Bilayers at the ILL 2019, Grenoble, France

Location of the general anesthetics in model membranes

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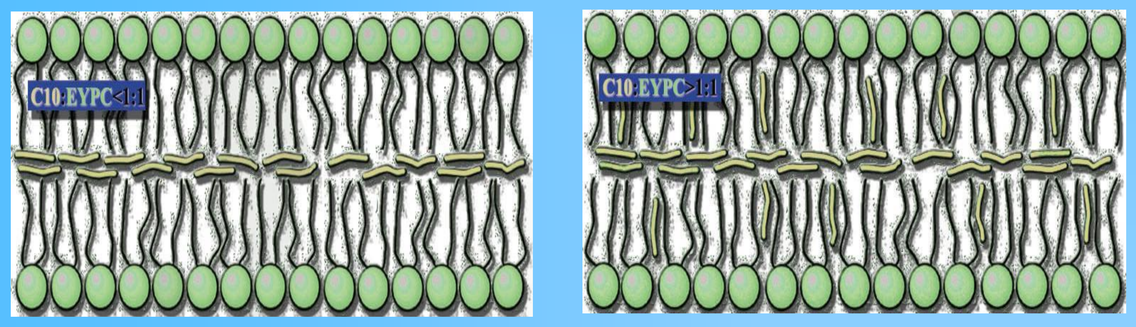
Motivation

alcanes and alifatic alcohols ⇒ anestetic effect
interactions between membrane constituents ⇒ structural changes
correlation: thickness ⇔ functions

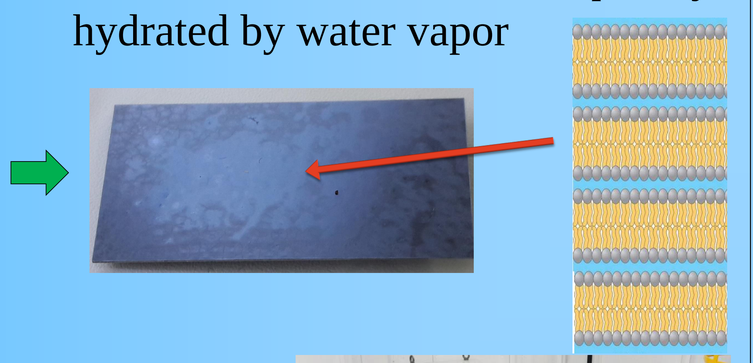


- Assumption: The location and orientation of decane molecules within the bilayer depends on their concentration

Sample preparation

- **n-decane** and **DOPC** mixed in organic solution in two different molar ratios **1:1**, **2:1**
- decane molecules employed: deuterium-**labeled** and **unlabeled**

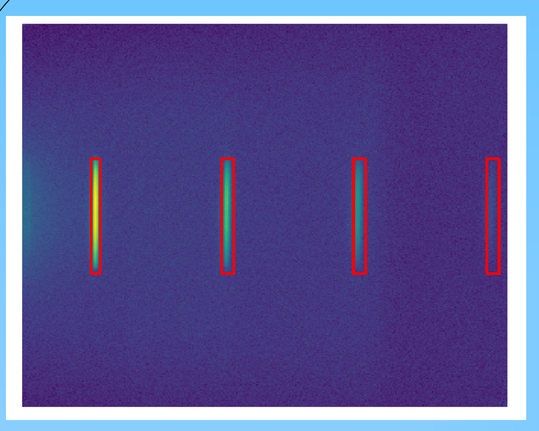
- After the evaporation of the organic solvent, model bilayers were formed and subsequently hydrated by water vapor



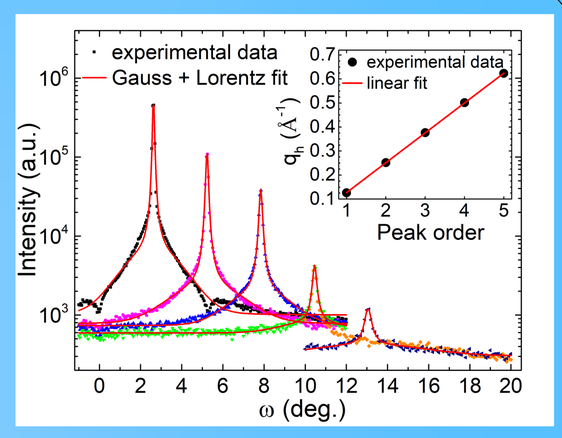
Experiment

- D16 - Small momentum transfer diffractometer, ILL, ($\lambda = 4.55$ Å)
- Samples rocked at fixed detector position
- Four different H_2O:D_2O scattering contrasts utilized

