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Advanced Small-angle Scattering Modeling of Lipid Bilayers: From Symmetric to Asymmetric Membranes

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Cell membranes are complex lipid-protein systems. Their biophysical properties are studied using model membranes, typically symmetric bilayers of a few lipid species. Structural characterization relies on small-angle scattering (SAS), using X-rays (SAXS) or neutrons (SANS), which provide complementary insights. Asymmetric phospholipid vesicles have also been recently investigated [1,2].

SAXS and SANS exploit different contrast mechanisms: SAXS detects electron density variations, while SANS highlights molecular components via isotopic contrast. For large-radius vesicles, both techniques approximate the signal of a planar membrane, representing the Fourier transform of the density profile perpendicular to the bilayer.

The Modified Scattering Density Profile (MSDP) model describes this profile through lipid chemical group distributions weighted by their scattering densities. This approach has been extended to asymmetric membranes, leading to the Asymmetric Scattering Density Profile (ASDP) model. Theoretical aspects and SAS simulations using GENFIT will be discussed [3,4].

[1] F. H. Heberle et al., *Langmuir* 32, 5195 (2016).

[2] M. Doktorova et al., *Nat. Prot.* 13, 2086 (2018).

[3] R. D. Rosa et al., *Biochim. Biophys. Acta* 1860, 2299 (2018).

[4] F. Spinozzi et al., *J. Appl. Crystallogr.* 47, 1132 (2014).