Location of the general anesthetics in model membranes

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Motivation
- alkanes and alifatic alcohols
- anesthetic 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
- \textbf{n-decane} and DOPC mixed in organic solution in two different molar ratios \textit{1:1, 2:1}
- decane molecules employed: deuterium-\textbf{labeled} and \textbf{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, (\(\lambda = 4.55 \text{ Å}\))
- Samples rocked at fixed detector position
- Four different H\textsubscript{2}O:D\textsubscript{2}O 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.

Difference of the corresponding NSLD profiles
- Distribution of the label
- Area ~ amount of the label

Conclusions
- \textbf{n-decane} – located in the hydrocarbon chains, mainly in the centre of bilayer
- No significant change in \textbf{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