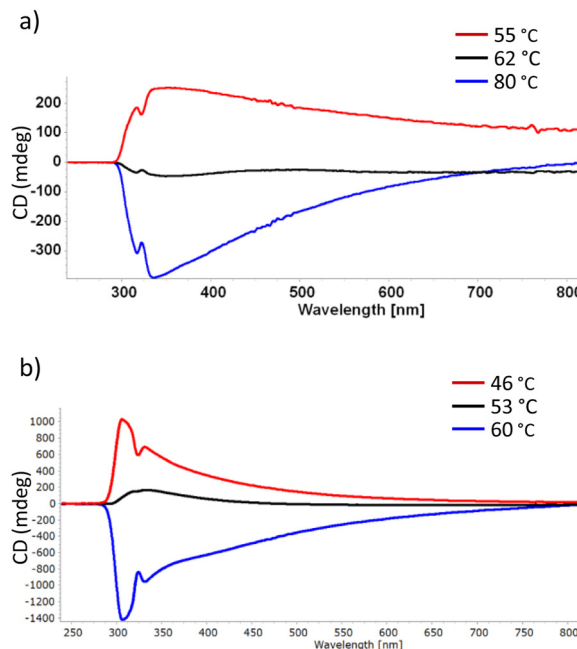
cholesteric phase with 85 mol% (**S**)-**BNOH-7-BB** were recorded at 93 °C, 90 °C, and 85 °C during the cooling cycle (Fig. 6b). At 93 °C, the CD spectrum exhibits a negative band, indicating a left-handed helical sense of the chiral nematic structure.<sup>44,45</sup> On the contrary, at 85 °C, the CD band becomes positive, and the helix is right-handed. At the intermediate temperature of 90 °C, the CD spectrum shows an almost flat line, suggesting that the structure is achiral.

The slight discrepancy in helix inversion temperature observed using POM and CD can be attributed to the different experimental setups used for temperature measurement. It is important to note that the shape and sign of the CD signals are both independent of the rotation angle and remain unchanged when the sample is flipped. The CD spectra support the optical observations and confirm that, as temperature decreases, the twist handedness changes from left to right across the entire composition range, as observed with the pure components. In addition, the results show that the helix inversion temperature can be varied by adjusting the mixing ratio of the chiral materials. However, the variation range is limited by the helix inversion temperatures of the pure components.

To assess the ability of these chiral compounds to impart this unique property to an achiral host, we investigated mixtures containing approximately 50 mol% of each chiral compound in three different achiral hosts, namely 4-hexyloxy cyanobiphenyl (6OCB), 4-(octyloxy)phenyl 4-octyloxybenzoate (8OPEP), and a mixture of 40 wt% of 4-cyanobiphenyl-4'-butylbenzoate in 4-cyanobiphenyl-4'-hexylbenzoate (PEPP-N) (Fig. S8). All three achiral hosts exhibit an enantiotropic nematic phase (N). Additionally, 8OPEP undergoes a transition from the nematic phase to the smectic phase at 73 °C. These achiral hosts were chosen for their structural similarity to the chiral compounds, which facilitates mixing. The results are summarized in Table 2.

**Table 2** Helix inversion temperatures of the CLC phase of mixtures containing (*S*)-naphthyl-3-hydroxypropanoic mesogens and different achiral LCs

Chiral compound	Mol%	$T_{P_{\infty}}$ (°C)
6OCB		
( <i>S</i> )- <b>BNOH-5-CB</b>	50	$N_R^* \Leftrightarrow 75 - 76 \Leftrightarrow N_L^*$
( <i>S</i> )- <b>BNOH-C6</b>	50	$N^*$
( <i>S</i> )- <b>BNOH-7-BB</b>	50	$N_L^*$
( <i>S</i> )- <b>BNOH-7-NB</b>	50	$N_L^*$
8OPEP		
( <i>S</i> )- <b>BNOH-5-CB</b>	52	$N_R^* \Leftrightarrow 85 - 86 \Leftrightarrow N_L^*$
( <i>S</i> )- <b>BNOH-C6</b>	51	$N_R^* \Leftrightarrow 55 - 56 \Leftrightarrow N_L^*$
( <i>S</i> )- <b>BNOH-7-BB</b>	50	$N_R^* \Leftrightarrow 62 - 63 \Leftrightarrow N_L^*$
( <i>S</i> )- <b>BNOH-7-NB</b>	49	$N_R^* \Leftrightarrow 77 - 80 \Leftrightarrow N_L^*$
PEPP-N		
( <i>S</i> )- <b>BNOH-5-CB</b>	50	$N_R^* \Leftrightarrow 111 - 112 \Leftrightarrow N_L^*$
( <i>S</i> )- <b>BNOH-C6</b>	48	$N_L^*$
( <i>S</i> )- <b>BNOH-7-BB</b>	49	$N_L^*$
( <i>S</i> )- <b>BNOH-7-NB</b>	45	$N_L^*$



**Fig. 7** (a) CD spectra of the **BNOH-7-BB\_8OPEP** (50 mol%) mixture at 55 °C (red), 62 °C (black), and 80 °C (blue). (b) CD spectra of the **BNOH-C6\_8OPEP** (51 mol%) mixture at 60 °C (blue), 53 °C (black), and 46 °C (red).

