Electronic Supplementary Material (ESI) for MedChemComm.

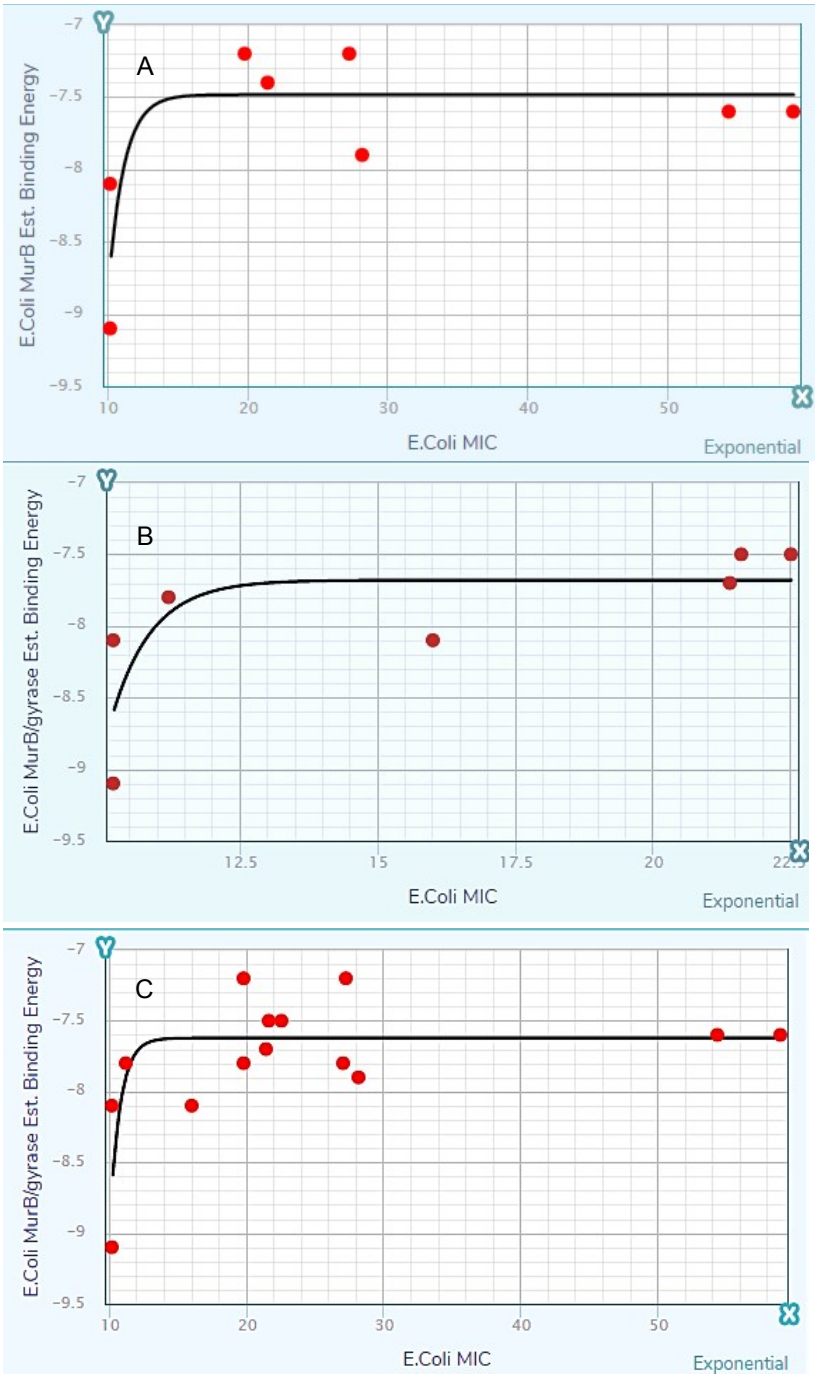

Figure S1. A. Best curve for the correlation of Estimated Binding Energy against *E.coli* MurB and *E.coli* MIC for the compounds with lower estimated Binding Energy to Mur B compared to gyrase. R^2=0.6829. B. Best curve for the correlation of the lowest Estimated Binding Energy against *E.coli* MurB or gyrase (the lowest one) and *E.coli* MIC, for compounds with clogP <4,000. R^2=5934. C. best curve for the correlation of the lowest Estimated Binding Energy against *E.coli* MurB or gyrase with *E.coli* MIC, for all compound with no clogP restrictions. R^2=0.5571, p=0.02529.

