The computational prediction of binding rate constants (kon and koff) for small molecules and druglike compounds is an active challenge for the molecular simulation community. This cover artwork represents a hybrid molecular dynamics, Brownian dynamics, and milestoning approach for the efficient calculation of these kinetic parameters and the subsequent ranking of compounds based on their kinetics. Depicted is the model host-guest system, ß- cyclodextrin with a series of seven ligands that spanning range of chemical functionalities.