

Figure S1. (A) Structure of the GABA_B receptor extracellular Venus flytrap domain (PDB ID, 4MS4). (B) Docked conformation of baclofen in the GABA_B receptor is shown. Interacting residues of the GABA_B receptor are represented as dashed lines and labeled. GABA_B, γ -aminobutyric acid B.

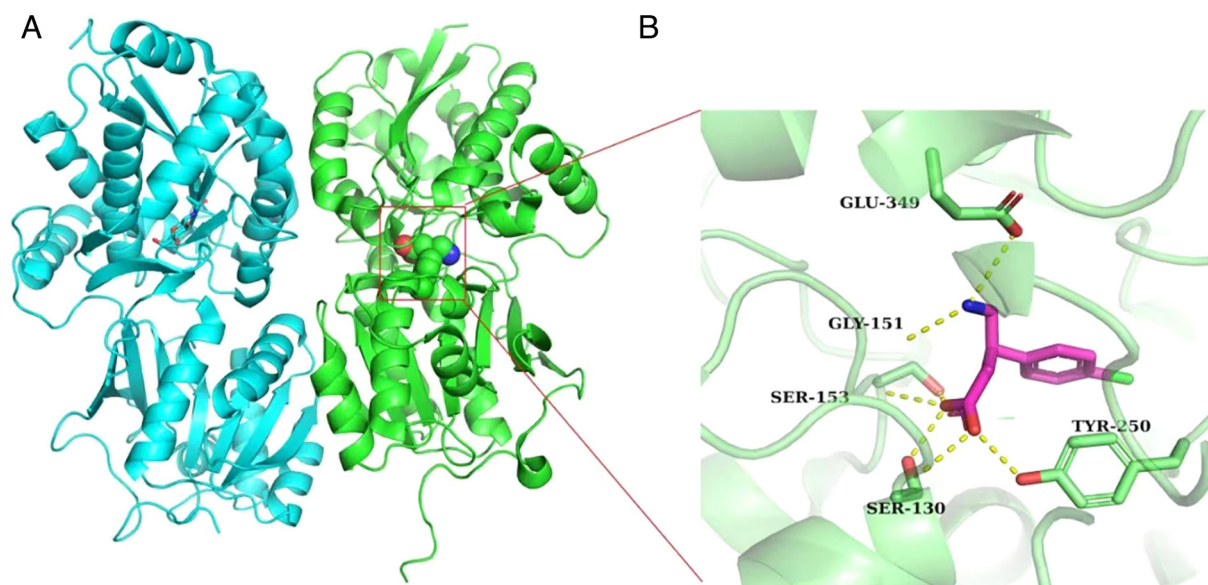


Figure S2. Docked conformations of the three selected compounds superimposed on to baclofen. The colors represent the following: Baclofen, green; compound with PubChem ID 450432, magenta; compound with ID 6448, blue; and compound with ID 6057, orange.

