

NMR as a tool for simultaneous study of diastereoisomeric inclusion complexes formed by racemic mixture of 4'-hydroxyflavanone and heptakis-(2,6-O-dimethyl)- α -cyclodextrin

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The complexes formed by (\pm)-4'-hydroxyflavanone (OHFL) and heptakis-(2,6-O-dimethyl)- α -cyclodextrin (DM- α -CD) were obtained using the racemic mixture of OHFL. These complexes were able to be studied due to their enantiodifferentiation by $^1\text{H-NMR}$ spectroscopy. Stoichiometry, association constants and thermodynamic parameters were obtained from these NMR data, and inclusion geometries were proposed from ROESY and docking experiments. The results show that diastereoisomeric complexes can be studied even when they are formed by enantiomeric mixtures. © 2010 Springer Science+Business Media B.V.