Chiral Recognition of Derivatives Based on the Ergot Alkaloid Terguride

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Intermolecular forces have always been object of interest, but, how they act, in concert, to discriminate between molecules, has been increasingly studied with the development of the concept of molecular recognition. An aspect of molecular recognition is chiral recognition. Here molecules are not expected to differentiate on the basis of physicochemical properties. They can only be discerned when they give rise to slightly different diastereomeric interaction once they associate with another chiral molecule. Chiral recognition is the basis of chiral chromatography. In fact, liquid chromatography requires a chiral stationary phase that interacts in an enantio- discriminative way with passing analyte in the mobile phase. The enantioselective absorption can be fairly understood, when the nature of the interactions between the species involved can be specified.

Here, the forces, that occur in the formation of the molecular complex between the selector and the more retained enantiomer of the analytes, are investigated from combining chromatographic studies and the analysis of structures in the solid state. This method is employed to derive a model of discrimination for the chiral selector (5*R*,8*S*,10*R*)-N1-allyl-N2'-diethyl-terguride, **1**, and for the analogous derivatives N2'-dimethyl, **2**, and N2'-diisopropyl, **3**, since they show different efficiency in the separation of racemates of the same classes of carboxylic acids. The crystal structures of the molecular complexes **1**/(**S**)-dansyl-tryptophan and **3**/(**S**)-naproxen will be discussed with other complexes to determine the differences in the mechanism of the enantiodiscriminative process.

Keywords: crystal structures, molecular complexes, chiral recognition