

*Supporting Information for:*

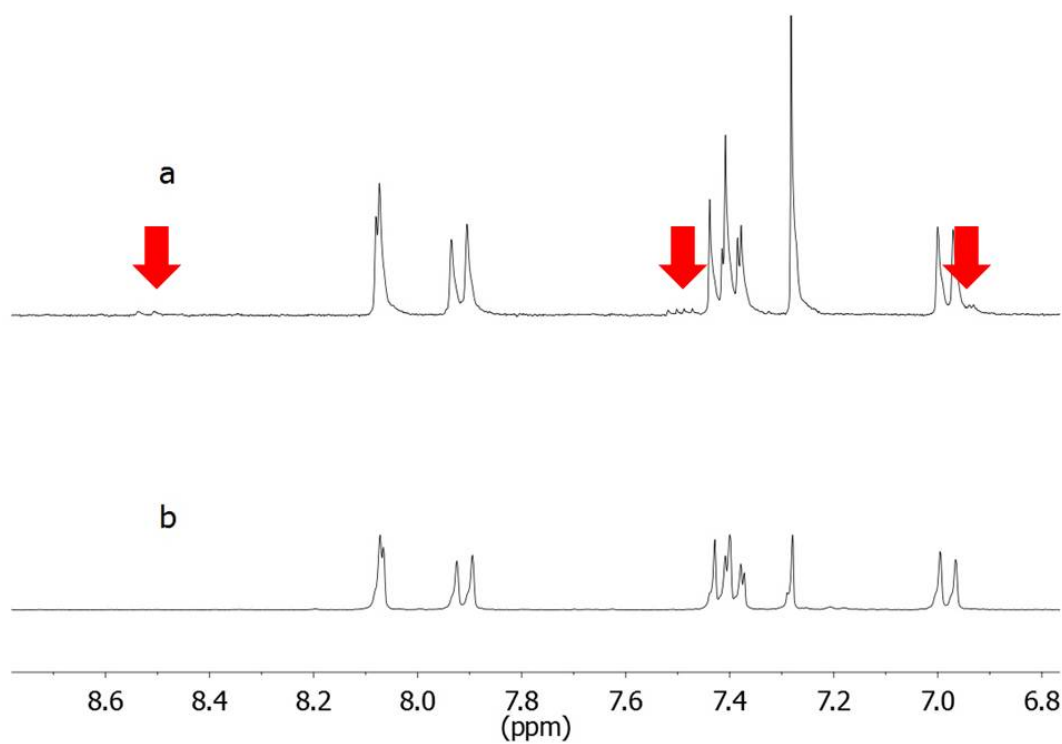
## **Crystal structure analyses facilitate understanding of synthetic protocols in the preparation of 6,6'- dibromo substituted BINOL compounds**

*Marco Agnes,<sup>a,b</sup> Alessandro Sorrenti,<sup>a</sup> Dario Pasini,<sup>b</sup> Klaus Wurst,<sup>c</sup> and  
David B. Amabilino<sup>a</sup>*

