

Electronic Supplementary Information

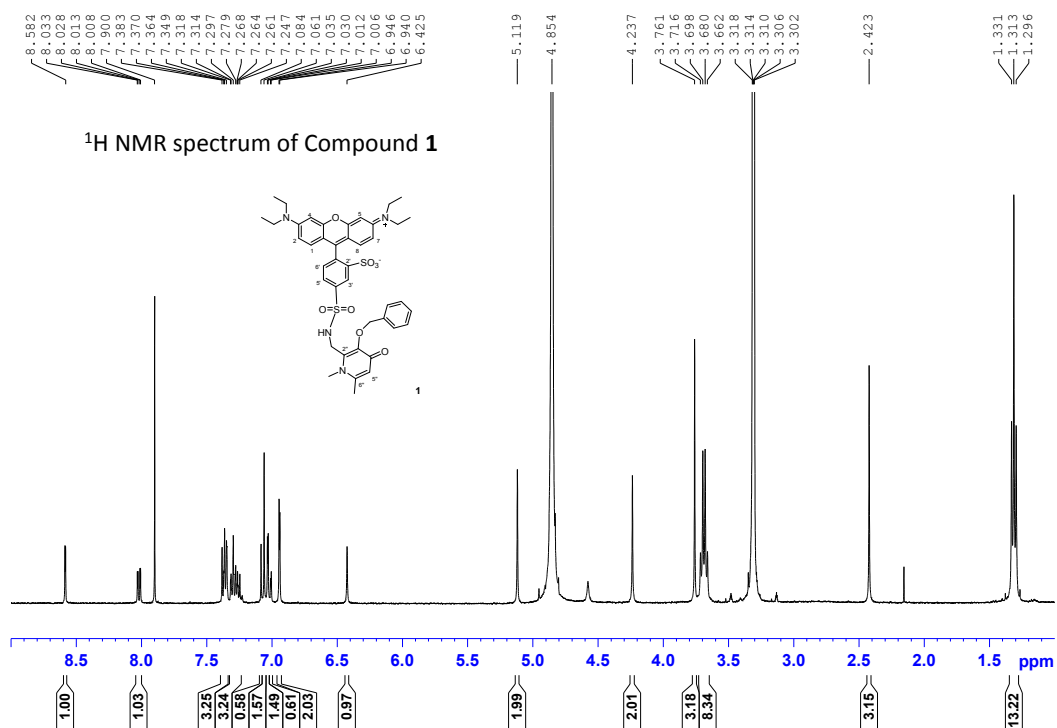


Figure S1. 400.15 MHz ¹H spectrum of compound **1**.

