Title (4)	:	**Molecular dynamics-driven exploration of peptides targeting SARS-CoV-2, with special attention on ACE2, S protein, Mpro, and PLpro: A review**
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Abstract	:	Molecular dynamics (MD) simulation is a computational technique that analyzes the movement of a system of particles over a given period. MD can provide detailed information about the fluctuations and conformational changes of biomolecules at the atomic level over time. In recent years, MD has been widely applied to the discovery of peptides and peptide-like molecules that may serve as severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) inhibitors. This review summarizes recent advances in such explorations, focusing on four protein targets: angiotensin-converting enzyme 2 (ACE2), spike protein (S protein), main protease (Mpro), and papain-like protease (PLpro). These four proteins are important druggable targets of SARS-CoV-2 because of their roles in viral entry, maturation, and infectivity of the virus. A review of the literature revealed that ACE2, S protein, and Mpro have received more attention in MD research than PLpro. Inhibitors of the four targets identified by MD simulations included peptides derived from food and other bioresources, peptides designed using the targets as templates, and peptide-like molecules retrieved from databases. Many of the inhibitors have yet to be validated in experimental assays for potency. Nevertheless, the role of MD simulation as an efficient tool in the early stages of anti-SARS-CoV-2 drug discovery agents has been demonstrated.