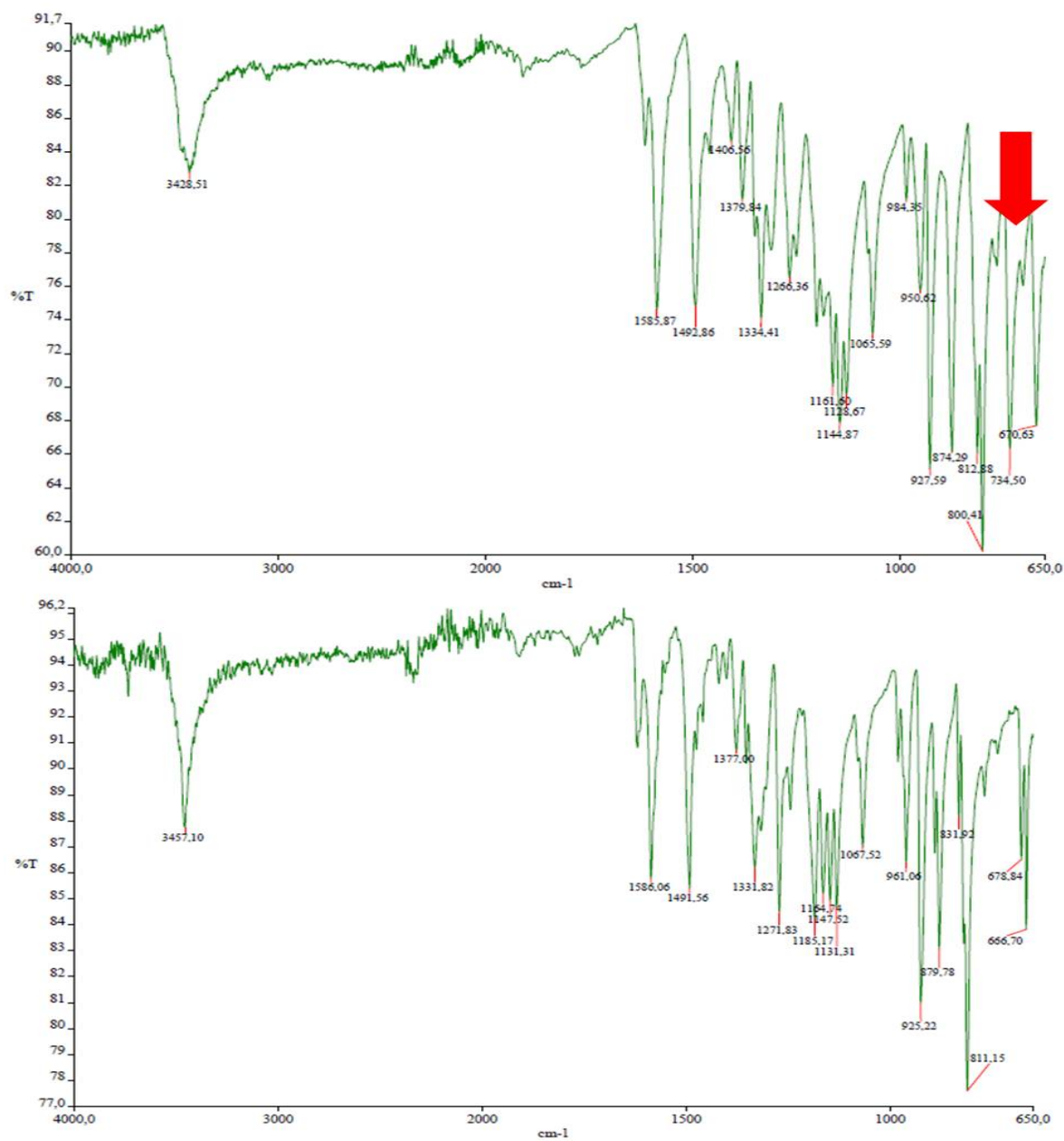
<sup>a</sup> *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus Universitari de Bellaterra, 08193  
Cerdanyola del Vallès, Catalonia - Spain, Fax: (+34) 93-5805729*

<sup>b</sup> *Department of Chemistry and INSTM Research Unit, University of Pavia, Viale Taramelli, 10 - 27100 -  
Pavia - Italy.*

