NMR as a tool for simultaneous study of diasteroisomeric inclusion complexes, part 2: Complexes formed by racemic mixture of 4?- hydroxyflavanone and two cyclodextrins

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Complexes formed by (±)-4?-hydroxyflavanone (OHFL) and the cyclodextrins ?-cyclodextrin and (2-hydroxypropyl)-?-CD were obtained using the racemic mixture of the OHFL. These complexes were able to be studied due to their enantiodifferentiation by 1H-NMR spectroscopy. Stoichiometry, association constants and thermodynamic parameters were obtained from these NMR data, and inclusion geometries were proposed from ROESY spectra. The results show a 1:1 stoichiometry, K a values decrease with increasing temperature, a spontaneous and exothermic complexes formation, and that ROESY spectra cannot differentiate between enantiomers, and therefore the estimated inclusion geometries were proposed for the mixture of diasteroisomeric complexes.