

**Biophysical study on the interaction of model membranes with a nonsteroidal antiinflammatory drug.**

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We combined calorimetry, ESR, ATR-FTIR and molecular docking to study the effects of ibuprofen, a nonsteroidal antiinflammatory drug, on DMPC bilayers. Ibuprofen influences the membrane thermotropic phase behaviour, abolishing the pre-transition, decreasing the main-transition temperature and promoting gel-to-fluid phase coexistence. It loosens the packing of DMPC interfacial region in the gel state and leaves unperturbed the chain flexibility in the fluid state. Ibuprofen also leads to a higher polarhead hydration and favours hydrogen bond formation with solvent molecules. The drug adopts different anchoring modes (interaction energy is about -6 kcal/mol) by binding through non-specific interactions at the hydrophilic/hydrophobic membrane interface.