

Conformation of Luteinizing Hormone Releasing Hormone as Studied by ^1H NMR

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NMR studies on the structure of the luteinizing hormone releasing hormone (LHRH) in aqueous buffer and trifluoroethanol (TFE)/aqueous buffer (1:1, v/v) solution were performed. The NMR data under these conditions suggested a unique conformation which includes a β -I turn of the Tyr5-Arg8 segment and an unusual turn of Ser4-Gly6 segment staggered with the β -I turn. The Arg8-Gly10 region is in an extended form. This conformation was most stable in TFE/aqueous buffer at pH 7. Restrained molecular modeling calculation showed that the N-terminal pGlu1-Ser4 region forms an additional bend, making the overall feature of the pGlu1-Arg8 region helical. In this conformation, the apolar side chains of Trp3 and Leu7 are located in close proximity and they are apart from the polar side chains.