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IN SILICO GUIDED SYNTHESIS OF TWIN TARGETED BENZIMIDAZOLE-1,2,4-TRIAZOLE MOLECULAR HYBRIDS AS ANTIFUNGAL AGENTS

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Abstract—*A series of novel benzimidazole-1,2,4-triazole molecular hybrids (1-24) were designed as tubulin and lanosterol 14α-demethylase inhibitors and rationally screened in silico to predict the molecules of great antifungal potential. Molecular docking in active site of tubulin revealed stronger binding of all the designed molecules in comparison to the standard, carbendazim with docking score of -6.12Kcal/mol. The docking of compounds 13 and 15 exposed best binding in the active site of tubulin as indicated by their appreciable docking score of -8.12 and -7.59Kcal/mol, respectively. Lanosterol 14α-demethylase could be inhibited well by compounds 13 and 15 with better docking score of -10.11 and -10.24Kcal/mol than that of standard propiconazole (-9.12Kcal/mol). Chemo-informatics analysis envisaged that all these compounds obeyed the Lipinski's rule. The compounds 13 and 15 were selected for synthesis, on the basis of in silico results, following a multistep protocol and their structures were ascertained by IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopy. Their antifungal evaluation studies against Fusarium verticillioides, Drechslera oryzae and Curvularia lunata revealed greater antifungal potency of hybrid 13 than the standards used with ED_{50} values of 21, 15 and 15μg/ml, respectively.*