

Supporting Information for "Solvent-Tunable Inversion of Chirality Transfer from Carbon to Copper", Marie Hutin and Jonathan R. Nitschke*

Preparation of 1. Into a 50 ml Schlenk flask was added (S)-(-)-3-amino-1,2-propanediol (10.3 mg, 0.11 mmol) dissolved in methanol (1 ml), 6-methyl-pyridine-2-carbaldehyde (13.7 mg, 0.11 mmol) dissolved in methanol (1 ml), (21.4 mg, 0.057 mmol) of $\text{Cu}(\text{NCMe})_4\text{O}_3\text{SCF}_3$, and methanol (3 ml). The flask was sealed, and traces of residual dioxygen were eliminated by five evacuation / argon fill cycles. The reaction was stirred at room temperature for 3 hours. Volatiles were then removed under dynamic vacuum, giving an isolated yield of 88% (30 mg, 0.05 mmol) of a red-orange solid, which was pure by NMR. ^1H NMR (500 MHz, 298 K, $\text{DMSO}-d^6$; H_P , H_M = signal attributed to (*P*) and (*M*) diastereomer, respectively): δ = 8.80 ppm (s, 2 H_P , imine), 8.77 ppm (s, 2 H_M , imine), 8.08 ppm (m, 2 H_P + 2 H_M , 5-pyridyl), 7.87 ppm (m, 2 H_P + 2 H_M , 6- pyridyl), 7.65 ppm (m, 2 H_P + 2 H_M , 4- pyridyl), 4.89 ppm (d, J = 4.5 Hz, 2 H_P , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 4.74 ppm (d, J = 5.0 Hz, 2 H_M , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 4.68 ppm (m, 2 H_P + 2 H_M , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 3.99 ppm (d, J = 10.0 Hz, 2 H_M , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 3.95 ppm (d, J = 8.5 Hz, 2 H_P , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 3.70 ppm (m, 4 H_P + 4 H_M , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$, $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 3.36 ppm (m, 4 H_P + 4 H_M , $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 2.18 ppm (s, 6 H_P , methyl), 2.17 ppm (s, 6 H_M , methyl). ^{13}C NMR (125.77 MHz, 298 K, $\text{DMSO}-d^6$): δ (ppm) = 162.9, 162.5, 157.6, 157.3, 149.8, 138.5, 138.4, 127.7, 127.6, 124.4, 124.2, 71.3, 71.1, 63.7, 63.4, 63.1, 62.8, 23.9. ^1H NMR (400 MHz, 298 K, CD_2Cl_2): δ = 8.68 ppm (s, 2H, imine), 7.96 ppm (t, J = 7.5 Hz, 2H, 5- pyridyl), 7.70 ppm (d, J = 7.0 Hz, 2H, 6- pyridyl), 7.53 ppm (d, J = 7.5 Hz, 2H, 4- pyridyl), 4.66 ppm (br s, 2H, hydroxyl), 3.90 ppm (br m, 8H, $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$, $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$, hydroxyl), 3.52 ppm (m, 4H, $\text{C}=\text{NCH}_2\text{CHOHCH}_2\text{OH}$), 2.30 ppm (s, 6H, methyl). ^{13}C NMR (100.62 MHz, 298 K, CD_2Cl_2): δ (ppm) = 163.1, 157.9, 150.0, 138.1, 127.8, 124.5, 71.8, 64.3, 62.9, 24.5. ESI-MS: m/z = 451.4 ($[\text{I}]^+$). UV-Vis (dichloromethane; $\lambda(\text{nm})$, ϵ ($\text{M}^{-1}\text{cm}^{-1}$)): 475, 6.1×10^3 ; 286, 1.80×10^4 ; 252, 1.84×10^4 ; 236, 1.71×10^4 . CD (dichloromethane, 20°C; $\lambda(\text{nm})$, $\Delta\epsilon$ ($\text{M}^{-1}\text{cm}^{-1}$)): 467, +2.21; 297, -10.51; 260, +9.04; 224, +3.93. CD (dimethylsulfoxide, 20°C; $\lambda(\text{nm})$, $\Delta\epsilon$ ($\text{M}^{-1}\text{cm}^{-1}$)): 484, -0.36; 301, +1.20; 262, -4.01.

