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A Conformational Exploration of Dissymmetric Macrolides Antibiotics

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Abstract: Conformational analysis of the macrolides from 12 to 22 links was carried out using molecular mechanics. Calculations indicate that each studied macrocycle presents eight families of preferential conformers. They result from the combination of the conformations of the two systems diene and α ,β - unsaturated ester. Among these conformers three families (F5, F6 and F3) have the lowest energy. The two families F5 and F6 adopt an s-cis conformation of the ester function and s-trans of the diene system with a pseudo-parallel arrangement of the two systems for the first family and a pseudo-antiparallel for the second. The third family F3 presents a s-trans conformation for the two systems. An important stereoselectivity of the complexed macrocycles was obtained.

Key Words: macrolide, molecular mechanics, conformational analysis, and tricarbonyliron.

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