Studying of chiral recognition mechanisms using experimental and theoretical methods

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This research aims to study the mechanisms of chiral recognition based on chiral substances and chiral selectors, particularly cyclodextrins. Since chiral recognition is based on intermolecular interactions, studying its recognition mechanisms requires multifaceted approaches and various research methods. One of the methods is capillary electrophoresis, which allows us to study the affinity of enantiomers of substances for cyclodextrin. In addition, the study allows us to determine the structure of the complex in solutions, which is possible with nuclear magnetic resonance spectroscopy, in particular, ROESY (Rotating-frame nuclear Overhauser Effect Specroscopy). Thus, the methods used allow us to obtain complementary information about the selector-selectand. On the one hand, through capillary electrophoresis, we establish that enantioselective interactions (chiral discrimination) occur, and through nuclear magnetic spectroscopy, we understand what determines this discrimination. [1] In this study, the binding of some basic drugs to cyclodextrins by electrophoresis was studied.

References

[1] B. Chankvetadze, *J. Chromatogr A*,1567 **2018**, 2-25