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BOOK OF ABSTRACTS

Studies on the Conformational Transitions in Flexible Systems of Peptides

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Reaction paths (RPs) leading to conformational transitions in flexible molecular systems (e.g. peptides) are important in the characterization of the most stable conformations and in the determination of the height of the transition barrier. One of the methods for studying such transitions is a molecular dynamics calculation. The other possibility is to find the RP on the potential energy sur (PES). Recently, two main global curve-variational methods are available for generating RPs on PESs. The one is an algorithm modified by Czerminski and Elber [1], and the other is the DDRP method [2]. PESs of the conformational transitions of di-, tri-, tetra-peptide models and small peptide fragments were generated by different force fields. RPs of the conformational transitions were studied by the two methods with the procedure given in Ref.[1] implemented in the program package TINKER [3] and the results were compared to those obtained by the DDRP method [2] interd with a molecular mechanics program used in Ref. [3]. [1] R. Czerminski and R. Elber, Proc. Nat. Acad. Sci. USA, 1989, 86 6963. [2] M.I. Bán, Gy. Dömötör and L.L. Stachó, J. Mol. Struct. (Theochem), 1994, 311, 29. [3] J.W. Ponder, TINKER: Software Tools for Molecular Design, Version 3.6, 1998.