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Computational simulation of the effect of quantum chemical parameters on the molecular docking of HMG-CoA reductase drugs

Faten Mahmoud Ahmed Atlam
Tanta University, Egypt

Density functional theory (B3LYP-6-31G(d)) was performed to study the effect of molecular and electronic structures, of 2-cyclopropyl-4-thiophenyl-quinoline mevalonolactones as potential hypocholesterolemic inhibitors, on their biological activities and discuss the correlation between the inhibition efficiency and quantum chemical parameters. Molecular docking was performed to investigate the mode of interactions between the investigated inhibitors and the active sites of the target Hydroxymethylglutaryl-Coenzyme A (HMG-CoA) reductase. The results could suggest further structural modifications to discover more potent and selective HMG-CoA reductase inhibitors. The catalytic active sites of HMGR have a positive electrostatic potential which is complemented with a negative electrostatic potential of the investigated drugs to form a stabilized complex. The presence of lipophobic groups, such as quinoline nucleus, cyclopropyl and substituted thiophenyl groups as well as a lactone moiety, is important for binding to the active sites. A good correlation between the experimental and theoretical data confirms that the quantum chemical methods and molecular docking studies are successful tools for enriching screening experiments aimed at the discovery of novel bioactive compounds.

faten_atlam@yahoo.com

Comparative study of sitagliptin analysis on halogenated stationary phases in pharmaceutical formulation

Hebatallah A Wagdy[1] and **Hassan Y Aboul-Enein**[2]
[1]British University in Egypt (BUE), Egypt
[2]National Research Center (NRC), Egypt

Sitagliptin [(2R)-1-(2,4,5-trifluorophenyl)-4-oxo-4-[3- (trifluoromethyl)-5,6 dihydro [1,2,4] triazolo [4, 3-a] pyrazin-7(8H)- yl] butan-2-amine] is an antidiabetic drug, it corresponds the dipeptidyl peptidase-4 (DPP-4) inhibitor. Although it was developed since 2006, only few methods were reported in literature for its analysis. None one of these methods have reported its analysis on the newly developed halogenated stationary phases namely; pentabromobenzyl (PBr) and pentafluorophenyl (PFP) columns. This investigation illustrates a comparison between the separation as well as the mechanism(s) involved in the separation of sitagliptine on PBr and PFP columns which include interactive forces such as hydrogen bonding, pi-pi-stackking and dispersion force interaction. In this method, standard solutions were prepared by dissolving the analyte in methanol and mobile phase and so is the pharmaceutical tablet formulation. The HPLC conditions used were: a mobile phase composed of phosphate buffer (pH-3.5): ACN (60:40v/v), the flow rate was 1 ml/min, the detection wavelength was 260 nm. The pKa of sitagliptin was calculated using ACD/Labs software® was 7.19. The results showed difference in analysis time and solvent consumption between the 2 columns used in this study. Furthermore, this study led to better understanding of the mechanism of action involved in these newly developed halogenated stationary phase regarding the studied analyte and mobile phase/column parameters.

Hebatallah.wagdy@bue.edu.eg

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