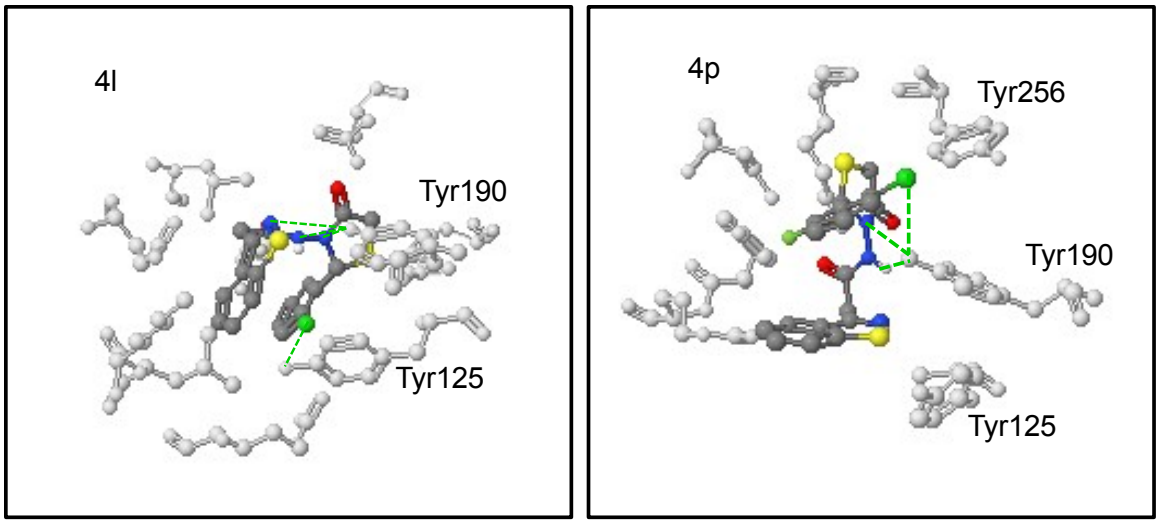

Figure S2. Docking of compounds 4l and 4p in the active site of E.coli MurB.

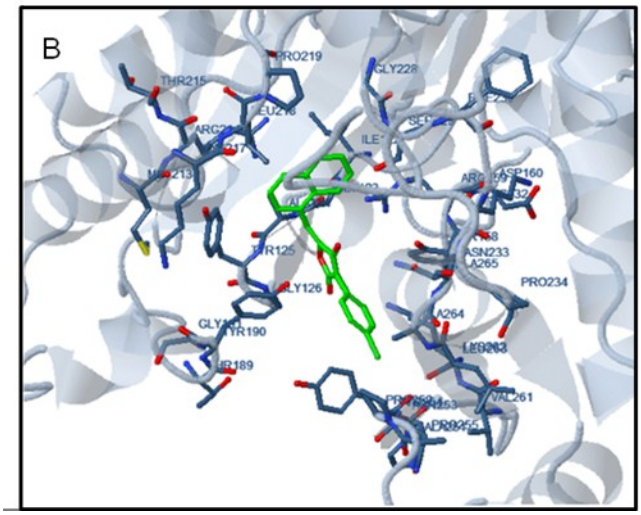

Figure S3. Docking of the inhibitor (5Z)-3-(4-chlorophenyl)-4-hydroxy-5-(1-naphthylmethylene)furan-2(5H)-one, in the active site of *E.Coli* MurB.

