Supporting Information

to the paper entitled

Effect of a methyl group on the spontaneous resolution of a square-pyramidal coordination compound: crystal packing and conglomerate formation

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Table S1 Summary of the crystallographic data for **1** (*Δ* enantiomer)

Formula	$C_{17}H_{21}CuN_3O_3$
Formula weight	378.91
Temperature	100(2) K
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.3456(5)
b/Å	11.2047(8)
c/Å	20.0815(15)
α/°	90
β/°	90
γ/°	90
V/Å^3	1652.8(2)
Z	4
D_{calc}/g cm^{-3}	1.523
μ/mm^{-1}	1.342
F(000)	788
R(int)	0.0321
Total Reflections	8722
Flack parameter	0.005(11)
Unique reflections	3607
$I > 2\sigma(I)$	3474
*R*1, *wR*2	0.0281, 0.0727

Table S2 Coordination bonds (Å) and angles (º) for **1** (*Δ* enantiomer)

Cu1−O11	1.909(1)
Cu1−N19	1.983(2)
Cu1−O38	1.998(2)
Cu1−N31	1.982(2)
Cu1−N22	2.325(2)
O11−Cu1−N19	95.21(7)
N19−Cu1−O38	90.53(7)
O38−Cu1−N31	82.08(7)
N31−Cu1−O11	93.03(7)
O11−Cu1−N22	107.50(7)
N19−Cu1−N22	83.30(8)
O38−Cu1−N22	98.08(7)
N31−Cu1−N22	94.08(7)