Data evaluation



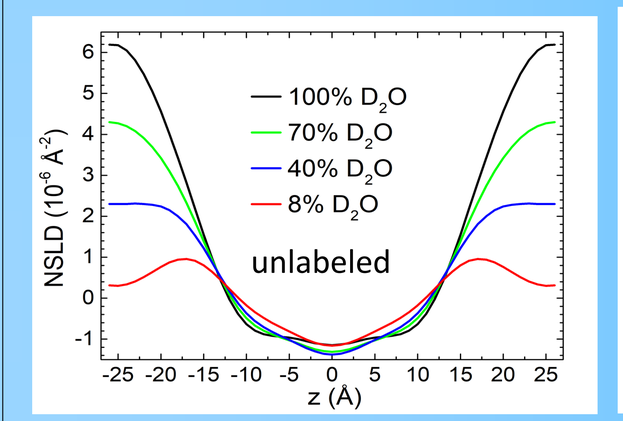
Determination of inter-layer repeat distance (d-spacing) $d = 2\pi n/q$

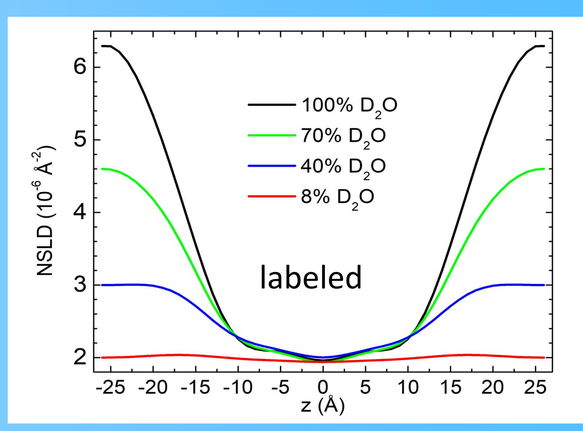


- Fitting the rocking curves to the Gauss + Lorentz function
- Determination of form factor related to the area of the peak

Bilayer profile reconstruction

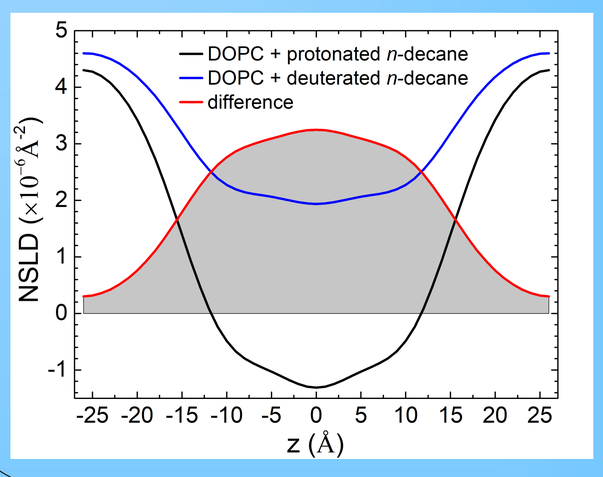
Neutron scattering length density profiles are related to the scattering form factors through their Fourier inversion.





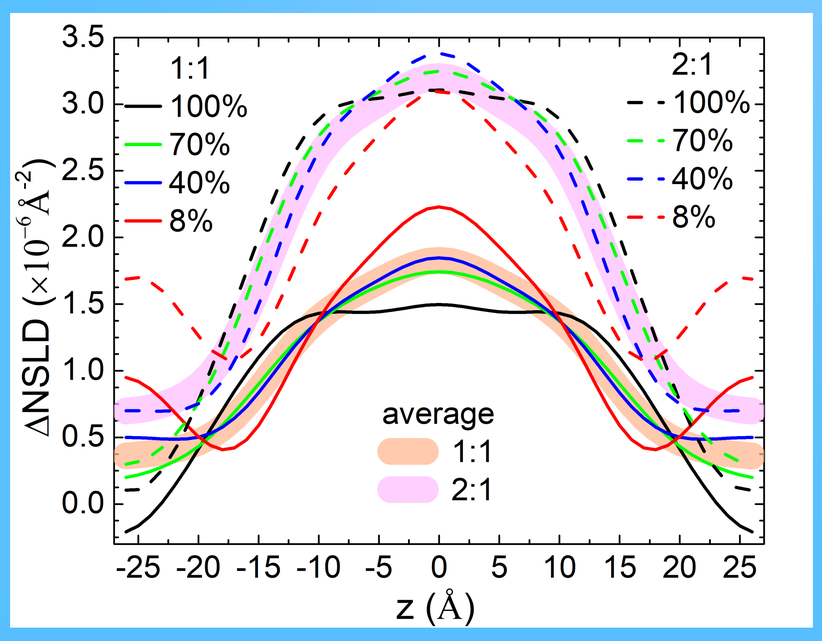
Profiles of bilayer NSLDs corresponding to different H_2O:D_2O contrast variants of system containing unlabeled and labeled n-decane molecules.

Difference of the corresponding NSLD profiles



- Distribution of the label
- Area ~ ammount of the label

Conclusions



- n-decane – located in the hydrocarbon chains, mainly in the centre of bilayer
- No significant change in n-decane distribution when compared systems with 1:1 and 2:1 decane:DOPC molar ratios
- Areas under the curves – correspond to the ammount of label utilised
- Results - supported by molecular dynamics simulations

Acknowledgement

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