



# LOCATION OF THE GENERAL ANESTHETICS IN MODEL MEMBRANES

Zreče  
2018

Pavol Hrubovčák  
Tomáš Kondela  
Norbert Kučerka

# Motivation

- **Alkanes** and aliphatic alcohols – **anesthetic** properties
- **Origin** of this behavior – **unknown** by now
- It is supposed that the effect is induced by **interactions** between **constituents** within cell **membrane**
- The **change** of membrane **structure** – significantly affects **functional** properties of membrane
- **objective** – investigate the **influence** of decane molecules on the **change** of membrane **structure**, hence the change of specific functions of biologic membrane

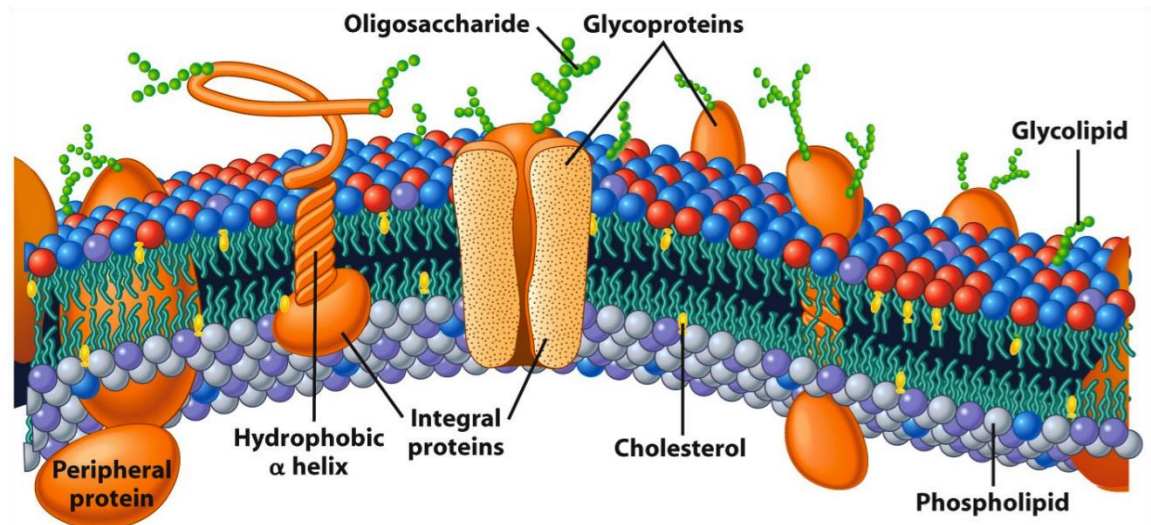
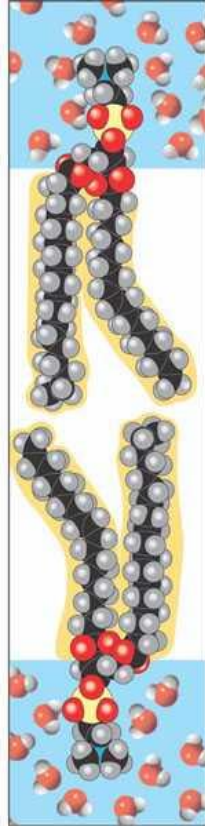
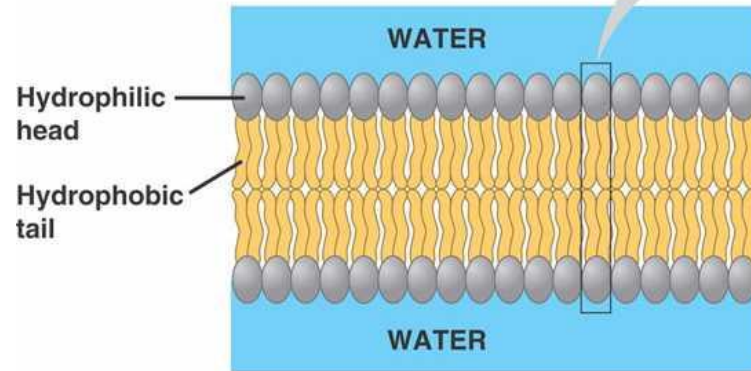
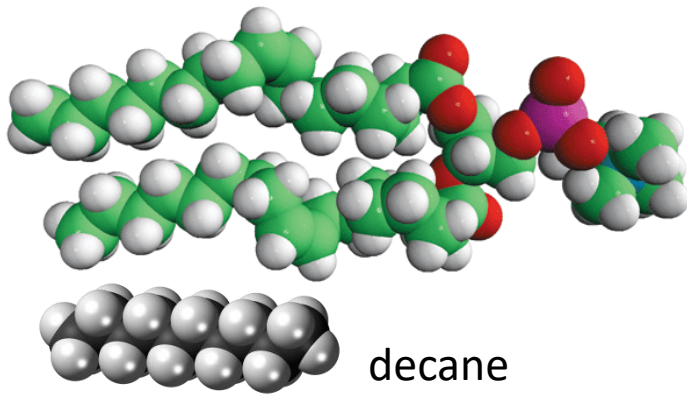


