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Comparative modeling of serotonin receptors 5ht2a and 5ht2c and *In-silico* investigation of whether they can be potential off-target to ethinylestradiol

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The side effects of contraceptives in general and combined oral contraceptives (COC) in particular are numerous and are limiting factors in many cases leading to cease their use. At the same time the combined oral contraceptives or synthetic estrogens are increasingly being used in Medicine today. Weight gain, migraine and depression are some of the side effects of COC and also three of them are associated with disorder in serotonin level. Here we hypothesized that EthinylEstradiol (EE) may affect serotonin function by binding to serotonin receptors as off-target ones (realizing that serotonin receptors and estrogen receptors coexist in a wide varieties of tissues); hence explaining the mechanism by which the aforementioned side effects take place. Having known that the receptors` tertiary structures are not solved yet, the only choice was to construct the 3D of receptors based on previously solved ones using comparative modeling techniques. the homology models for serotonin receptors (5ht2a and 5ht2c) were generated using I-TASSER web server and MOE program (Molecular operating environment), and then the structures were compared using Dalilite web server against a high resolution beta2 adrenergic receptor 2RH1, accordingly the best one was that predicted by I-TASSER web server. The binding sites predicted by I-TASSER for both receptors, were highly consistent with those predicted by others. Molecular docking of the ligands was performed using PatchDock web server and SYBYL-X program. The final results strongly support our hypothesis furthermore it highlights the issue of target specificity and how important is it when synthesizing any drug.

Biography

Rehab Yousif finished her MSC in Molecular medicine July 2012 with distinction degree from Institute of Endemic Diseases (IEND), University of Khartoum. She is a teaching assistant in the department of Pharmaceutical Microbiology, Faculty of Pharmacy, University of Khartoum.

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Bilayer tablets of conventional paracetamol and sr aceclofenac: Formulation and *invito* evaluation

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The objective of the present work was to formulate the bilayer tablets consisting conventional immediate release paracetamol and sustained release aceclofenac. Aceclofenac in combination with paracetamol is generally indicated for acute pain, chronic treatment of rheumatoid arthritis and ankylosing spondylitis. Among different batches prepared by the wet granulation technique, the optimized batch of paracetamol using super disintegrant sodium starch glycolate for the immediate release layer and methocel K4M polymer used for aceclofenac sustained release layer were selected for the compression of bilayer tablets. The tablets were evaluated for physicochemical properties. All the values were found to be within the limits. There was no drug-excipient interaction which was confirmed by IR Spectrum. And in vitro release studies (which were estimated by the UV simultaneous estimation method) showed a release of 80% paracetamol within 15mins. And aceclofenac sustained release layer was found to releasing the drug for more than 8 hours. The dissolution profiles were compared with the reference marketed products and the F2 value was in between 50-100. The results obtained shows that there is not much difference between the marketed products and our formulated bilayer tablets of conventional paracetamol and sustained release aceclofenac tablets.

Keywords: Bilayer tablets, paracetamol, aceclofenac, sustained release and UV simultaneous estimation method.

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