It is well known that the biological properties of compounds are directly related to the configuration of their stereogenic centers. Therefore, the determination of the compound spatial structure, including its configuration, is crucial for better understanding of the mode of action of bioactive compounds and the design of new drugs. The nuclear Overhauser effect has been shown to be highly useful in NMR spectroscopy for characterizing and refining organic chemical structures. However, the results are not always conclusive.

During the presentation the most common problems associated with the acquisition and interpretation of NOE data will be discussed. Other alternative measurement parameters (chemical shifts and coupling constants $J_{\text{HH}}$), which are usually neglected when assigning configuration, will be presented. Also RDS (residual dipolar coupling) measurements, that are an alternative to NOE measurements, will be briefly explained.

The second part of the presentation will be devoted to determining the relative configuration of $\beta$-lactams. Recently we have found that the assignment of relative configuration at the bridgehead carbon atom of bicyclic carbapenams can be easily achieved by analyzing chemical shifts of the geminal protons of the methylene group at the C-3 carbon atom. This observation can be attributed to the influence of the anisotropy of the neighboring carbonyl group and can be easily correlated with the configuration at the bridgehead carbon atom.

The study showed that the proposed simple relationship can also be used for other azabicyclic compounds.

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References:


The form of presentation proposed by the Author:
oral (15 min)