Lipid bilayers are essential constituents of living cells enabling cell compartmentalization and affecting membrane protein function. It is therefore important to understand how the molecular structure and dynamics of simple lipid bilayer models are affected by a number of factors, such as the incorporation of molecules of interest in a given bilayer (e.g. other lipids, drugs, peptides or proteins) or by simply varying intensive properties. This presentation will focus on how to use molecular dynamics simulations and solid-state nuclear magnetic spectroscopy in this context, two of the most prominent techniques at present for studying soft matter.