Figure S1 Molecular structure of the *Δ* enantiomer of compound **1**

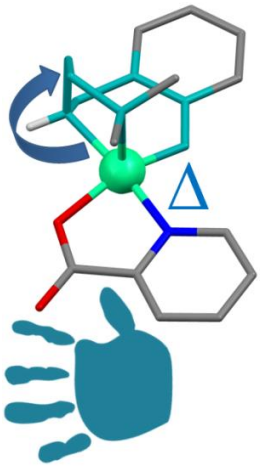

Figure S2 UV-Vis spectrum of a millimolar methanolic solution of **1**

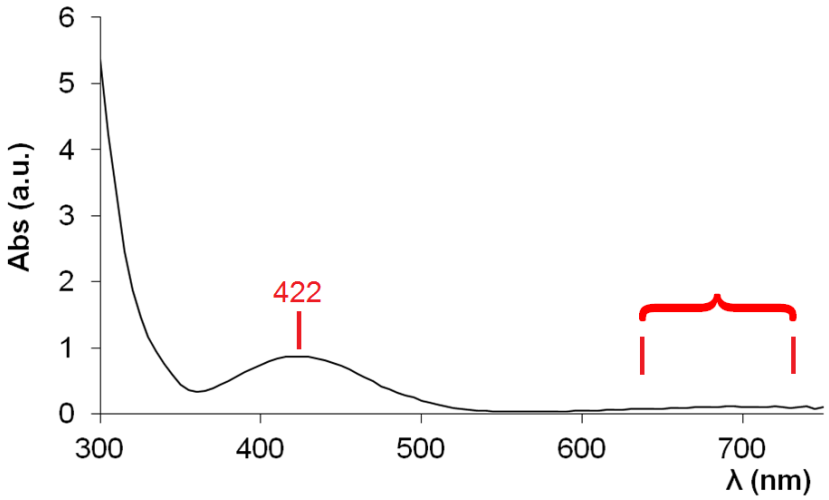

Figure S3. Solid-state CD spectrum of the other enantiomer of **1-*Δ***

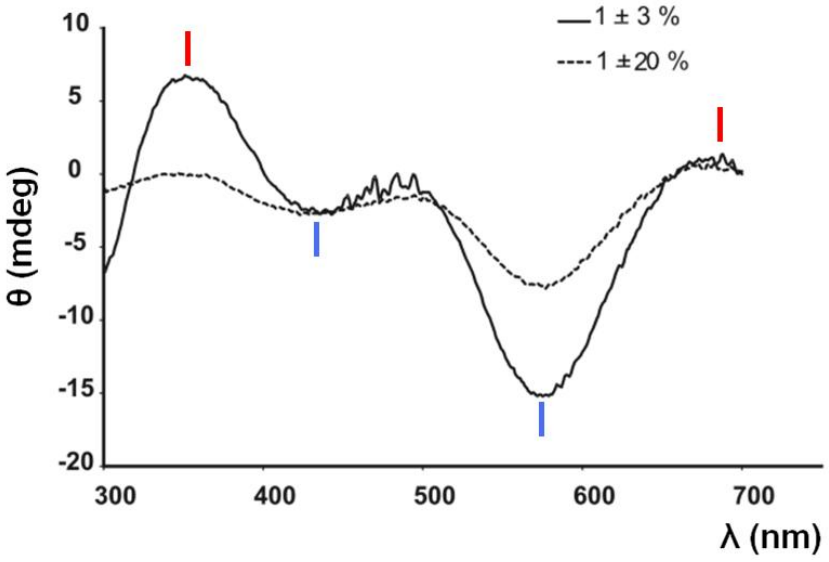

Figure S4 Solution CD spectrum of **1** (1×10^{-3} M in methanol)

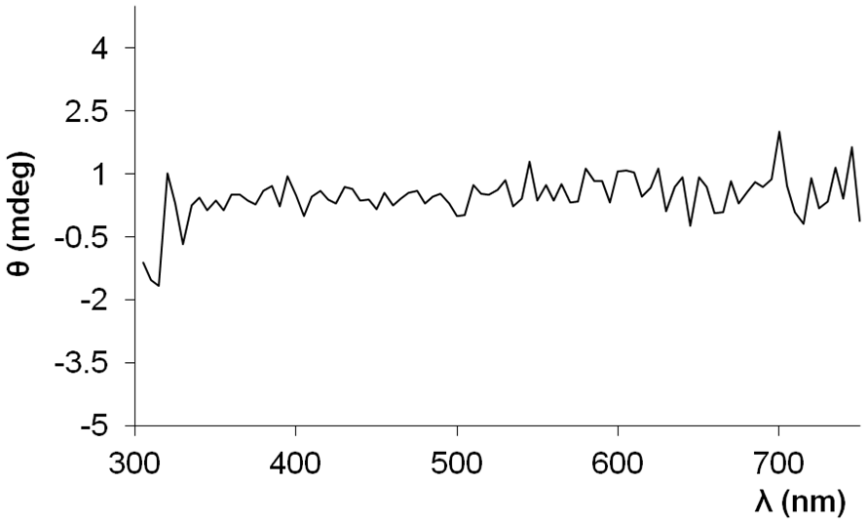

Figure S5. Solution CD spectrum of **2** (1×10^{-3} M in methanol)

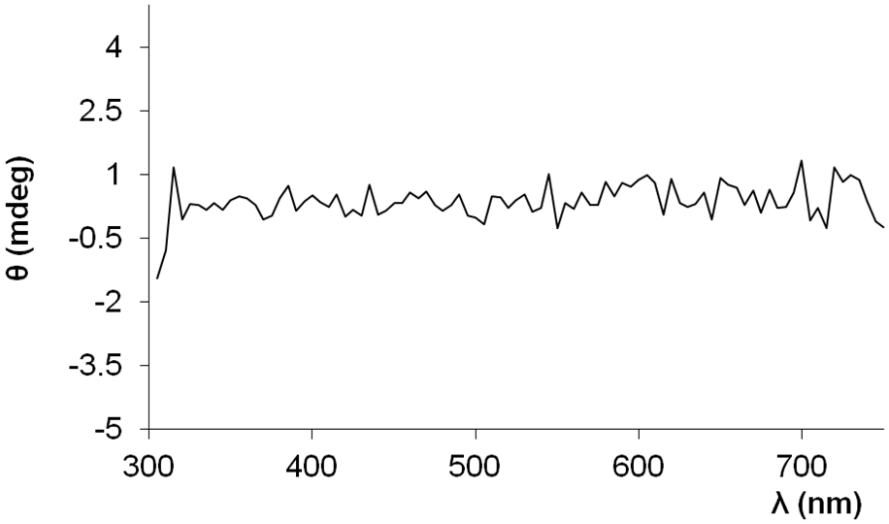

Figure S6. Solution (**A**) and solid-state (**B**) UV-Vis spectra of **2**