NMR Spectrum of 1 in CD_2Cl_2 :

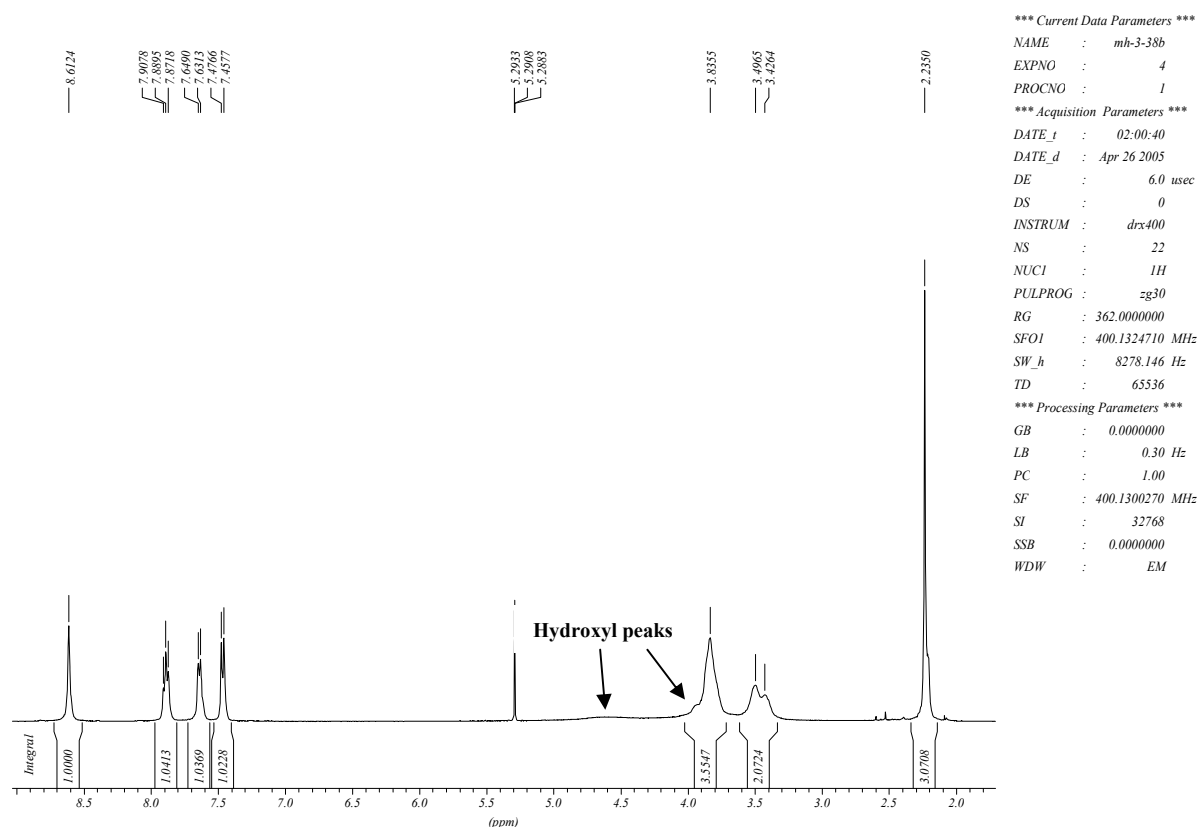


Fig. S1. NMR Spectrum of 1 in CD_2Cl_2

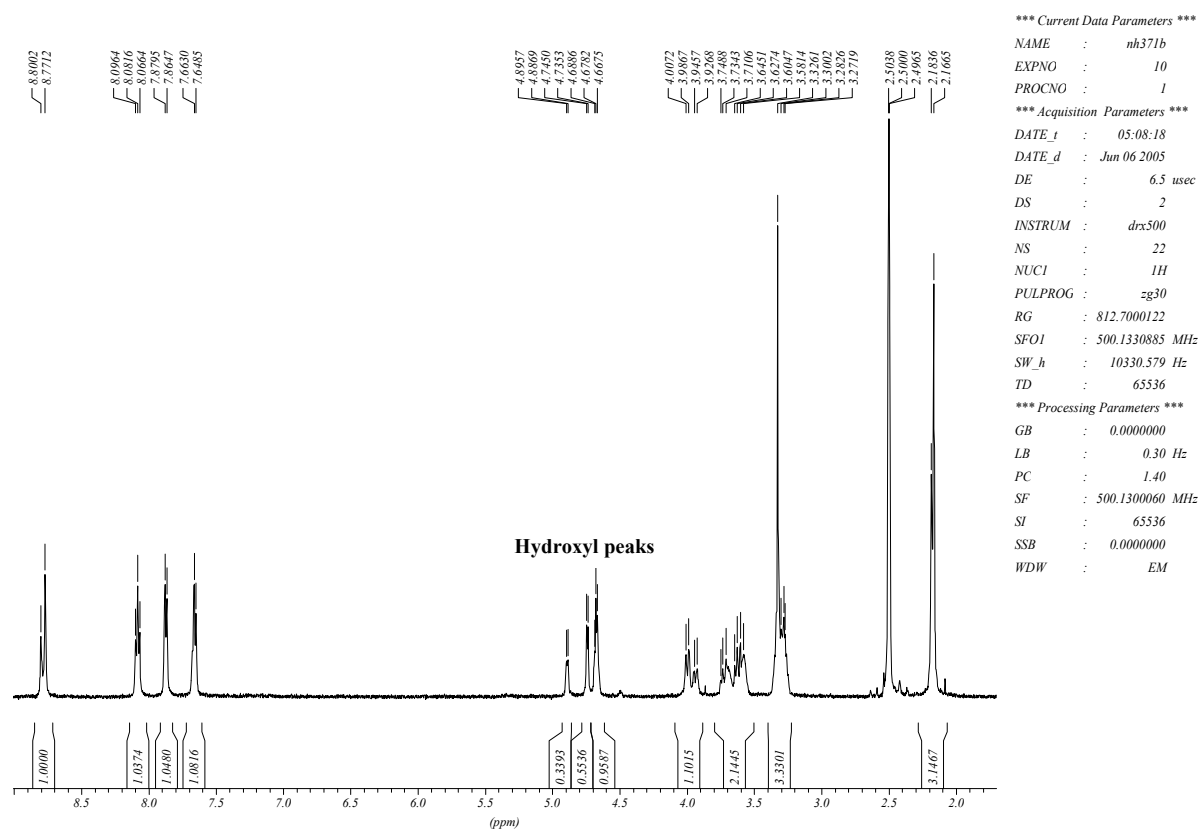


