Binding Pocket Prediction of Glutamate Binding Site on Glycine Receptor

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In the mammalian brainstem and spinal cord, synaptic excitation and inhibition are mediated by the excitatory transmitter glutamate, which acts on iontropic glutamate receptor-gated cationic channels, and the inhibitory transmitter glycine acting on glycine receptor (GlyR)-gated chloride channels. According to the literatures, that glutamate and several of its analog ligands potentiate GlyR-gated chloride currents in cultured spinal neurons. This potentiation is not dependent on activation of any known iontropic or metabotropic glutamate receptors, and manifests as an increase in single channel open probability in single channel recordings. From past study, which indicate that glutamate may allosterically potentiate GlyR-gated chloride channel. In this study, we use iGEMDOCK and *Accelry* Discovery Studio 2.5 to compute and predict of glutamate binding pocket of the brain neurotransmitter glycine receptor chloride channels, in order to analyze glutamate binding points and its interacted force on glycine receptor. We searched Gly alpha 1 of the Protein Data Bank and found the experiment-related protein (Code: 1T3E) to do the docking simulation. In the calculation of anhydrous environment, it is convenient to calculate because there is no interference of the water molecules. By adding water molecules influence and calculate docking of protein and drug affect the docking scores. So the docking scores were obtained more worst than the original.