Supporting Information for:

Crystal structure analyses facilitate understanding of synthetic protocols in the preparation of 6,6’-dibromo substituted BINOL compounds

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Figure S1. $^1$H-NMR spectra of (RS)-2 before (a) and after crystallization from toluene/cyclohexane (b).
Figure S2. IR spectra of (R)-2 before (top) and after crystallization from toluene/n-hexane (bottom).
Figure S3 Optical microscope images of compound $(R)$-2 crystallized from CH$_2$Cl$_2$/cyclohexane and purified.

Figure S4 Optical microscope images of compound $(R)$-2 crystallized from toluene/n-hexane and purified.

Figure S5 Optical microscope images of compound $(RS)$-2 crystallized from toluene/cyclohexane and purified.
Figure S6: Optical microscope images of compound (RS)-3 crystallized from CHCl₃/EtOH and still with regioisomerically impurities.

Figure S7: Optical microscope images of compound (R)-3 crystallized from CHCl₃/EtOH and purified.

Figure S8: Optical microscope images of compound (RS)-4 crystallized from CH₂Cl₂/EtOH and regioisomerically impure.
Figure S9 Solution state circular dichroism spectra of the \( R \) enantiomers of compounds \( 2 \) (in EtOH), \( 3 \) and \( 4 \) (both in MeCN).
Copies of NMR spectra of compound (RS)-4

$^1$H NMR

![NMR spectra image]
$^{13}$C NMR

$^{13}$C NMR (DEPT)
Hydrogen bonds for \((R)-2\) and \((RS)-2\)

Table S1. Hydrogen bonds for \((R)-2\) \([\text{Å and }^\circ]\) in \(P2_12_12_1\).

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>(&lt;(DHA))</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(1)-H(1O)...O(2)#1</td>
<td>0.831(19)</td>
<td>2.13(2)</td>
<td>2.934(4)</td>
<td>164(5)</td>
</tr>
<tr>
<td>O(2)-H(2O)...Br(1)#2</td>
<td>0.823(19)</td>
<td>2.74(4)</td>
<td>3.353(3)</td>
<td>133(4)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y+1/2,-z+1/2    #2 x+1/2,-y+3/2,-z

Table S2. Hydrogen bonds for \((RS)-2\) \([\text{Å and }^\circ]\) in \(P2_1/n\).

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>(&lt;(DHA))</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(1)-H(1O)...O(2)#1</td>
<td>0.820(19)</td>
<td>2.14(3)</td>
<td>2.840(3)</td>
<td>143(4)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y+1/2,-z+1/2