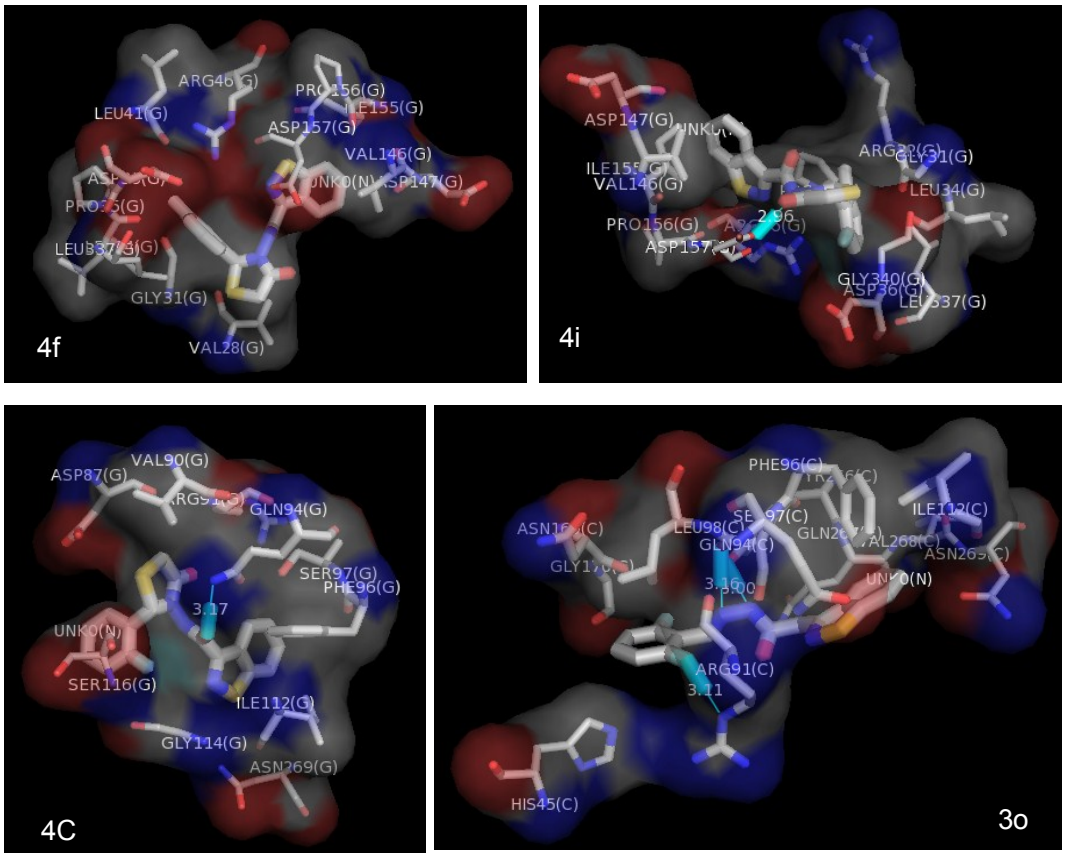

Figure S4. Docking of the compounds 4f, 4i, 4c and 3o in E.Coli gyrase.

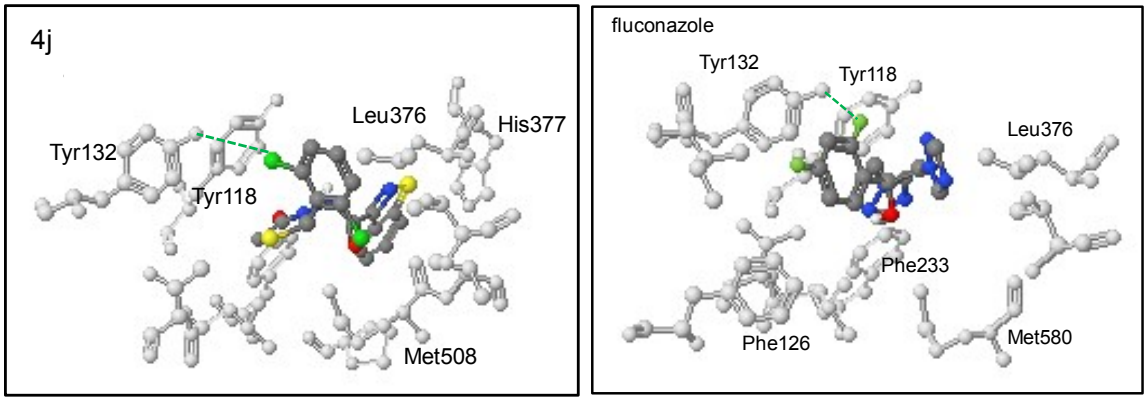

Figure S5. Docking of compound 4j and fluconazole to the active site of *Candida Alpicans* 14a-lanosterol demethylase (ERG11) (PBD ID:2v2z)