# ABSTRACT

Development of antibiotic-resistant and virulent microbes has diverted the attention of pharmacologists towards natural antimicrobials from herbal origin as an alternative treatment to synthetic drugs. Purpose of current study was the selection, identification and evaluation of new lead compounds (inhibitors) having potential of anti-*Pateurella multocida* activity by using natural compounds. For this purpose different targeted enzymes of *P. multocida* were selected to use as receptor molecules and virtual screening was performed against them by using VegaZZ, Patchdock software and "NPASS" databases to identify new compounds as potential inhibitors of DNA Gyrase and Sialyltransferase. Docked complexes then subjected to PDBSum. Results were interpreted on basis of binding affinity of receptor binding site amino acids with ligands, druglikeness score and on the physicochemical properties. According to screening results 2 compounds such as NPC235059, NPC271437 showed the potential as inhibitor of Sialyltransferase. While the compounds NPC165755, NPC139891 were selected as lead drug against the DNA gyrase. Derivatives of one of the lead compound selected for each receptor NPC235059 (Cinnamaldehyde) and NPC139891 (coumarin) were made to obtain the improved Physicochemical properties and more interactions. Results of derivatives compared with lead compounds displayed greater interactions and improved ADMET properties. Furthermore source of these screened compounds were found in natural herbs and antibacterial activity of these herbal plants (marjoram, cinnamon) extracts were investigated against multidrug resistant *P. multocida*. Among the herbal extracts cinnamaldehyde extract showed highest anti-*Pasteurella multocida* activity. The findings from this study document that natural herbs can be used as an alternative treatment of *Pasteurella multocida* infections.