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***Application of mass spectrometry in the characterization
of selected chiral heterocyclic compounds***

Mass Spectrometry (MS) is one of the most commonly used and the most universal analytical methods applied in the chemical analysis. The exact molecular weight of a chemical compound, obtained by this method is necessary, not only in compound characteristic but, mainly in determine of unknown compounds structures, establishing the qualitative and quantitative composition of the mixtures. The increasing of the sensitivity and resolution of the instruments, as well improvement in the data analysis, has opened new dimensions in description of complex organic and inorganic systems.

The aim of my PhD thesis was characterization of small bioorganic molecules by MS, mainly derivatives of diethyl 1,2-diaminoalkylphosphonates, oxazolidinone and short peptides. A common feature of selected systems is the presence of the heterocyclic ring in the structure of which has at least one asymmetric center.

The literature part of my PhD thesis describes the possibilities of application of modern MS techniques. In this part of dissertation the most important ionizations techniques, mainly applied to characterization of the chiral compounds are reviewed. Different types of analyzers are reported. The main chapter is devoted to the methods of distinguish the enantiomeric compounds. The analysis of this kind of compounds is a great challenge for other spectroscopic techniques and may lead to many difficulties. At the end, the possibilities of application of the modern MS in distinguish of diastereoisomers structure was presented. This chapter contains the complete introduction to the exploration the diastereoisomers which is the main theme of my dissertation.

My studies proved, it was apparent that mass spectrometry is powerful technique for differentiating the diastereoisomers of diethyl 5-substituted (2-thioxo-imidazolidin-4-yl)phosphonates, which can be regarded as masked diethyl 1,2-diaminoalkylphosphonates. I

have confirmed that computational chemistry is a useful, complementary tool for mass spectrometry studies. This method gives the additional insight into the MS-type fragmentation.

Azides belong to the group of highly reactive compounds. Chiral azides can not be easily characterized by spectroscopic methods. During the course of my thesis, I showed that the mass spectrometry is an excellent technique for this kind of analysis.

The last part of my studies demonstrated the exceptional usability and complementarity of mass spectrometry with other instrumental methods, such as *Solid State Nuclear Magnetic Resonance* (SS NMR), during the evaluation of reaction products in the thermal decomposition of short peptides in the solid phase (2,5-diketopiperazine). The mechanism of the formation of diketopiperazine was also described.

The results of my studies showed that mass spectrometry is a very attractive and outstanding analytical method that can be used for elucidation of many research problems which are difficult to solve by standard techniques.