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Understanding the principles of diastereomeric complexes of chiral urea derivatives

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The separation processes of chiral compounds attract considerable interest, as it in many cases represents the only way how to obtain chiral catalysts, drugs or their precursors. The effectivity of such separations is usually checked employing HPLC methods using the separation on chiral phase. These methods are time and solvent consuming and in many cases are not capable bringing acceptable results. Especially when dealing with carboxylic acids, amines or alcohols, the appropriate separation method is not always readily accessible.

On the other hand, the enantiomers of such compounds can be visible by MNR, when using NMR shift reagents. The urea derivatives are capable of hydrogen bonding towards free electron pairs of the heteroatom present in the chiral substrate leading to the formation of diastereomeric complexes. The understanding of the structure and principles of formation of these complexes gives rise to widely useful methodologies of checking the percentage of individual enantiomers of the substrate.

The main target of this work based on the NMR studies is to elucidate the structural principles which are responsible for the action of the chiral selectors at hand, and thus to be able to predict the new promising structures useful as NMR shift reagents.

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