Abstract

Medicinal herbs have strong therapeutic potential because of the presence of phytochemicals in them. During the past few years, the global problem of antibiotic resistance has become a major health concern leading towards the search for new alternatives of antibiotics. In this regard, herbal compounds are the most appropriate options to be considered. In the present study, three herbal compounds i.e., gymnemic acid, eugenol and shogaol were extracted from medicinal herbs i.e., *Gymnema sylvestre* (gur mar), *Syzygium aromaticum* (clove), and *Zingiber officinale* (ginger) respectively. The fractions of extracted phytochemicals were used for the formation of silver nanoparticles (AgNps) i.e., gymnemic acid AgNp, eugenol AgNp, and shogaol AgNp, characterized by UV-vis and FTIR spectroscopy. Antibacterial potential of extracted herbal compounds and their silver nanoparticles was investigated by disc diffusion and broth dilution assay against gram positive (*Staphylococcus aureus, Methicillin resistant Staphylococcus aureus*) and gram negative bacteria (*Escherichia coli, Salmonella enterica,* and *Klebsiella sp.*). *In silico* study was also conducted to determine the effect of selected herbal compounds against bacterial targets i.e., 4CKL, 6J90, 7KHQ and 3DWK. The results of antibacterial screening reveals the highest antibacterial potential of eugenol (MBC: 250µl) as compared to other extracted compounds and their silver nanoparticles against all the selected bacteria. The *in silico* docking results also revealed eugenol as the most suitable compound on the basis of lowest binding energy and highest number of interactions with all the targets. However, the drug likeliness score of eugenol was -0.74 i.e., in the range of non-drug like compounds. It is due to the presence of double bond side chain at 4C of benzene ring. If this side chain is replaced with some other functional groups such as -OH, its drug likeliness increases. Therefore, as result of study, eugenol can be used as best antibacterial agent, however, for oral intake, its analogue such as 2-(4-hydroxy-3-methoxyphenyl)ethane-1,1diol with drug likeliness score -0.05 is more preferable drug candidate.