New and mild method for the synthesis of alprazolam and diazepam and computational study of binding mode of them to $GABA_A$ receptor

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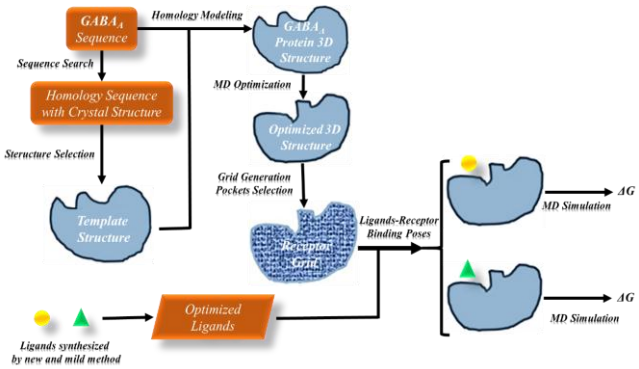

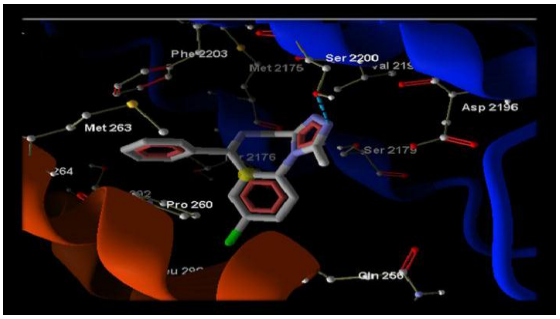

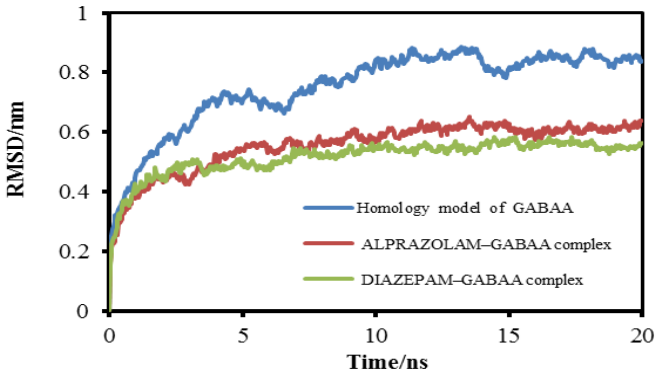

In the current study, alprazolam and diazepam were synthesized in a new and mild condition in the framework of green chemistry. Also, in order to find the 3D structure of $GABA_A$ and investigate possible interactions alprazolam and diazepam with active site of $GABA_A$, a template sequence was selected for homology modeling. The initial 3D structure obtained from homology modeling was optimized using MD simulation. Then, alprazolam and diazepam were docked into the receptor. Finally, the ligand binding free energy for the complex was calculated based on the MD simulations.