ABSTRACT

Skin diseases are the most common infection in humans as well as in animals caused by fungi like yeast, mould and dermatophytes. In this study, in silico analysis of 20 phytocompounds was carried out for their efficacy as antidermatophytic agents using the receptor 1, 3 - β -D-Glucan synthase. The 3D structure of the receptor obtained using Modeller9V8 was validated with Procheck, where Ramachandran plot showed 80.3% of residues in the most favoured region. The phytocompounds and the drugs Echinocandin B and Caspofungin were docked with 1, 3 - β -D-Glucan synthase using Glide. Though all the 20 compounds exhibited lesser energy than both Echinocandin B (-3.3Kcal/mol) and Caspofungin (-1.68 Kcal/mol), Quercetin-3-O-rutinoside exhibited very less energy (-11.56 Kcal/mol). Further, comparing to synthetic drugs, the entire compounds selected for this study showed high interaction with the modeled protein. Hence, the present study concludes that the efficacy of all phytocompounds used in this study act against dermatophyes and which will be very helpful to the researchers working in the area of dermatophye drug developments