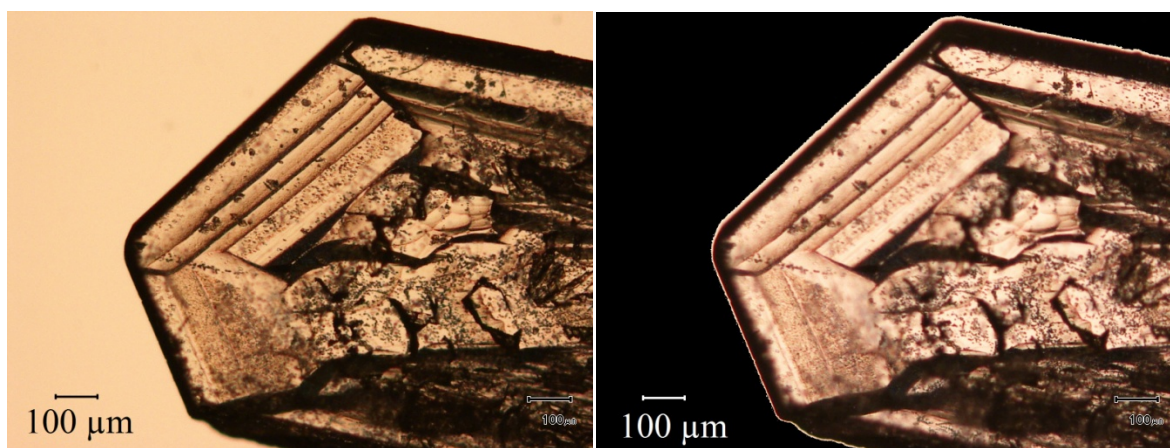
<sup>c</sup> *Institut für Anorganische Chemie, Innrain 80/82, A-6020 Innsbruck, Austria*



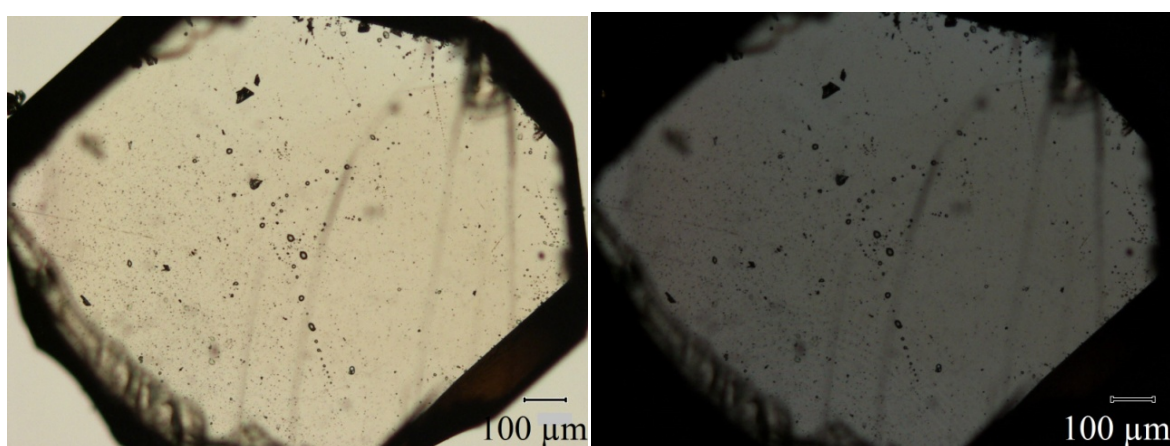
**Figure S1.** <sup>1</sup>H-NMR spectra of (*RS*)-**2** before (a) and after crystallization from toluene/cyclohexane (b).