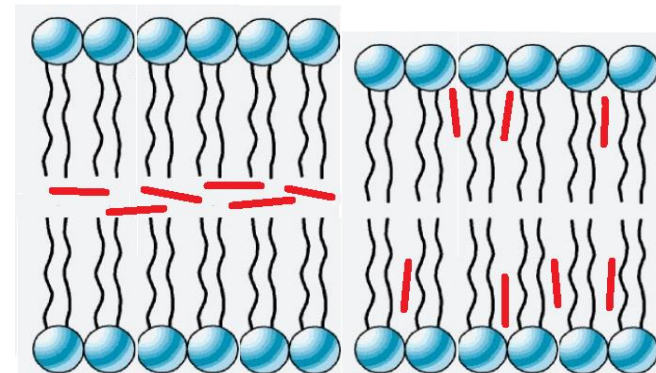
Figure 4-4c Cell and Molecular Biology, 5/e (© 2008 John Wiley & Sons)

# Model of biologic membrane

- Bilayer of phospholipides (amphiphilic molecules)
- DOPC (1,2-**Dioleoyl**-sn-glycero-3-phosphocholine)



- Previous studies show that the concentration of decane in cell membrane affects spatial distribution and orientation of decane molecules
- 2 hypotheses of decane localization
  - **center**; perpendicular to hydrophobic chains
  - **parallel** to chains
- Solution – labeling of decane molecules

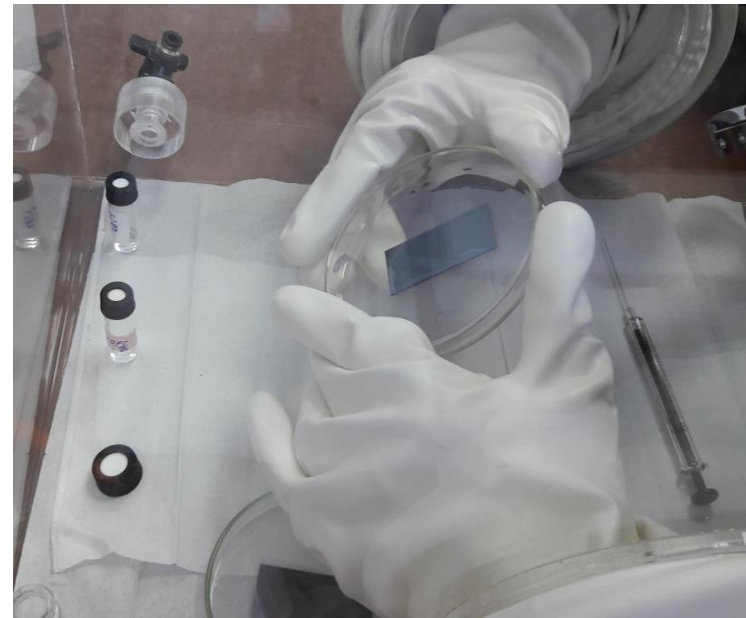


# Samples' preparation

1.) **Solution** of organic solvent with DOPC and decane (homogeneous mixture)

