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Structure Elucidation of Bioactive Compounds by Means of Circular Dichroism Spectroscopy

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It is well known that the biological properties of bioactive compounds are closely related to their stereostructure as well as their physicochemical and chemical properties. Thus, the development of practical methods allowing for the unequivocal and reliable determination of the absolute configuration is actively researched. The high level of interest in this subject is, not withstanding the other reasons, related to the fact that the enantiomers of a particular bio-active compound may demonstrate differences of up to several orders of magnitude in their pharmaceutical effects and potency at the same receptor. The fact that one of the enantiomers is usually more active than its counterpart, which may even be toxic, necessitates the need to use enantiomerically pure products to avoid adverse effects. In this context, the chiroptical methods and the circular dichroism (CD) spectroscopy specifically, appear to be sensitive, fast, and convenient methods for the stereochemical assignment provided that the compounds studied are chiral and non-racemic. During the present lecture, the most recent results on the application of electronic circular dichroism spectroscopy in the structure elucidation of a broad variety of important bioactive compounds will be presented. The scope of the present lecture includes, among others, β-lactam antibiotics, amino acids, amino alcohols, vitamins, and carbohydrates. For the representative derivatives, the CD spectra computed applying the time-dependent density functional theory (TDDFT) will be compared to the experimental CD curves. The high sensitivity of the CD spectroscopy to the minor structural changes will be demonstrated.