

EXPLORING THE EFFECT OF ANAESTHETIC GASES ON BIOMEMBRANES

LORNA M. STIMSON^{1*}, ILPO VATTULAINEN², TOMASZ RÓG¹
and MIKKO KARTTUNEN¹

¹Biophysics & Statistical Mechanics Group, Laboratory of Computational Engineering, P. O. Box 9203, FIN-02015 Helsinki University of Technology, Finland, ²Laboratory of Physics, P.O. Box 1100, FIN-02015, Helsinki University of Technology, Finland

General anaesthetics are able to induce a reversible loss of consciousness and response to painful stimuli. Molecular species from simple mono-atomic xenon gas to much larger and more complex structures may be potent general anaesthetics. In this work, we aim to investigate the hypothesis that general anaesthetics cause disruptions in the cellular membrane that are responsible for the anaesthetic effect [Eckenhoff, R.G. **Mol. Interv.** 1 (2002) 258]. It has been shown that such changes in the lipid bilayer cause alterations in the structure and function of embedded proteins. Of particular interest are mechanosensitive channel proteins, for example MscL, which in an open state, allow diffusion of small cations. The diffusion of these ions is fundamental for the control of the potential across the membrane and therefore to the conductance of nerve impulses [Cantor, R.S. **Toxicol. Lett.** 101 (1998) 451]. The initial investigations centre on the effect of xenon gas on the model membranes. We have carried out molecular dynamics simulations of DPPC bilayers consisting of 128 lipid and ~3000 water molecules. Xenon is then introduced into the solvent phase. We observe the rapid penetration of the bilayer by the gas and find that the xenon preferentially occupies the tail region. There is an increase in the area per lipid associated with accommodation of xenon and for highly saturated systems we observe a slight increase in the order of the hydrocarbon chains. Finally we compare our findings with previous studies on the effect of alcohol on bilayers [Patra, M. *et al.* submitted].

* E-mail: lorna@lce.hut.fi, Project homepage: www.softsimu.org