Technical Data of In Silico Analysis of the Interaction of Dietary Flavonoid Compounds against Spike-Glycoprotein and Proteases of SARS-CoV-2

ABSTRACT

The spike glycoprotein (S protein), 3-chymotrypsin-like protease (3CL-Pro), and papainlike protease (PL-Pro) of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) virus are widely targeted for the discovery of therapeutic compounds against this virus. Dietary flavonoid compounds were proposed as a candidate for safe therapy for COVID-19 patients. Nevertheless, wet lab experiments for high-throughput screening of the compounds are undoubtedly time and cost consuming. This study aims to screen dietary flavonoid compounds that bind to S protein, 3CL-Pro, and PL-Pro of SARS-CoV-2. For this purpose, protein structures of the receptor-binding domain (RBD) of S protein (6M0J), 3CL-Pro (6LU7), and PL-Pro (6W9C) were retrieved from the RCSB Protein Data Bank (PDB). Twelve dietary flavonoid compounds were selected for the studies on their binding affinity to the targeted proteins by global and local docking. The docking and molecular dynamic (MD) simulations were performed using YASARA software. Out of 12 compounds, the highest binding score was observed between hesperidin against RBD S protein (−9.98 kcal/mol), 3CL-Pro (−9.43 kcal/mol), and PL-Pro (−8.89 kcal/mol) in global docking. Interestingly, MD simulation revealed that the complex between 3CL-Pro and RBD S protein has better stability than PL-Pro. This study suggests that hesperidin might have versatile inhibitory properties against several essential proteins of SARS-CoV-2. This study, nevertheless, remains to be confirmed through in vitro and in vivo assays.