

^1H -NMR and ^{13}C -NMR investigation of complexes of Mn^{2+} with oxytocin analogues in $(^2\text{H}_6)$ dimethylsulfoxide.

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Streszczenie

Several oxytocin analogues were synthesised by substitution of the Pro residue with sarcosine or *N*-methylalanine, the glutamine residue with threonine and one of the cysteines with 2-mercaptopropionic acid. All the derivatives were investigated by NMR in dimethylsulfoxide solutions and evidence was obtained for similar preferred conformations in the solution free state. All peptides were shown to form complexes with Mn^{2+} in solution by the strong paramagnetic effects experienced by several proton resonances. Two structures could be determined, one formed by peptides containing threonine and the other by the remaining peptides. The two structures were delineated by molecular modelling using the Mn^{2+} -proton distances obtained by NMR as restraints.

Słowa kluczowe

oxytocin analogue, manganese(II), NMR, relaxation

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