THE WORLD OF PEPTIDES VIEWED THROUGH SOLID STATE NMR SPECTROSCOPY WINDOW

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Short peptides have recently attracted increasing attention in biology, chemistry of new materials, and medicine due to their specific features. The wealth of possible applications, the complexity of the systems studied and the need to understand the correlation between structure, dynamics and functions have prompted many research groups to seek universal analytical tools that provide maximum information with minimum effort. One of such instrumental technique that comes close to fulfilling these requirements is solid state NMR spectroscopy. The advantage of solid state NMR spectroscopy is that specific structural and dynamic aspects can be accurately described by using different pulse sequences and different viewing windows.

In the first part of the MMCE paper, the usefulness of tripeptides as standards for the developing of new NMR sequences will be briefly discussed. In particular attention will be paid to the problem of local molecular motion analysis, in particular for aromatic residues.

The second part will be devoted to demonstrating the power of solid-state NMR spectroscopy in the analysis of supramolecular structures formed by self-assembling peptides. Currently, there is an increasing interest in the use of self-organizing peptides in the development of new types of soft matter, such as hydrogels and organogels. Gelation and crystallization processes are intertwined, yet it is still not clear in what way. In this work, the attention is focused on understanding the relationship between these two phenomena with an aim to deliver a rational explanation for the fact of distinct behaviour of two cTyrTyr (cYY) diastereoisomers.

In the final part, we will present a unique and very effective approach for peptide cyclization in the condensed matter, a method combining the achievements of mechanochemistry and the topochemical concept. The progress of mechanosynthesis is controlled by advanced solid state NMR spectroscopy. The power of the method is proved with the use of four linear peptides Tyr-(D)Ala-Phe-Gly (signal sequence of neuropeptide Dermorphin), Tyr-Pro-Phe-Phe-OH (analogue of neuropeptide Endomorphin-2), ProPheProPhe·HCl and O-Benzyl derivative of Tyr-(D)Ala-Phe-Gly. Each of the used peptides adopts in the solid state a pseudocyclic conformation that meets the topochemical criteria allowing for the formation of new peptide bonds and the synthesis of cyclic compounds.

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