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Molecular dynamics model of melatonin and MT1 receptor

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Melatonin receptor (MT1) is an attractive target for elaboration of new drug candidates, but unfortunately is known to be unstable out of the membrane lipid bilayer, which makes the obtaining of a crystal structure by X-Ray diffraction (XRD) an elusive goal. Up to now, there is no published real structure suitable for docking of new ligands targeting this receptor. However, there are lots of model based on the data from crystallized rhodopsin, but they are too artificial for reasonable docking of drug-like candidate molecules. To overcome these drawbacks, we built an *in silico* molecular model of a melatonin receptor in membrane bilayer in water cell, with explicit water molecules. For that purpose, we used GROMACS molecular mechanics software with GROMOS force field and TYP3P water model. Calculations were carried out in periodic boundary conditions at 300 K and one bar pressure, physiological NaCl content and pH7. By the simulation, we caught the act of melatonin entering the receptor which enlightened a wide variety of interactions that can facilitate or to disturb the movement of melatonin to the hardly accessible active site of MT1. Molecular docking of the drug like candidates was performed on receptor model. The information can be used along with data obtained from the structure of melatonin-receptor complex to construct new analogs of melatonin, capable not only to activate the receptor but also to successfully manage their way to the MT1 binding site.

Biography

Violina T Angelova has completed her PhD in Organic Chemistry from Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Science, in 2004. She has 22 years of research experience and published more than 29 papers in reputed journals. Currently, she is an Associate Professor at the Faculty of Pharmacy, Medical University of Sofia.

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