A number of new molecular entities (NMEs) selected for full-scale development based on their safety and pharmacological data suffer from undesirable physicochemical and biopharmaceutical properties, which lead to poor pharmacokinetics and distribution after in vivo administration. An optimization of the preformulation studies to develop a dosage form with proper drug delivery system to achieve desirable pharmacokinetic and toxicological properties can aid in the accelerated development of these NMEs into therapies. Nanoparticulate drug delivery systems show a promising approach to obtain desirable druglike properties by altering the biopharmaceutics and pharmacokinetics properties of the molecule. Apart from the advantages of enhancing potential for systemic administration, nanoparticulate drug delivery systems can also be used for site-specific delivery, thus alleviating unwanted toxicity due to nonspecific distribution, improve patient compliance, and provide favorable clinical outcomes. This review summarizes some of the parameters and approaches that can be used to evaluate nanoparticulate drug delivery systems in early stages of formulation development.