The induction and stabilization of transmembrane pores by peptides

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Atomistic molecular dynamics simulation techniques have been used to examine the interaction of a range of pore-forming and cell-penetrating peptides with lipid membranes. Such systems are archetypical examples of self-organizing molecular systems leading to functional complexes. In general it had been assumed that the structured formed were highly regular. However, simulations of the spontaneous induction of transmembrane pores by the antimicrobial peptides Magainin and Melletin suggest that the pores are at least initially highly disordered casting doubt on the validity of current models (Leontiadou, Mark & Marrink, 2006; Sengupta *et al.*, 2008). In contrast in the case of the cell-penetrating peptides Penetrin and the TAT-peptide no spontaneous formation of transmembrane pores was observed. Instead, the simulations suggest that the peptides may enter the cell by micropinocytosis, whereby the peptides induce curvature in the membrane, ultimately leading to the formation of small vesicles within the cell that encapsulate the peptides (Yesylevskyy, Marrink & Mark, 2009).

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