



## About the Cover

Coronavirus SARS-CoV-2 infects host cells via binding to the cell receptor ACE2 with its spike proteins. Atomistic molecular dynamics simulations reveal that the receptor binding domain (RBD) of spike protein can tightly bind to both open and closed ACE2 receptors, mostly by specific interactions between RBD and ACE2 N-terminal helices. The water molecules residing at the RBD-ACE2 interface play critical roles in stabilizing the complex structure: on average about 15 water molecules are observed at the RBD-ACE2 interface. Some water molecules stay at the interface over 10 nanoseconds, suggesting that the significant contribution to the RBD binding. Engineered ACE2 proteins or peptides can be potential pharmaceutical molecules to interfere the infection of SARS-CoV-2. For details please refer to the article by Lupala et al. in pp. 61–72. We acknowledge Letpub for its professional scientific illustration service.