2.) **Deposition** of solution on Si wafer -> Rock & roll method

- solvent evaporation
- regular structure of thousands of parallel bilayers

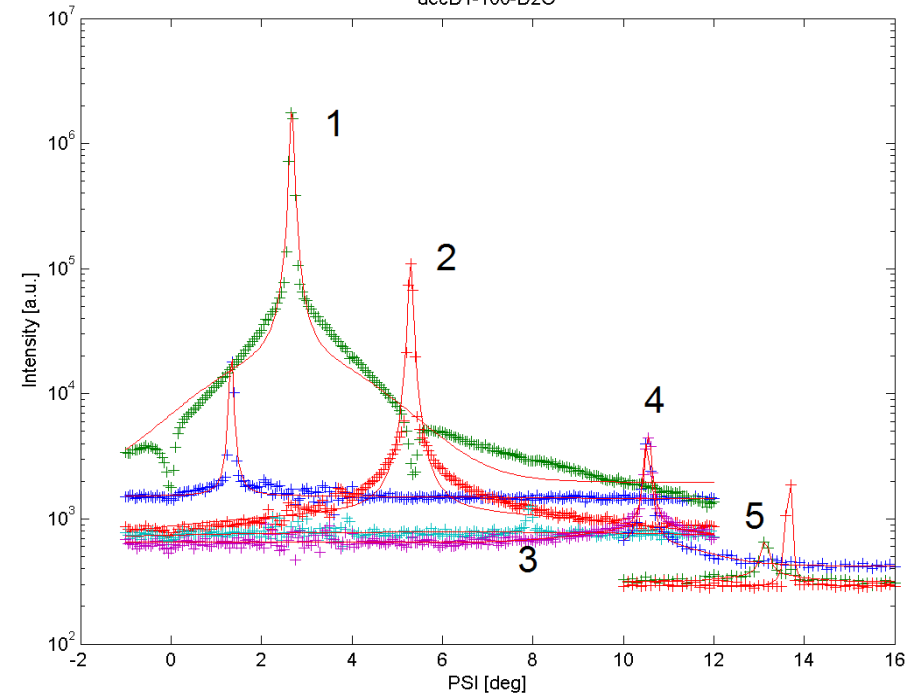
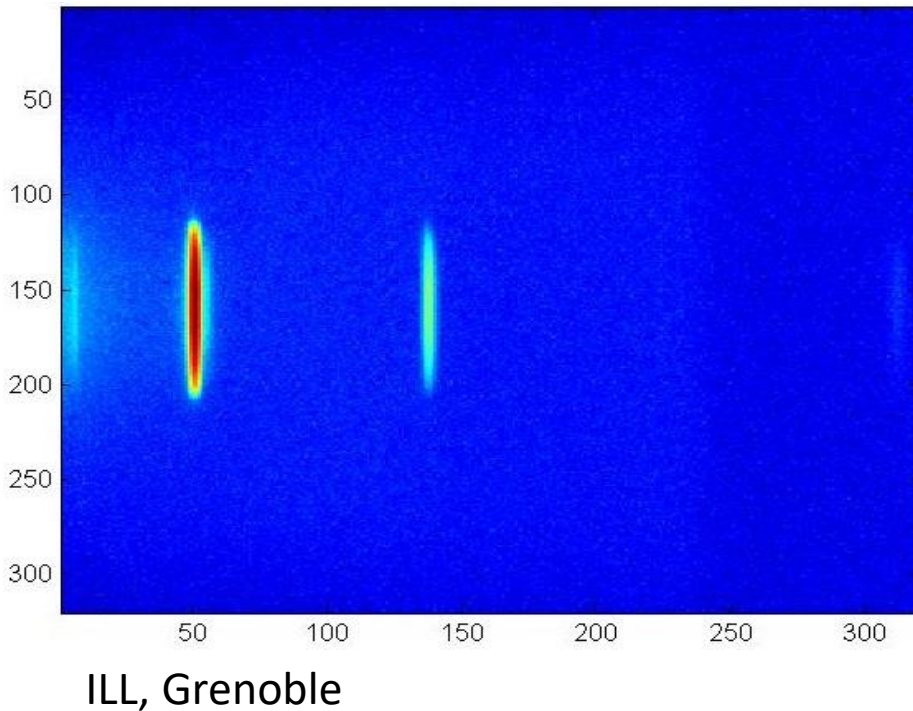
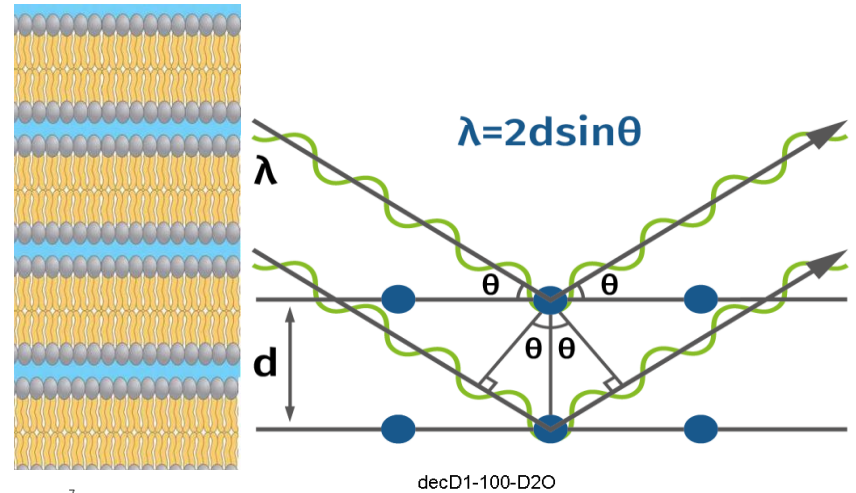


