KONFORMACIJSKA ANALIZA DISUPSTITUIRANIH
FEROCENSKIH PEPTIDA
CONFORMATIONAL ANALYSIS OF THE
DISUBSTITUTED FERROCENE PEPTIDES

Ivan KODRIN,1 Zlatko MIHALIĆ,1 Jasmina LAPIĆ2 and Vladimir RAPIĆ2
1Laboratory of Organic Chemistry, Faculty of Science, University of Zagreb,
Horvatovac 102a, 10000 Zagreb, Croatia
2Faculty of Food Technology and Biotechnology, Pierottijeva 6, 10000 Zagreb, Croatia

Ferrocene peptides have many conformers due to the internal rotations about single bonds and rotation of the cyclopentadienyl rings with the respect to the Cp-Fe-Cp axis.[1,2,3] In this study we present the results of the detailed conformational analysis of previously synthesized asymmetrical 1,1'-disubstituted ferrocene peptides of the MeCO-Fn-CO-AA-XMe ester and amide type (Fn=ferrocene-1,1'-diyl; AA=l-α-amino acid, Gly, Ala or Val, R=H, Me or i-Pr; X=O, NH).

We have conducted a full conformational space search of the studied compounds using different variants of the Monte Carlo method and force fields not necessarily parameterized for the ferrocene moiety. Thus obtained structures served as starting geometries for further energy minimizations at quantum-mechanics level of theory. The resulting Boltzmann distribution of conformers in vacuum, chloroform and DMSO, together with analysis of the general structural characteristics of the most stable conformers, provides some new insights into the intramolecular interactions in these compounds, as well as their relative importance for overall conformers stability.