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Poster presentation

Molecular dynamics simulations studies of aurein 1.2 analogs in water and TFE/water

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Aurein 1.2 is an antimicrobial and anticancer peptide isolated from an Australian frog [1]. The structural properties of aurein 1.2 analogs, a small alpha helix peptide, are studied in water and TFE/water by molecular dynamic simulations. A series of 10 nanosecond molecular dynamics simulations have been performed on F13G analog of aurein 1.2 and retro analog aurein 1.2 in water and TFE/water. F13G analog exhibits a higher variation in its conformation than the native peptide. The importance of F13 of aurein 1.2 is further supported by our molecular dynamic simulations. The alpha helical conformation of the peptide is decreased through the 10 ns duration of the simulation in retro aurein 1.2.different extents of variability in the conformation exhibited by the retro and the native peptides, imply heterogeneous conformation propensities for the two peptides it is possible that the retro analog of aurein1.2 might not be functionally active. These results imply that positive charges, negative charges and hydrophobic residues are critical.

References

1. Rozek TL, Wegener KL, Bowie JH, Olver IN, Carver JA, Wallace JC, Tyler MJ: **The antibiotic and anticancer active aurein peptides from the Australian Bell Frogs Litoria aurea and Litoria raniformis.** *Eur J Biochem* 2000, **267:**5330-5341.