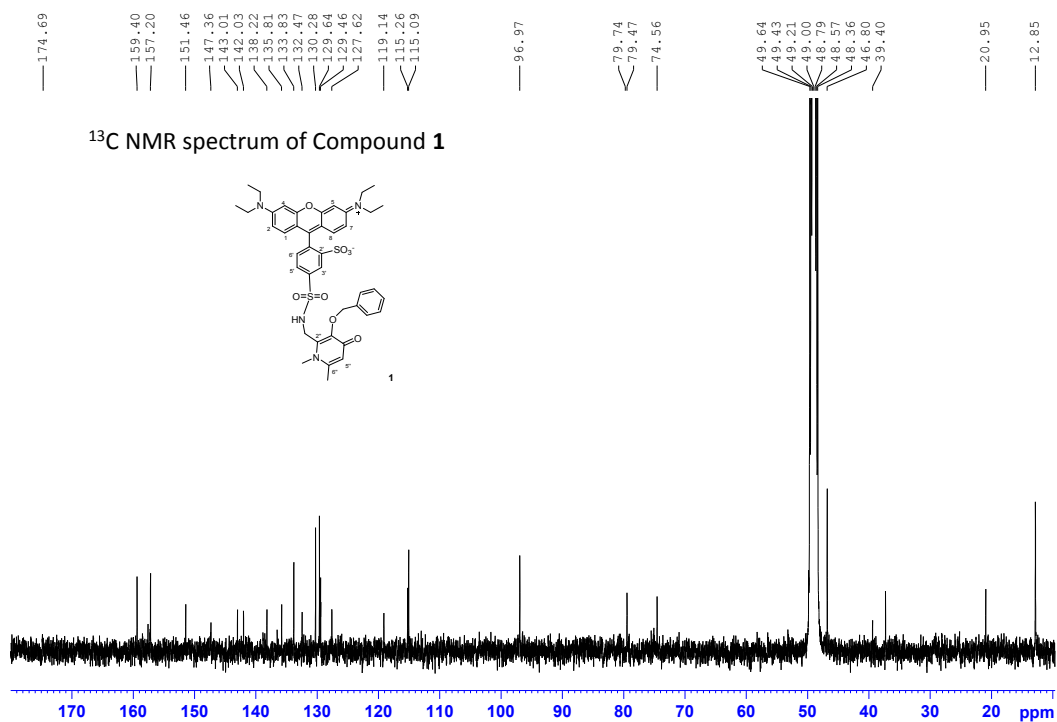


Figure S2. 400.15 MHz ¹³C spectrum of compound **1**.

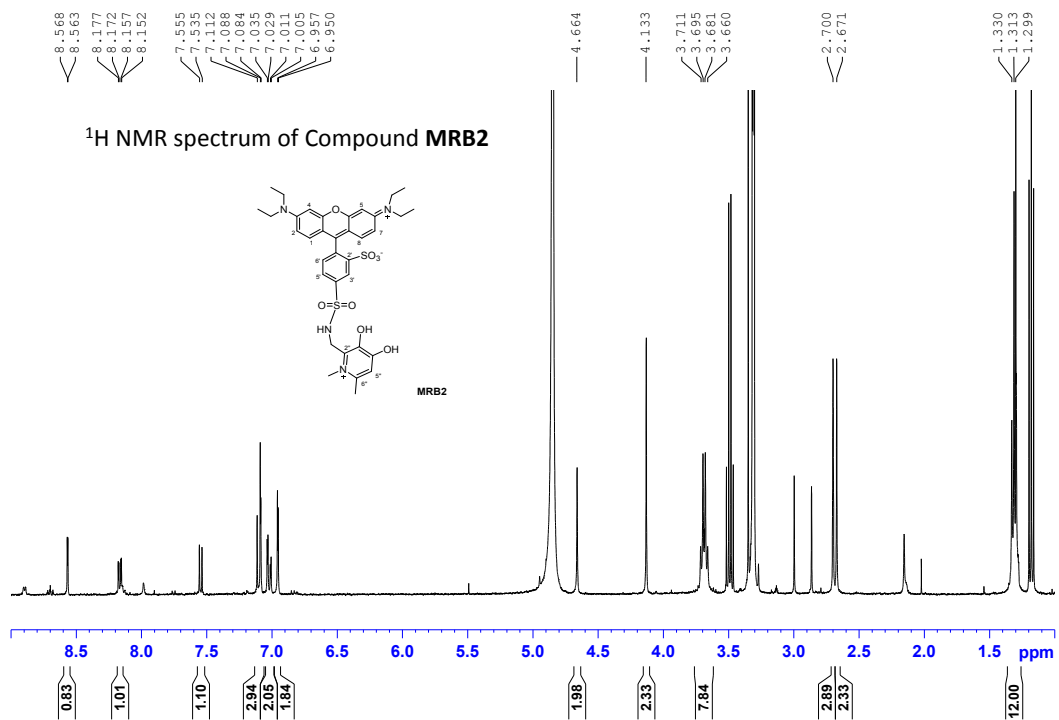


Figure S3. 400.15 MHz ¹H spectrum of compound MRB2.

