عنوان مقاله:

Simulation of Clonazepam and Diazepam in DPPC membrane: Investigation of the movement

محل انتشار:

بیستمین کنفرانس شیمی فیزیک ایران (IPCC20) (سال: 1396)

تعداد صفحات اصل مقاله: 3

نویسندگان:

Khaled Azizi - *Department of Chemistry, University of Kurdistan, Sanandaj, Iran- Research center of Nanotechnology, University of Kurdistan, ۶۶۱۷۷-۱۵۱۷۵, Sanandaj, Iran*

Mokhtar Ganjali Koli - *Department of Chemistry, University of Kurdistan, Sanandaj, Iran- Research center of Nanotechnology, University of Kurdistan, ۶۶۱۷۷-۱۵۱۷۵, Sanandaj, Iran*

خلاصه مقاله:

Mobility of DPPC molecules in the presence of two kinds of benzodiazepines (BZDs) (Diazepam;Clonazepam) within model membranes was investigated by molecular dynamics simulation. Observations can beexplained by more free space in the Clonazepam containing system that leads to more movement of DPPC molecules inthis system. Mobility of Diazepam in DPPC membrane is more than Clonazepam. It seems the presences of bulkyatoms like Oxygen and Nitrogen in the structure of Clonazepam caused less movement of this molecule. More abilityof Clonazepam molecules in establishing the hydrogen bond is another reason for slower movement of this molecule inDPPC membrane.

کلمات کلیدی:

Benzodiazepines, Molecular dynamics simulation, Mean Square Displacement, Membrane