Advanced sampling techniques allow the computational investigation of a range of equilibrium and kinetic phenomena in complex systems. In this talk I will illustrate the application of such methods to the study of dynamics and equilibrium water sorption in protein powders, hydrophobically-induced evaporation near model substrates, and cold unfolding of proteins. The insights gained from these computational studies shed light on the behavior of proteins under extreme conditions (temperature, dehydration). They also provide helpful information for the design of processes for the long-term storage of proteins in pharmaceutical applications, and for the maintenance and repair of biological substrates such as skin or hair.