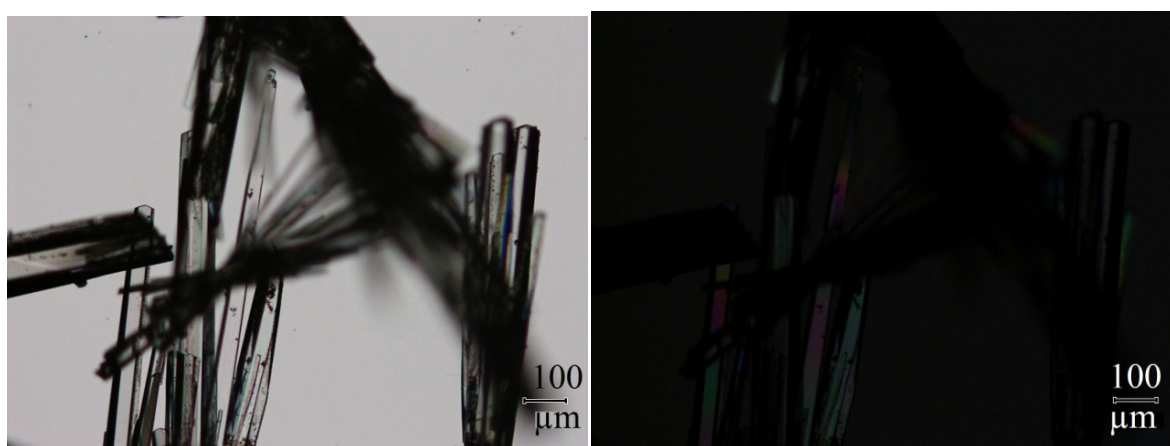
**Figure S2.** IR spectra of (*R*)-**2** before (top) and after crystallization from toluene/*n*-hexane (bottom).



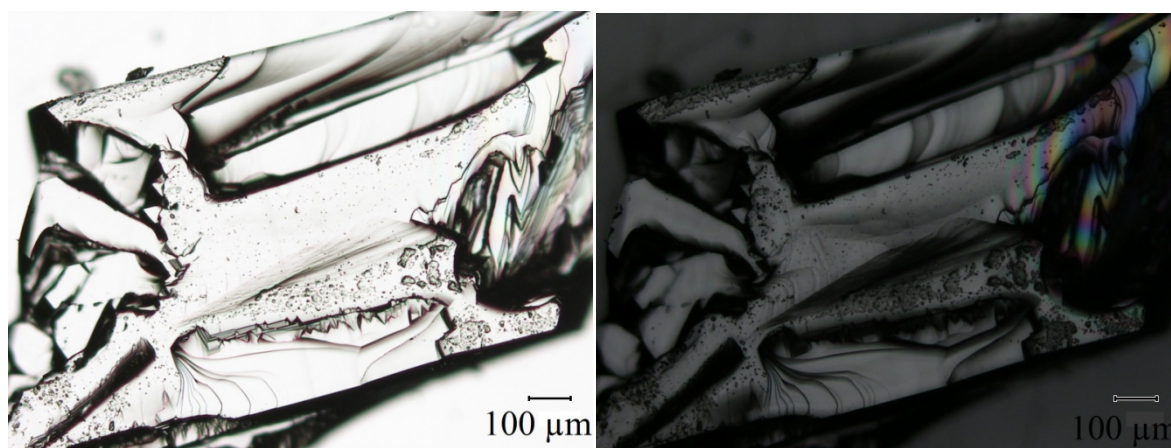
**Figure S3** Optical microscope images of compound (*R*)-2 crystallized from CH<sub>2</sub>Cl<sub>2</sub>/cyclohexane and purified.



