Characterization of protein-ligand complexes using molecular dynamics simulations by consideration of $GABA_A$ protein as receptor and Lavender compounds as ligand

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Abstract:

$GABA_A$ receptors are a class of receptors that respond to the neurotransmitter gamma-aminobutyricacid (GABA), the chief inhibitory neurotransmitter in the vertebrate central nervous system, which are ligand-gated ion channels and are known as ion tropic receptors [1-5]. Lavender is a species of flowering plants in the mint family and is native to the mountainous zones of the Mediterranean and flourishes throughout southern Europe, Australia, and the United States. This herb has been used as a remedy for a range of ailments from insomnia and anxiety to depression and fatigue. This plant is grown mainly for the production of lavender's oil which has antiseptic and anti-inflammatory properties. A number of studies have reported that this oil may be beneficial in a variety of conditions, including insomnia, hair loss, anxiety, stress, and postoperative pain [6, 7]. This plant is being studied for antibacterial and antiviral properties [8]. In this work, we have simulated and studied the complexes of different chemical compounds found in the lavender extract with GABA protein as receptor. Our Simulations are based on molecular dynamics (MD) approach through force fields and GROMACS package is used to do MD simulations to locate sites with favorable interaction energy.

Keywords: $GABA_A$ receptors, Lavender plant, Molecular dynamics, GROMACS

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