

SHOULD MODEL RESEARCH ON LIPID MEMBRANES TAKE INTO ACCOUNT THE DIPOLE CHARACTER OF LIPID POLAR HEADS?

KRYSTIAN KUBICA

The Department of Physics and Biophysics, Agriculture University, 50-375
Wrocław, Poland, e-mail: kubica@ozi.ar.wroc.pl

Taking into consideration the dipole structure of the polar heads of model membrane molecules, even in a simplified way, allowed ripple phase modeling to be performed [1]. The current model is constructed on assumptions which reflect the real membrane properties much better:

- each molecule modeling a lipid consists of two hydrocarbon chains and one dipole,
- the chain closer to the polar head is shorter by two C-C bonds,
- the chains can assume one of 10 distinct conformations,
- all the molecules can rotate 180° around an axis perpendicular to the membrane surface,
- the whole molecule can move along the normal to the membrane surface to a two C-C bond projection,
- the dipoles can assume one of two tilts: 78° and 30°,
- the dipoles can rotate towards their 6 nearest neighbors,
- the dipoles interact with their nearest dipoles and with the neighbours of the latter.

These assumptions take into consideration environmental aspects: ionic force, dielectric permeability, and temperature.

Only if the dielectric permeability of the membrane polar parts is significantly smaller than the water dielectric permeability does a membrane model not have to take into account the changeability of the tilt between dipoles and the membrane surface. This result becomes especially significant when the dielectric permeability approaches a value of $\epsilon=80$.

REFERENCE

1. Kubica, K. Monte Carlo simulation towards ripple phase modelling. **Computers and Chemistry** 25 (2001) 245-250.