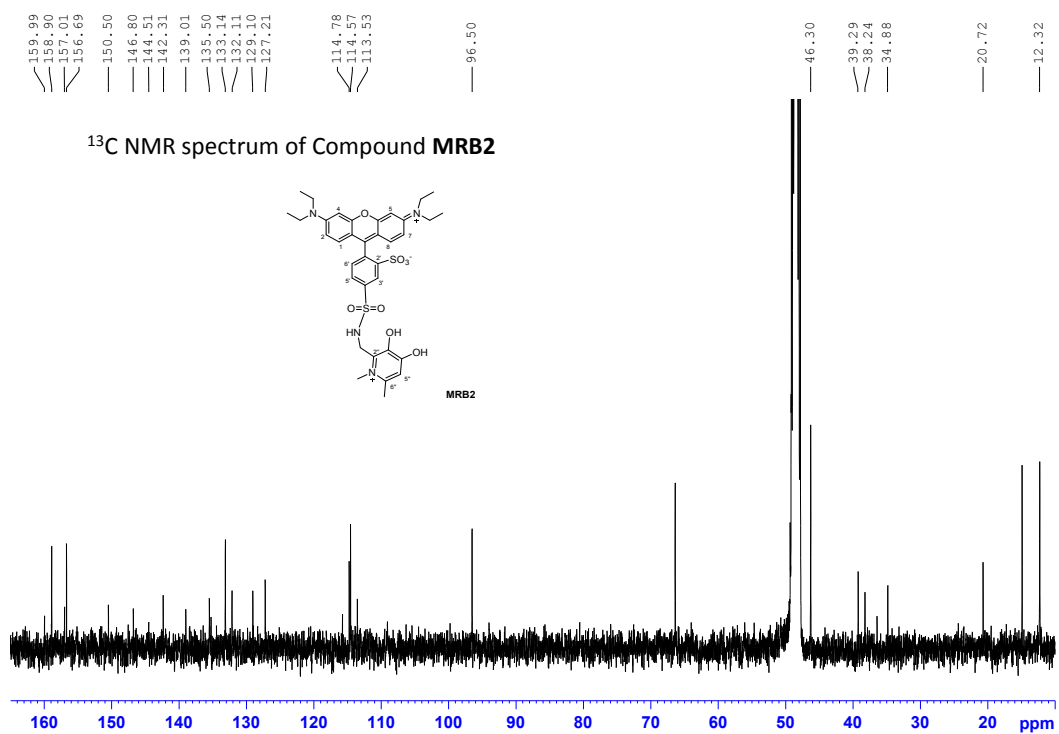


Figure S4. 400.15 MHz ¹³C spectrum of compound MRB2.

