Infectious diseases have become an inevitable truth of life and antibiotics are available for treatment. But from past few years the development of resistance against antibiotics has been major concern all over the world which highlights the dire need to find alternatives. Herbs having therapeutic properties could be considered as finest option. The present study is based on both in silico and in-vivo approaches to find the drug candidates against certain bacteria. Target proteins 4OR7, 5L75, 1ND4 of Klebsiella pneumoniae and 6M1S. 5HZU of Pseudomonas aeruginosa were selected and docked against database comprising of 606 herbal compounds. The in silico study revealed that ursolic acid. oleanolic acid and beta-sitosterol, exhibit low binding energy and good number of interactions with the selected targets, as final hit compounds. In this study, herbal compounds including, ursolic acid from Malus domestica (apple), oleanolic acid and betasitosterol from Olea europaea (olive plant) were extracted and fractioned in different organic solvents. The antibacterial activity of the extracted herbal fractions was checked by agar well diffusion method against K. pneumoniae and P. aeruginosa. Thin layer chromatography (TLC) was performed to confirm the presence of the desired compounds. Beta-sitosterol and oleanolic acid showed zones of inhibition against K. pneumoniae and P. aeruginosa respectively. However, ursolic acid showed activity against both the selected strains. Therefore, the three compounds screened in this study are suggested as potential drug leads and can be developed as possible antibacterial drug against different bacterial strains.