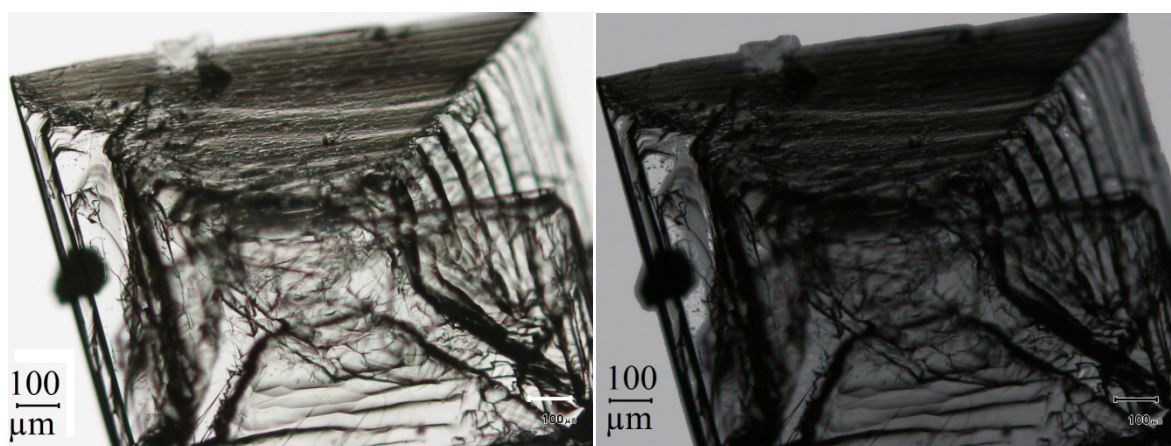
**Figure S4** Optical microscope images of compound (*R*)-2 crystallized from toluene/n-hexane and purified.



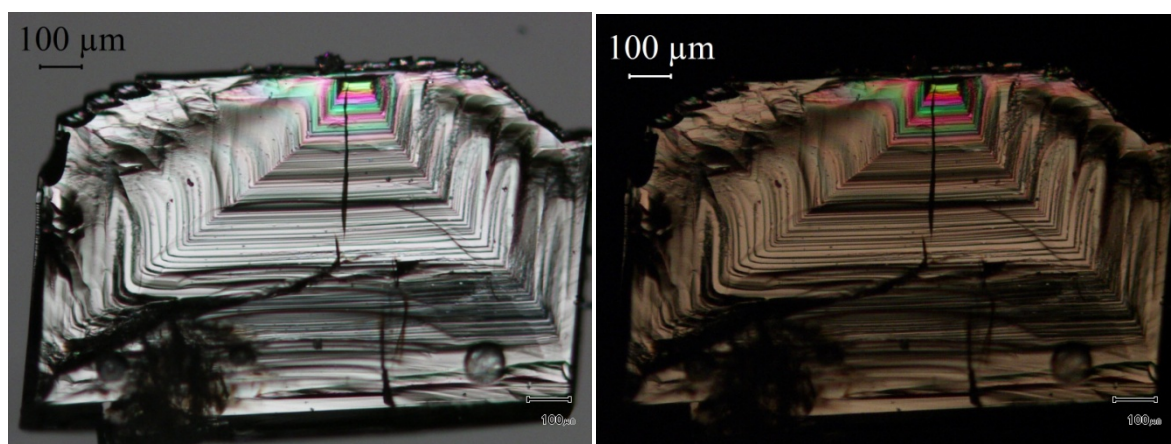
**Figure S5** Optical microscope images of compound (*RS*)-2 crystallized from toluene/cyclohexane and purified.



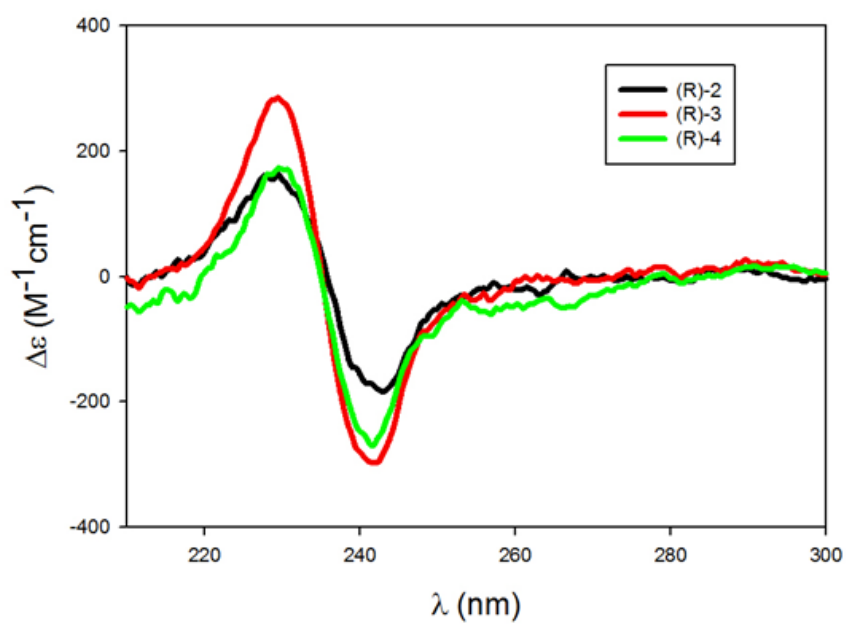
**Figure S6** Optical microscope images of compound (*RS*)-**3** crystallized from CHCl<sub>3</sub>/EtOH and still with regioisomerically impurities.