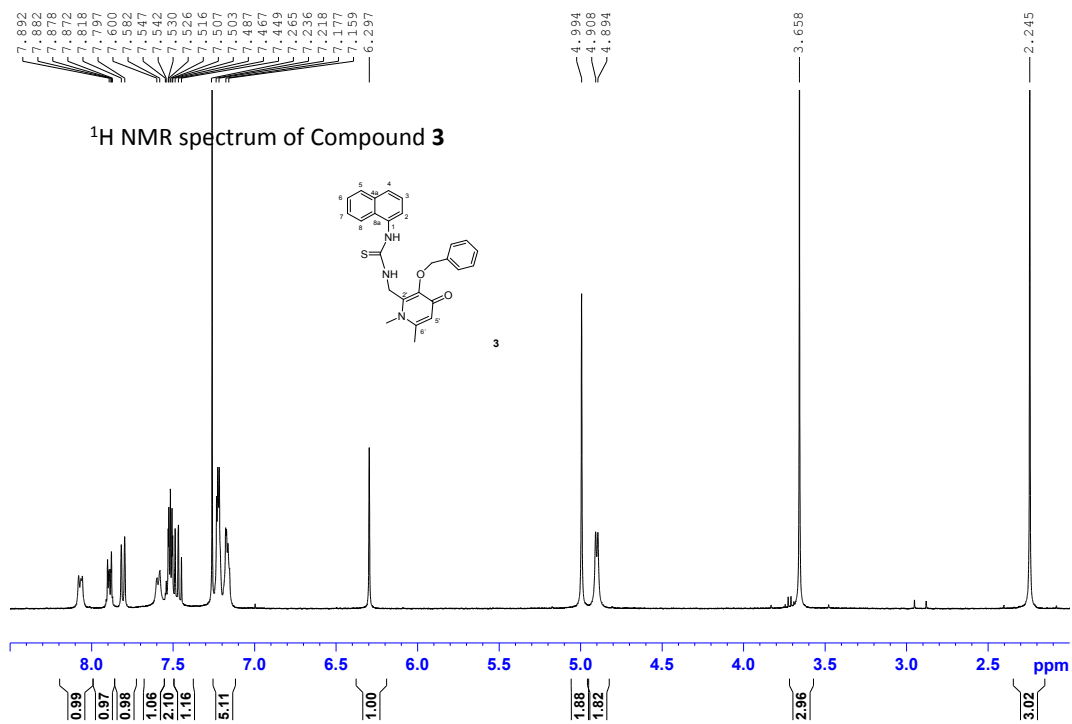


Figure S5. 400.15 MHz ¹H spectrum of compound 3.

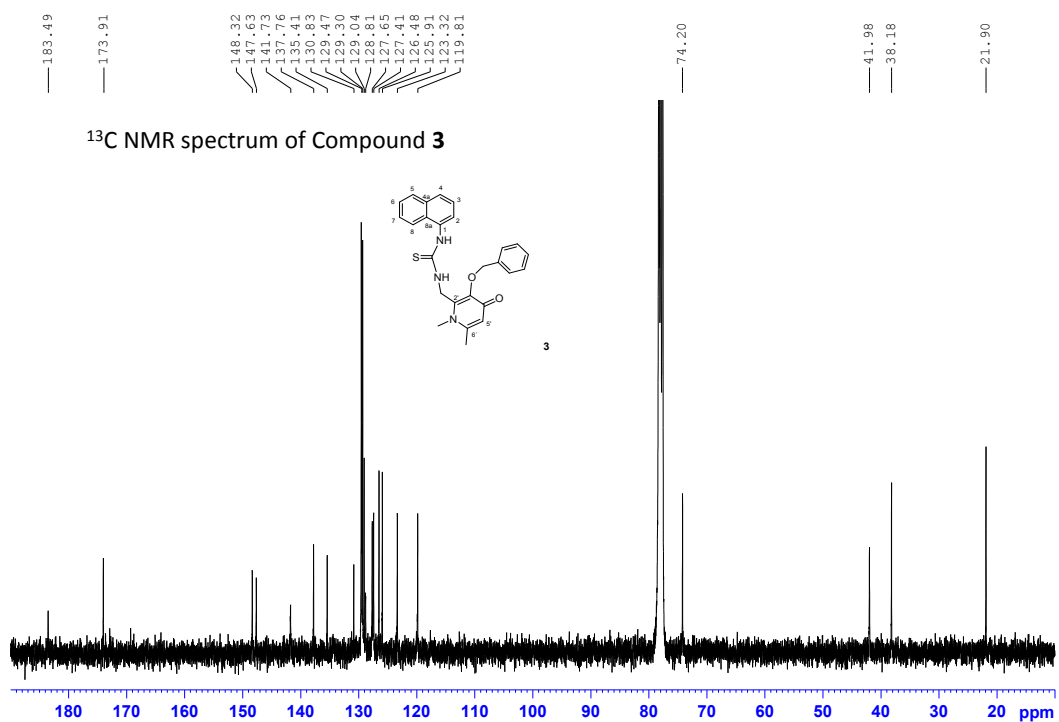


Figure S6. 400.15 MHz ¹³C spectrum of compound 3.

