Computational probing of Nigella sativa bioactive metabolites against chikungunya nsP2 cysteine protease

ABSTRACT

Background and Aim: Instances of chikungunya reported throughout the world in the past two decades of the present century. There is a lack of effective medicine or vaccine for chikungunya treatment. Non-structural protein, the nsP2 cysteine protease (nsP2pro) is an attractive target for inhibitors. It is a key enzyme for proteolytic cleavage of polyprotein precursors and produces functional proteins for replication and multiplication of the virus. Bioactive metabolites from Nigella sativa L; a popular spice and well-known medicinal plant, were selected for the current study against nsP2pro to search for potent non-toxic natural inhibitors of nsP2pro. Experimental: procedure Out of 54 bioactive metabolites from N. sativa 27 qualified drug likeliness properties. Virtual screening of 27 selected molecules was performed using AutoDock Vina. Top four molecules Kaempferol, (-)-Epicatechin, (+)-Catechin, and Apigenin with the least binding energy were taken for molecular docking employing AUTODOCK4. These metabolites were subjected to molecular dynamics simulation and MMPBSA, and the resilience of protein–ligand complexes had been assessed in terms of RMSD, RMSF, Rg, SASA, and hydrogen bonding. Results and Conclusions: Drug likeliness, molecular docking, molecular dynamics simulation properties, and MMPBSA analyses made clear that Kaempferol, (-)- Epicatechin, (+)- Catechin, and Apigenin all seem to be potential nsP2pro potent inhibitors and strong candidates for chikungunya virus drug development.