Complex and evolving structures, often in fluid states, play a crucial role in the pharmaceutical industry. Selecting and combining the right ingredients in the right manner to obtain optimal properties are essential for success given the inherent challenges and a competitive market. With advances in modern simulation techniques and computer hardware, molecular modeling is starting to provide timely and invaluable information that is complementary to experimental characterization. This talk will provide a background on drug formulation challenges that molecular modeling can impact. For both small-molecule and biologics formulations, powerful simulation tools using atomistic or coarse-grained models permit the characterization of molecular interactions and nanoscale structuring, sometimes within otherwise disordered bulk systems (e.g., self-assembly of polymer-based structures, dissolving amorphous solid dispersions, liposomes and protein-excipient interactions). We will present some prototypical studies for both small molecule drugs and biologics.