**Figure S7:** Optical microscope images of compound (*R*)-**3** crystallized from CHCl<sub>3</sub>/EtOH and purified.



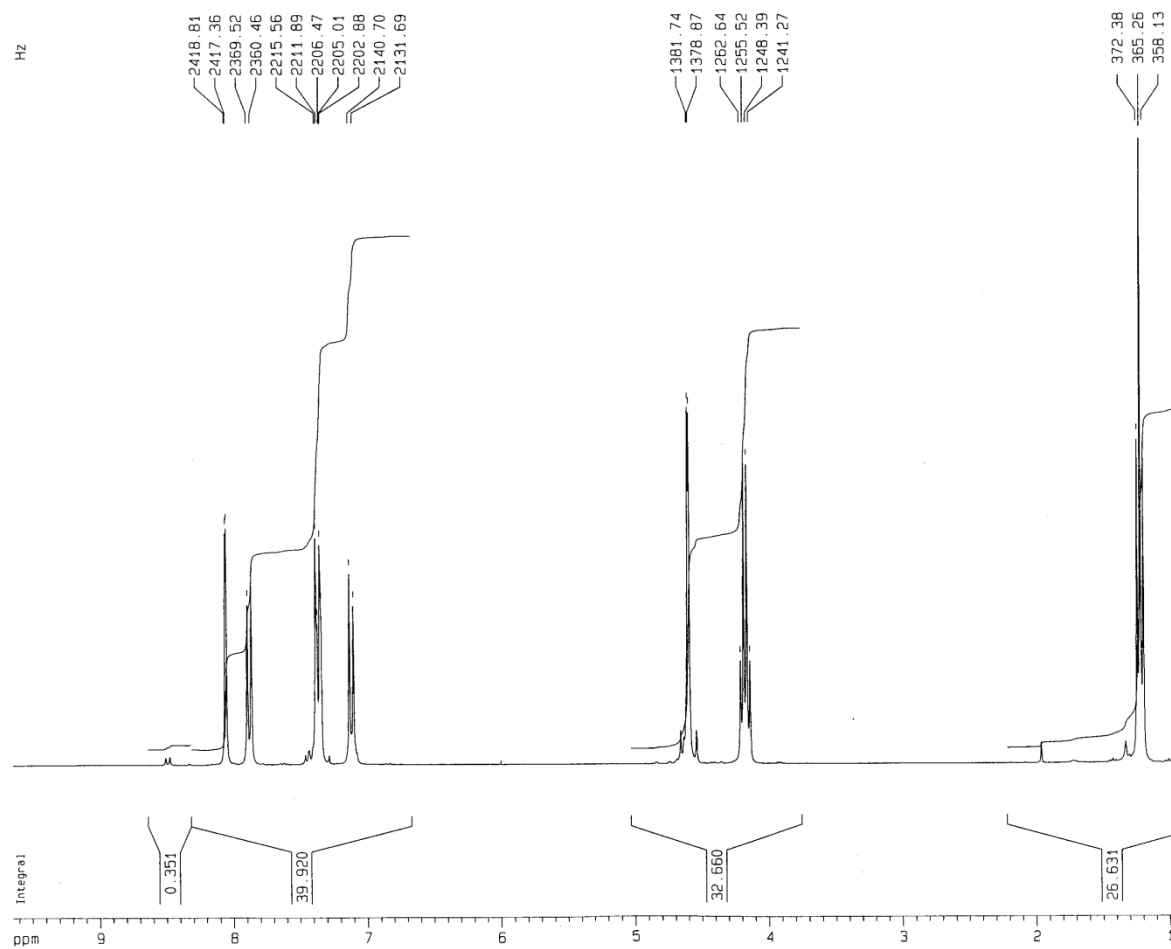
**Figure S8** Optical microscope images of compound (*RS*)-**4** crystallized from CH<sub>2</sub>Cl<sub>2</sub>/EtOH and regioisomerically impure.



