## عنوان مقاله:

In silico studies of rs1799971 (A118G) OPRM1 gene structural polymorphism binding to buprenorphine as an opioid addiction substrate

## محل انتشار:

سومین کنگره بین المللی و پانزدهمین کنگره ملی ژنتیک ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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## خلاصه مقاله:

Introduction: According to the previous studies, A118G has showed a critical role in the association studies of mu-opioid receptor 1 (OPRM1, MOR). We aimed to investigate homology modeling and docking analyses of rs1799971 (A118) in binding to buprenorphine as an opioid addiction substrate for the first time. Methods: The tertiary structures of human MOR protein in wild-type (Asn40) and mutant (Asp40) alleles of rs1799971 (A118G) were modeled by the chosen template (PDB ID: 4DJH) through Swiss Model, PS2, and Phyre2 online softwares. Then, best models (from Phyre2) were built after energy minimization by Swiss-PdbViewer ver. 4.1.0 software. The structures of designed models were then validated using RAMPAGE and ProSA softwares. Final models were visualized by Autodock ver. 1.5.6. To prepare the ligand for docking, energy minimization of ligands was performed using Hyperchem professional tool ver. 8.0.8. Active site of OPRM1 was predicted by COACH. Best conformation among 10 conformations was opted based on the lowest binding energy and H-Bonds in cluster. Finally, dominant and recessive complexes with same ligand were compared to each other. Results: In silico analyses of OPRM1 protein with buprenorphine as ligand showed that the best conformation of buprenorphine had more binding affinity to Asp40 (binding Energy=-8.46 kcal/mol with 2 Hydrogen bonds formation) compared to Asn40 model (binding Energy=-5.26 kcal/mol with lack of H-bond formation). Conclusion: Consequently, genotyping of A118G as a remarkable marker of opioid addiction may be helpful in buprenorphine administration and treatment among populations which have shown significant susceptibility to opioid addiction.

## کلمات کلیدی:

A118G, homology modeling, docking, buprenorphine, addiction.

## لینک ثابت مقاله در پایگاه سیویلیکا: