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Conformational Analysis of Pol-Rfamide II (Glu}^{1}-Trp^2-Leu^3-Lys^4-Gly^5-Arg^6-Phe^7-NH_2) Heptapeptide

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Abstract: The geometrical structure of the sea anemone and sea pansies neuropeptide Pol-RFamide II Glu^1-Trp^2-Leu^3-Lys^4-Gly^5-Arg^6-Phe^7-NH_2 was carried out by molecular mechanics (MM). The linkage bonds are characterised by the torsional angles ϕ, ψ and ω and the side groups characterised by the torsional angles χ_1, χ_2, χ_3,... subsequently. The energy-map for each monopeptide of the Pol-RFamide II was drawn in the range of -180° to 180° with increments of 20°. Conformation facilities for monopeptides were decided from these maps. These results were used in the analysis of the dipeptide Glu^1-Trp^2. Then, the Glu^1-Trp^2-Leu^3 tripeptide was examined by using the calculated results for dipeptide. Conformational analysis of the Glu^1-Trp^2-Leu^3-Lys^4 tetrapeptide was performed using the low-energy values of the tripeptide. The geometrical structure of Glu^1-Trp^2-Leu^3-Lys^4-Gly^5-Arg^6-Phe^7-NH_2 neuropeptide was determined by rotating the tetrapeptide Glu^1-Trp^2-Leu^3-Lys^4 and the dipeptide Arg^6-Phe^7-NH_2 about the monopeptide Gly^5 due to the minimisation of energy.

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