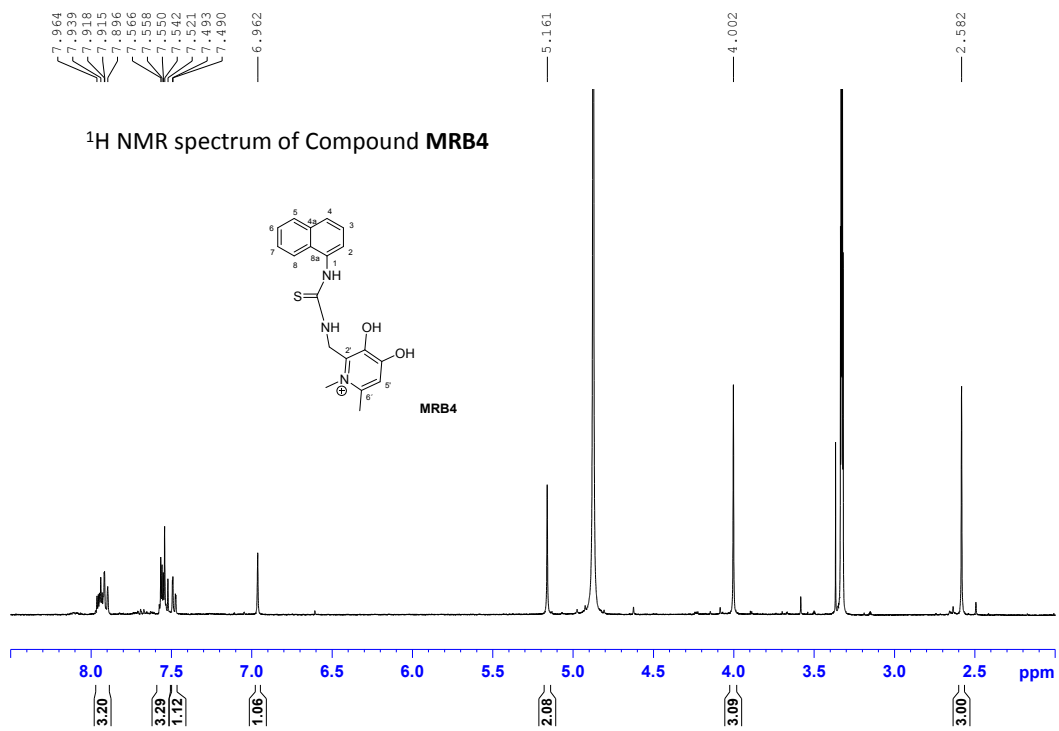


Figure S7. 400.15 MHz ¹H spectrum of compound MRB4.