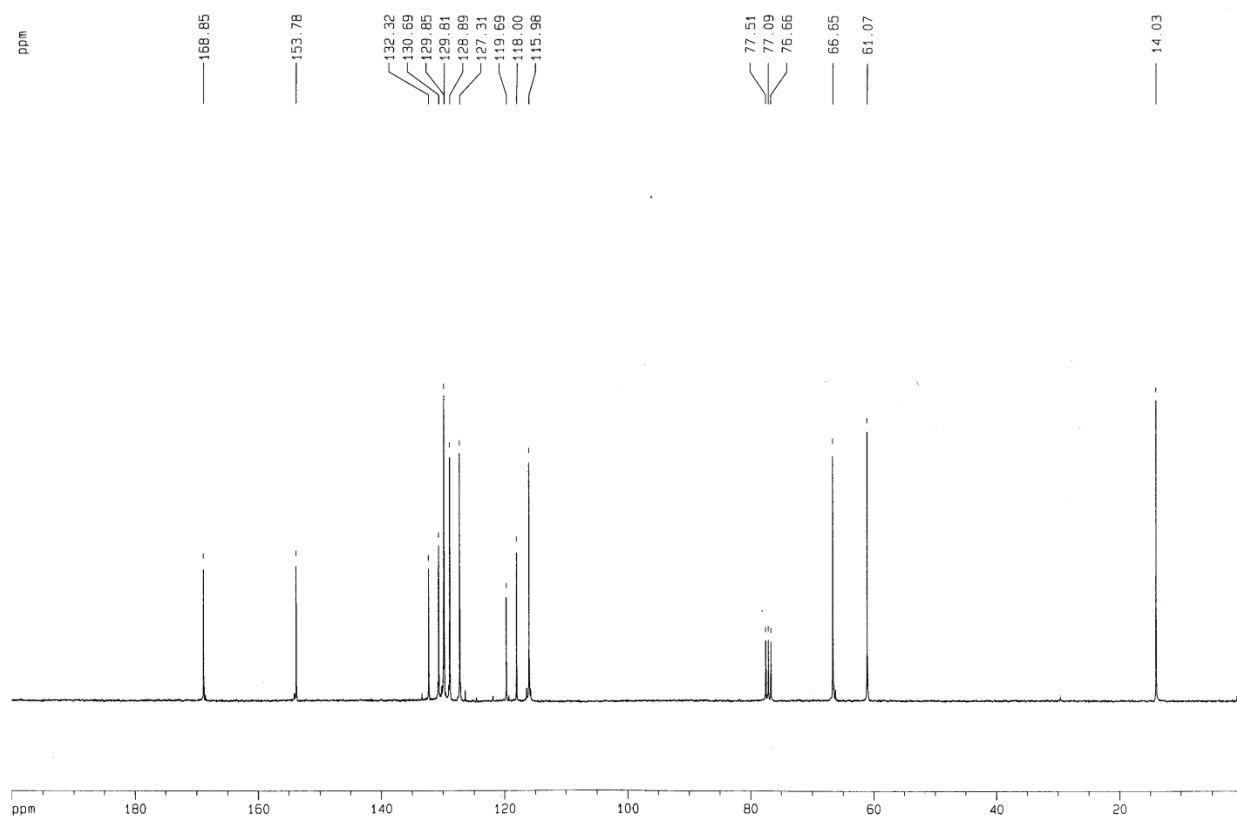
**Figure S9** Solution state circular dichroism spectra of the *R* enantiomers of compounds **2** (in EtOH), **3** and **4** (both in MeCN).

