NMR can be used as an analytical tool for determining enantiomeric excesses of chiral molecules with use of a suitable chiral chemical shift agent. In this work we study determination of enantiomeric excesses of Ibuprofen (guest molecule) with non-chiral porphirinogen DiBrBzOxP (host molecule) using ^{1}H-NMR spectroscopy, and we report the mechanism of this phenomenon.
Method is based on a formation of host-guest complex of chiral guest with achiral host signaling chiral information. This complex formation cause splitting of DiBrBzOxP's β-proton NMR resonances linearly with enantiomeric excess of the Ibuprofen. NMR studies also revealed that water acts as a inhibitor for complex formation. Considering this inhibition properties of water, association constant of DiBrBzOxP with Ibuprofen using NMR titration was determined $K_a = 6.02 mol/l^{-1}$. To understand the binding mechanism of complex, DFT computations have been performed. M06-L/6-31G(d,p) revealed two stable conformers for this complex. To verify that found structures correspond to reality, their GIAO/M06-L/6-31++G(d,p) calculated chemical shift tensors were compared to experimental values. SVD analysis of UV/vis and Raman analysis of DiBrBzOxP titrated with trifluoroacetic acid revealed existence of three different protonated forms, that might have different association constants for Ibuprofen complex.