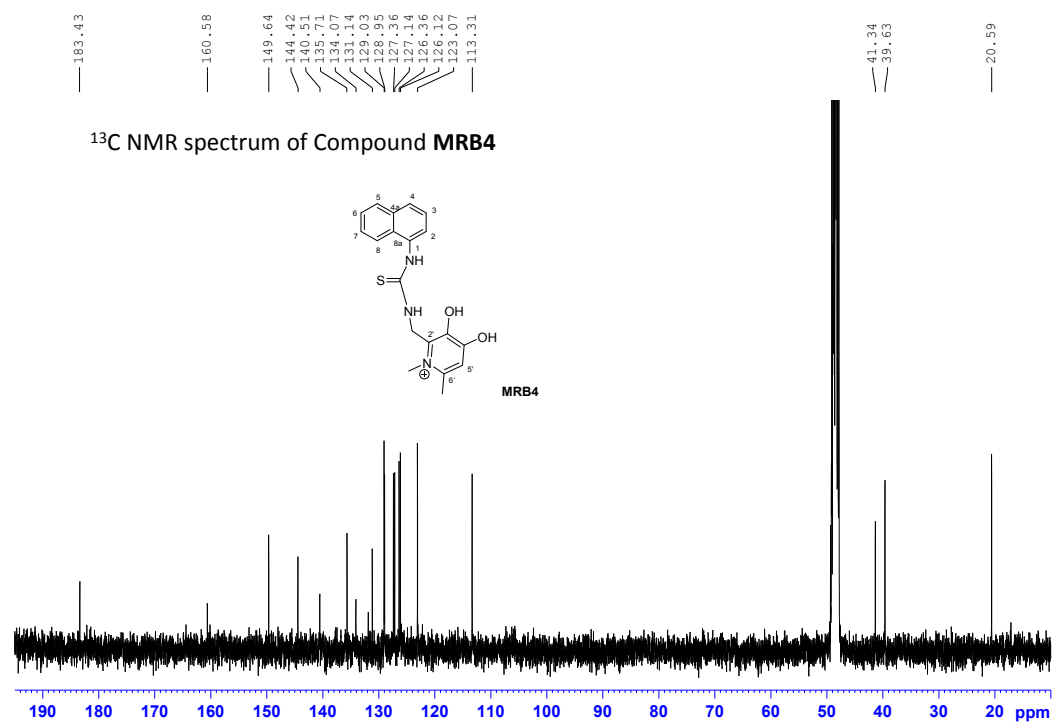


Figure S8. 400.15 MHz ¹³C spectrum of compound MRB4.

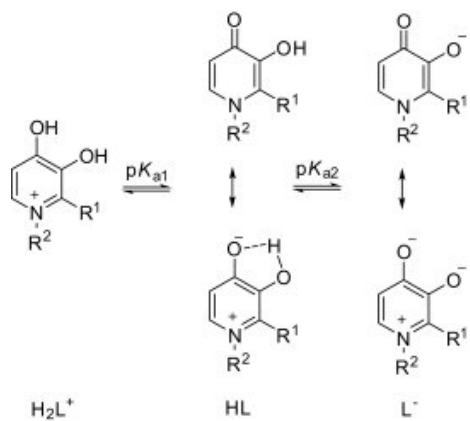


Figure S9. Dissociation equilibria of 3,4-HPO chelators in aqueous solution.

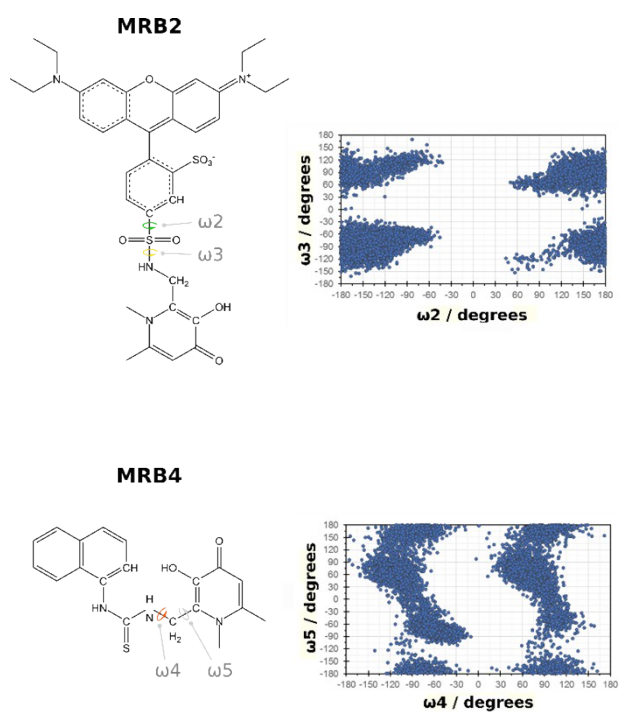


Figure S10. 2D maps of the dihedral values of the two most flexible torsions for compounds MRB2 and MRB4, along the MD simulations.