POM observations of mixtures with 6OCB revealed that helix inversion occurs only in the **BNOH-5-CB\_6OCB** mixture, whereas the **BNOH-7-BB\_6OCB** and **BNOH-7-NB\_6OCB** mixtures display only the left-handed CLC phase. Upon cooling from the isotropic melt, the **BNOH-C6\_6OCB** mixture displays the CLC phase within only a fraction of a degree, immediately followed by the  $SmA^*$  phase, despite both mixture components being exclusively nematogens.

When the achiral host was changed from 6OCB to 8OPEP, an aromatic ester-type LC, helix inversion was observed for all four mixtures. The change from the high-temperature left-handed helix to the low-temperature right-handed helix was confirmed by both POM<sup>46</sup> and CD spectroscopy, as illustrated by the CD spectra of the **BNOH-7-BB\_8OPEP** and **BNOH-C6\_8OPEP** mixtures (Fig. 7).

With the achiral PEPP-N host, which has both cyanobiphenyl and aromatic ester moieties, helix inversion was only detected in the **BNOH-5-CB\_PEPP-N** mixture. The **BNOH-C6\_PEPP-N**, **BNOH-7-BB\_PEPP-N**, and **BNOH-7-NB\_PEPP-N** mixtures exhibit a left-handed cholesteric phase followed by a  $SmA^*$  phase. Induction of the smectic phase in binary mixtures involving cyanobiphenyl and aromatic ester-type components has been reported previously.<sup>47,48</sup> However, determining why the  $SmA^*$  phase appears in mixtures of PEPP-N and **BNOH-C6\_6OCB** is beyond the scope of this study.

These findings demonstrate that the ability to impart the property of temperature-induced helix inversion from a chiral guest to an achiral host depends on their specific interactions. In the same nematic host, the chirality transfer is affected by the short-range interactions between guest and host, as well as



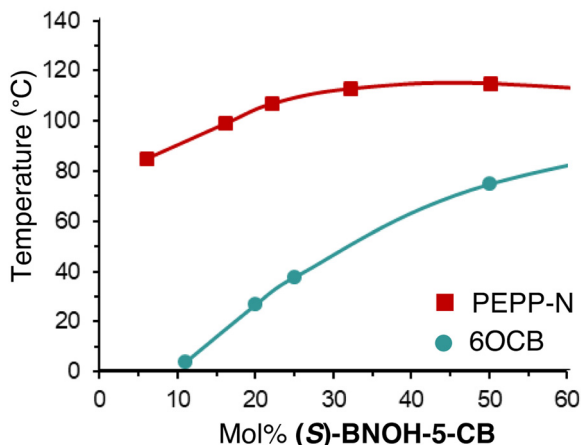


Fig. 8 Dependence of the temperature of helix inversion on the concentration of (S)-BNOH-5-CB in the binary mixtures of BNOH-5-CB\_6OCB (●) and BNOH-5-CB\_PEPP-N (■).

the orientational order of the chiral guest in the nematic environment.<sup>49,50</sup> While (S)-BNOH-5-CB, which has both ester and cyanobiphenyl units, successfully imparts helix inversion to all three achiral hosts, (S)-BNOH-C6, (S)-BNOH-7-BB, and (S)-BNOH-7-NB, which just have ester-type mesogenic units, promote helix inversion in the achiral host 8OPEP only. This suggests that short-range interactions between the structurally similar mesogenic units of guest and host enhance the transfer of temperature-dependent helix inversion. In contrast, specific interactions between unlike mesogenic units induce the formation of the SmA\* phase. Therefore, the concentration of chiral guest required for helix inversion could be reduced by using an appropriate combination of chiral guest and nematic host.

To test this assumption and investigate how a reduction of concentration of the chiral guest affects the helix inversion temperature, we studied binary mixtures of BNOH-5-CB\_6OCB and BNOH-5-CB\_PEPP-N in the concentration range of 6 to 50 mol% of (S)-BNOH-5-CB. We chose the achiral hosts, 6OCB and PEPP-N, because, unlike 8OPEP, they only exhibit the nematic phase and not the smectic phase, which could hinder helix inversion in mixtures with low concentrations of the chiral guest. The dependence of the helix inversion temperature on the concentrations of (S)-BNOH-5-CB in 6OCB and PEPP-N is presented in Fig. 8.