3.) **Hydratation** of membranes

In total: 4 couples of samples (labeled/unlabeled) of different contrast

# Principles of experiment

- multilayers -> **diffraction**
- **neutrons** (Instead of X-ray)
- High quality of samples



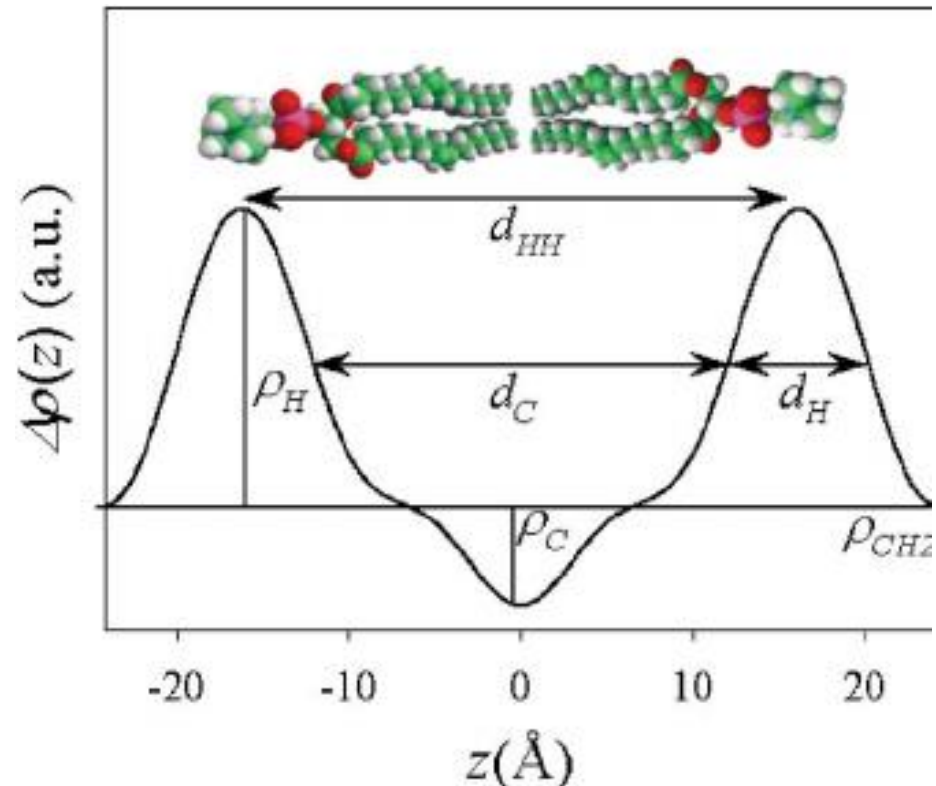
# Bilayer profile

- *Diffraction pattern* -> reconstruction of bilayer profile
- *Relation*  $I(\mathbf{q}) \sim \rho(\mathbf{r})$  scattering length density of unit cell

$\rho(\mathbf{r})$  – characteristic for each particular structure (H<sub>2</sub>O, D<sub>2</sub>O, hydrophilic/hydrophobic DOPC groups, ...)

