# Angular dynamic simulates incorporation of peptides into implicit lipid bilayer

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The Monte-Carlo procedure and Molecular Dynamics (MD) are used to model interactions between membrane lipids and peptides, proteins or drugs and reveal how structures change when they insert and try to match themselves up with the different membrane areas. Instead of these classic approaches, respectively too simplified and too time consuming, we performed *in silico* insertion of peptides in implicit lipid bilayers, using an Integral Membrane Protein and Lipid Association (IMPALA) program[1]. The program includes two powerful new features: first, the Charge Potential (CP), which takes into account the charge density throughout the membrane and second, the Angular Dynamic Procedure (ADP), which allows the structure to deform during insertion. This method improves the precision of the model and, with regard to the MD, decreases calculation time. With IMPALA-CP-ADP, we rapidly and correctly simulated the insertion and the tilt of peptides with different lengths, charges and structures, in several membranes of different compositions and thicknesses. Our results support experimental data[2,3]. We showed for instance that it is energetically favourable for lysine to plunge their polar heads into a hydrophilic area instead of leaving them in hydrophobic one. Moreover, given the importance of the insertion of several molecules (peptides involved in different diseases for example) in membrane, one realises the importance of being able to rapidly and correctly simulate the insertion and orientation in membrane of any kind of protein or derivative.

1 Ducarme, P., M. Rahman & R. Brasseur, 1998. IMPALA: a simple restraint field to simulate the biological membrane in molecular structure studies, Proteins 30: 357-371.
2 Webb, R. J., J. M. East, R. P. Sharma & A. G. Lee, 1998. Hydrophobic mismatch and the incorporation of peptides into lipid bilayers: a possible mechanism for retention in the Golgi, Biochemistry 37: 673-679.
3. Bechinger, B., Zasloff, M., and Opella, S.J, 1998. Structure and dynamics of the antibiotic peptide PGLa in membranes by solution and solid-state nuclear magnetic resonance spectroscopy. Biophysical Journal 74: 981-987.