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Modeling studies of pyrazolo[3,4-d]pyrimidines as antiamoebic agents through docking and molecular dynamics simulations

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Amoebiasis, a common infection caused by a protozoan parasite *Entamoebahistolytica*, infects the large intestine of humans and in advance stage liver, brain and lung. It can cause abscesses, ulcers and may infect the bowel which can be highly fatal. Metronidazole (MNZ), the first line medicament against amoebiasis, is potentially carcinogenic to humans as it is genotoxic to human cells and shows significant side-effects. In the present work, *in-silico* molecular docking simulation have been performed on nine pyrazolo[3,4-d]pyrimidine molecules having no linker, and nine pyrazolo[3,4-d]pyrimidine molecules having trimethylene linker along with the reference drug metronidazole with O-acetyl-L-serine sulfhydrylase enzyme, the prime target for inhibiting the growth of *E. histolytica*. Without linker molecules 2 and 4 have been proven to be better inhibitors than metronidazole. Trimethylene linker molecules show improved binding capabilities among which molecules 15 and 16 supersede. Molecular dynamics simulation on the best docked poses of molecules 2, 4, 15, 16 andMNZhave been carried out for 10.2 ns using DESMOND which make obvious that the complexes remain stable during the course of dynamics. RMSD variations and energy calculations of the complexes through MD simulation show that molecule 4has the best stability and binding capability.

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