



1. Trajectory containing dodecylphosphocholine (DPC) micelles, clustered using a cutoff and minimum image convention over each frame.

2. Pair distances between each type of atom in DPC, within each cluster. All frames considered part of one equilibrium ensemble. Outputs  $r_{ij}$  histograms for all possible pairs of atom types in DPC.

3. Debye scattering equation which takes  $r_{ij}$  histograms:

$$I(Q)/I(Q_0) = \frac{\sum_{i,j} b_i b_j^* \frac{\sin(Qr_{ij})}{Qr_{ij}}}{\sum_{i,j} b_i b_j^* \frac{\sin(Q_0 r_{ij})}{Q_0 r_{ij}}}$$