Microscopy observations showed that the helix inversion temperature decreases with decreasing concentration of (S)-BNOH-5-CB in both achiral hosts. Regardless of the host type, all the mixtures maintain the change from the high-temperature left-handed helix to the low-temperature right-handed helix. In the BNOH-5-CB\_6OCB mixtures, the helix inversion temperature varies by as much as  $\approx 70$  K within the 11 to 50 mol% concentration range. Upon cooling, the BNOH-5-CB\_6OCB mixture with 6 mol% of (S)-BNOH-5-CB crystallizes at 48 °C, which is in fact higher than the helix inversion temperatures observed for the mixtures with 11 mol% and 25 mol% of the chiral guest.

The helix inversion temperatures of the BNOH-5-CB\_PEPP-N mixtures are higher than those of the BNOH-5-CB\_6OCB mixtures, spanning  $\approx 30$  K across the explored concentration range. The occurrence of helix inversion at 84 °C in the BNOH-5-CB\_PEPP-N mixture with 6 mol% of (S)-BNOH-5-CB demonstrates that helix inversion can be transferred even at guest concentrations as low as 6 mol%.

Both types of mixtures exhibit a significantly broader range of helix inversion temperatures than the 10 K range reported for CLC mixtures of (S)-1,2-propanediol esters<sup>28</sup> or the 20 K range observed for binary mixtures of (S)-BNOH-7-BB and (S)-BNOH-5-CB. Furthermore, the transition between helices of opposite handedness can be achieved within a given temperature range by adjusting the concentration of the chiral nematogen in the achiral host. Specifically, using the PEPP-N host brings the helix inversion temperature within the 84 °C to 114 °C range, while the 6OCB host brings it within the 4 °C to 74 °C range. These results represent an exciting opportunity for this new class of compounds for applications in the design of materials with tunable thermally-induced helical switching properties.

## Conclusion

This article presents a new class of liquid crystalline compounds with a single chiral center that exhibit reversible thermally-induced helix inversion in the cholesteric phase. The key structural fragment of these compounds is the (S)-naphthyl-3-hydroxypropanoic moiety, which is essential for their unique behavior. The helix inversion is attributed to the conformational freedom of the naphthyl group adjacent to the stereogenic center and to its orientation relative to the long molecular axis. However, the helix inversion temperature in pure compounds is affected by the structure of the alkyl ester moiety.

In mixtures of two chiral compounds, the helix inversion behavior remains limited to that of the pure compounds, as the helix inversion temperature depends on the composition yet remains between those of the pure chiral liquid crystals.

Furthermore, we demonstrated that the property of temperature-induced helix inversion, from a high-temperature left-handed helix to a low-temperature right-handed helix, could be transferred from a pure (S)-naphthyl-3-hydroxypropanoic chiral derivative to a structurally similar achiral nematic host. Additionally, our study revealed that the helix inversion temperature can be precisely adjusted across a wide range, from below room temperature up to 114 °C.

These new chiral mesogens offer great potential for further research and applications thanks to their unique properties, specifically their thermally-induced helix inversion, their ability to transfer this unique feature to an achiral host, and the wide temperature range over which this inversion can be adjusted. Moreover, structural modifications on the alkyl ester moiety do not disrupt the helix inversion, allowing for the tailoring of key properties, such as the helix inversion temperature,



interactions with the host, and even the incorporation of additional responsive functionalities.

Given the very limited number of CLCs exhibiting thermally-induced helix inversion,<sup>22,23</sup> these novel chiral mesogens provide new systems for experimental and theoretical studies aimed at understanding the mechanisms of transmission and amplification of chirality from the molecular to the supramolecular levels. The tunability of thermal helix inversion has great potential for designing new responsive liquid crystal systems, especially for applications where precise, temperature-controlled modulation of chirality and optical properties is essential.

## Author contributions

A. Ožegović, investigation, writing – original draft, writing – review & editing. A. Šimanović, investigation, writing – original draft. I. Dokli, investigation, writing – original draft, writing – review & editing. P. Davidson, investigation, writing – original draft, writing – review & editing. I. Dozov, investigation, writing – original draft, writing – review & editing. Jurica Novak, investigation, writing – original draft, writing – review & editing. A. Knežević, investigation, writing – original draft, writing – review & editing, funding acquisition. A. Lesac, conceptualization, investigation, writing – original draft, writing – review & editing, funding acquisition.

## Conflicts of interest

The authors have no conflicts of interest to declare.

## Data availability

The data supporting this article have been included as part of the SI. See DOI: <https://doi.org/10.1039/d5qm00456j>

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