# Copies of NMR spectra of compound (RS)-4

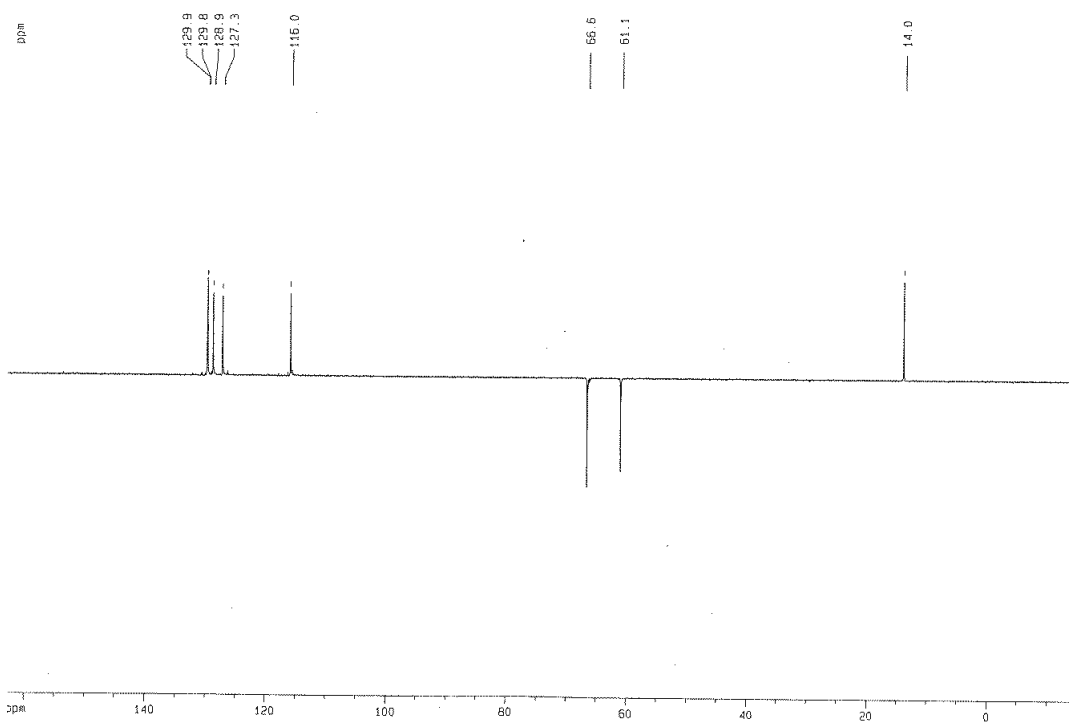
## <sup>1</sup>H NMR



# <sup>13</sup>C NMR



# <sup>13</sup>C NMR (DEPT)





## Hydrogen bonds for (*R*)-**2** and (*RS*)-**2**

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

---

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1)-H(1O)...O(2)#1	0.831(19)	2.13(2)	2.934(4)	164(5)
O(2)-H(2O)...Br(1)#2	0.823(19)	2.74(4)	3.353(3)	133(4)

---

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** [ $\text{\AA}$  and  $^\circ$ ] in  $P2_1/n$ .

---

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1)-H(1O)...O(2)#1	0.820(19)	2.14(3)	2.840(3)	143(4)

---

Symmetry transformations used to generate equivalent atoms:

#1  $-x-1/2, y+1/2, -z+1/2$