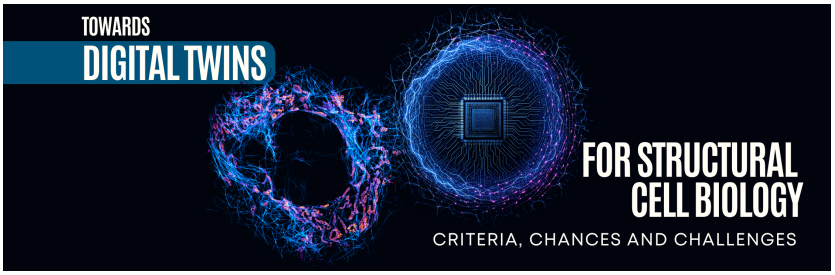

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Combining experiments and molecular simulations

We combine experiments with molecular simulations to learn more about a biomolecular system than we could from the individual methods alone. Ensemble and force-field refinement provide consistent, reproducible, and robust ways to do so. Biophysical experiments like SAXS, FRET, NMR, PELDOR/DEER provide ensemble averaged information. Although valuable by themselves, such information can be of low structural resolution and/or sparse and insufficient to reconstruct high-resolution structural biomolecular ensembles. Understanding of the structural ensemble gives mechanistic insight related to their functions. Molecular dynamics simulations can provide such high-resolution structural ensembles. Balancing force field inaccuracies and sampling errors limits their predictive power, though. We thus combine information from experiments and simulations in two ways. We refine the predicted structural ensembles directly or we refine the underlying force field by learning (atomistic) interactions. Both approaches are valuable tools for learning from experiments, simulations, or any machine learning method providing structural ensembles.

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