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Spatial structure of peptides determined by residual dipolar couplings analysis

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Abstract

The gated decoupled 13C NMR spectra of a dipeptide (Glu-Trp) and a tetrapeptide (NAc-Ser-P-e-Val-Gly-OMe) were recorded in D2O and in a lyotropic alignment medium (pentaethylene glycol monododecyl ether/n-hexanol). The residual dipolar couplings were extracted as the differences between the observed couplings for the magnetic nuclei dissolved in the latter and former media. Using a computational optimization, the spatial structures of the compounds were calculated starting from their respective low energy conformations obtained on a semiempirical basis. The uniformity of each conformation was confirmed by the solid-state 13C NMR spectra of powder samples. Differences between the starting structures and final ones, optimized when employing residual dipolar couplings, are discussed. Copyright © 2008 John Wiley & Sons, Ltd.

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Keywords

13C NMR, Lyotropic medium, NMR, Oligopeptides, Pentaethylene glycol monododecyl ether (C12E5), Residual dipolar couplings, Spatial structure