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Conformational Analysis of Linear Peptide (Glu^1-Leu^2-Leu^3-Gly^4-Gly^5-Arg^6-Phe^7NH_2)

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Abstract: Conformational energy-minimization of the Sea Anemone and Sea Pansy neuropeptide Pol-RFamide (Glu^1-Leu^2-Leu^3-Gly^4-Gly^5-Arg^6-Phe^7-NH_2) was carried out by molecular mechanics (MM). The linkage bonds were characterized by the torsion angles θ, ψ and ω and the side groups were characterized by the torsion angles χ_1, χ_2, χ_3\ldots The energy-map for each monopeptide of the Pol-RFamide I was drawn in the range of -180° to 180° with increments of 20°. Conformation facilities for monopeptides were determined from these maps. These results were used in the analysis of the dipeptide (Glu^1-Leu^2). Then, the (Glu^1-Leu^2-Leu^3) tripeptide was examined using the calculated results for the dipeptide. Conformational analysis of the (Glu^1-Leu^2-Leu^3-Gly^4) tetrapeptide was performed using the low-energy values for the tripeptide. The space structure of the (Glu^1-Leu^2-Leu^3-Gly^4-Gly^5-Arg^6-Phe^7-NH_2) neuropeptide was found as a result of minimization of energies by rotating the tetrapeptide (Glu^1-Leu^2-Leu^3-Gly^4) and the dipeptide (Arg^6-Phe^7-NH_2) about the monopeptide (Gly^5).

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