Fig. S1. NMR Spectrum of 1 in DMSO- d_6

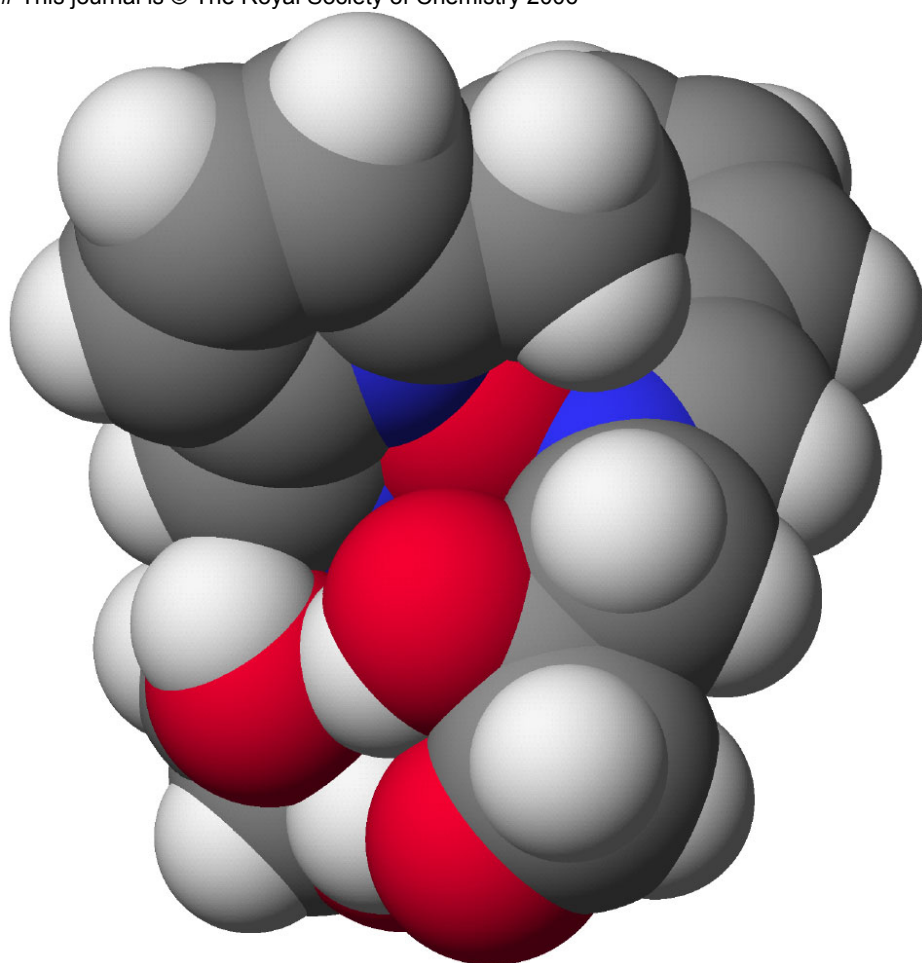


Fig. S3. Space-filling model of the proposed structure of **1** in dichloromethane