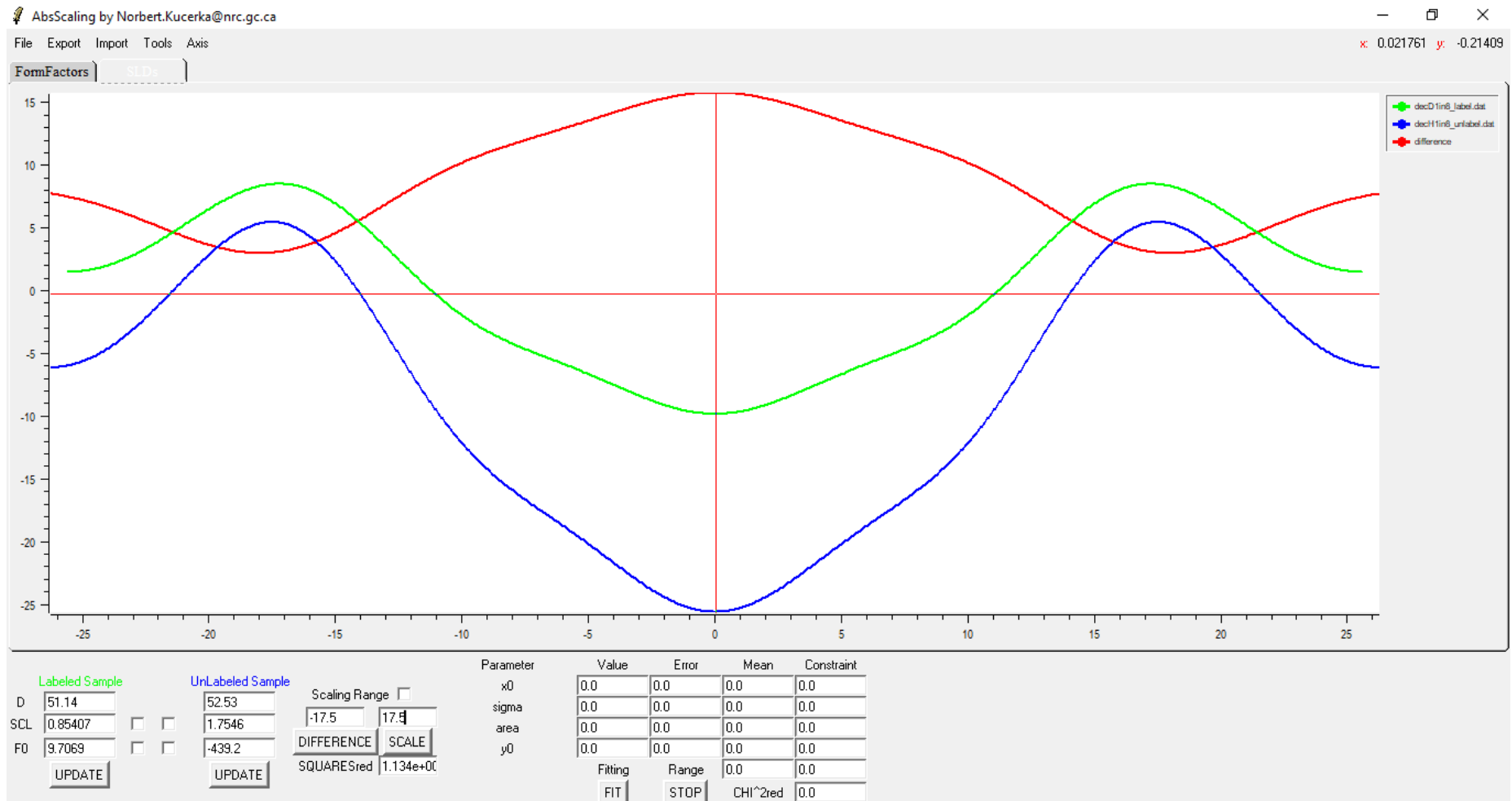


Recognition of positions of different structures



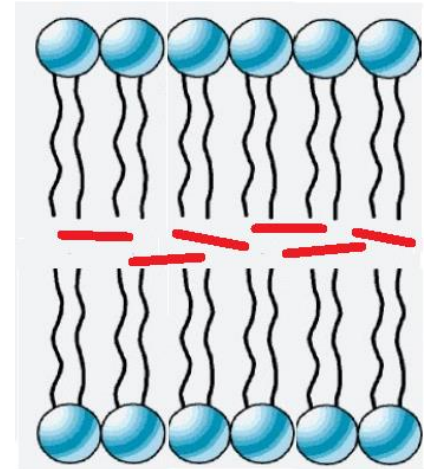
# Profiles of $\rho(r)$ for decane:DOPC 1:1

- Decane localization – **difference** of bilayer profiles containing **labelled** (deuterated) and **unlabelled** decane molecules



# Conclusions

- decane:DOPC 1:1
- decane location – in the center of bilayer
- Corroborated by
  - $\rho(r)$  profiles difference
  - simulations of molecular dynamics



## Further investigation

- Different concentrations of decane (lower/higher) and its influence on molecules' location



Thank you for attention