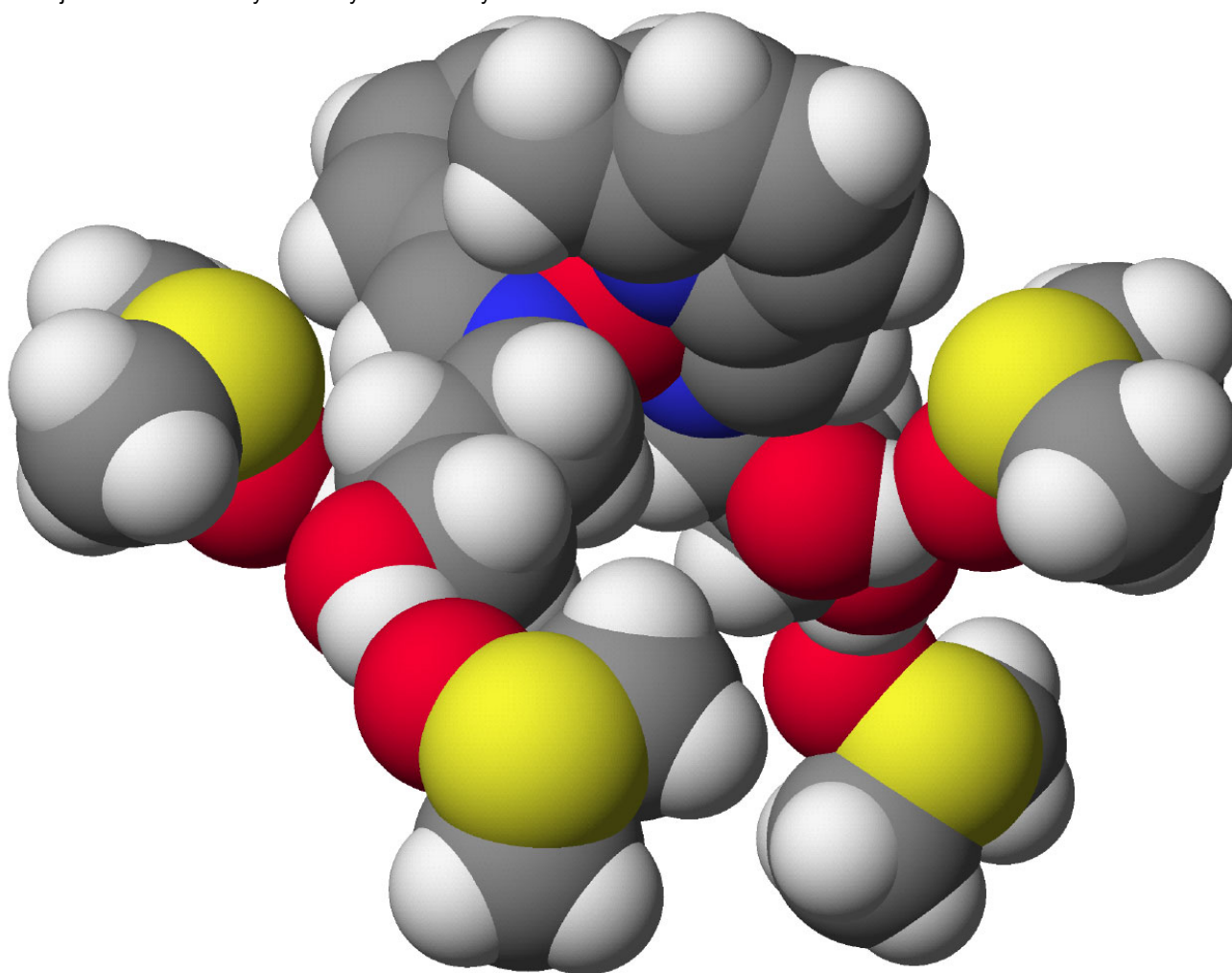


Fig. S4. Space-filling model of the proposed structure of **1** in DMSO