Joint International Conference and Expo on Industrial Pharmacy & 5th Global Pharmacovigilance Summit

April 28-29, 2016 Dubai, UAE

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. faten.atlam@science.tanta.edu.eg

The appropriate use of antibiotics in early children: The FP-MCRN study

Ettore Napoleone

Family Pediatricians-Medicines for Children Research Network, Italy

Paediatricians should be aware that the inappropriate use of antibiotics in early children (0 - 2 years) increases the risk of ADRs and drug resistance. Despite of it is well known that around 200% of the initial conduction of the second c and drug resistance. Despite of it is well known that around 80% of respiratory tract infections have a viral etiology, data about pharmaceutical prescription suggest an increasing consumption of antibiotics in this age group. The use of these drugs is not always based on scientific evidence, increasing problems in term of efficacy and safety of the therapy. In this context, Family Paediatricians -Medicines for Children Research Network (FP-MCRN) established with the aim of developing competence, infrastructure and education for paediatric clinical trials, plays a crucial role in paediatric Pharmacovigilance, thought a training and educational courses, a correct research methodology and very strong relationship with the families. The aim of the FP-MCRN-Study was to evaluate the prescription attitude related to antibiotics in the early paediatric population, to encourage the appropriate use of antibiotics and to inform paediatricians and families about the possible iatrogenic illnesses caused by their improper use. This study represents a territorial survey of the prescriptive appropriateness and safety of these drugs in the paediatric population, a necessary prerequisite to assess the risk-benefit ratio of their use. The study evaluated the antibiotic prescriptions in 4060 children (0-2 years) of 37 Family Pediatricians (FP) in 2013. During 2014 we achieved specific training and educational courses for FP and families on the appropriate use of antibiotics and on the possible iatrogenic illnesses caused by their improper use. The results obtained highlighted that 3369 children (83%) of the 4060 received at least one prescription of antibiotic during 2013. In particular, a total of 7.114 prescriptions were dispensed, with amoxicillin/clavulanic acid as the first-choice treatment in 33% of patients. This -very high- value of prevalence (83%) of the antibiotic prescriptions will be compared with the 2015 prescription data after FP-MCRN training and educational courses directed to the families and to the 37 FP. We will compared antibiotic ADRs too. The antibiotic over-prescription (prevalence-83%) exposes patients to an increased risks of side effects and drug resistance, both representing public health problems. Hence, the need to improve the activity of antibiotic prescribing, in particular in the early pediatric populations. The starting point must necessarily be cultural: An implementation of the culture of iatrogenic disease and a careful assessment of the correct diagnosis and therapy.

ettorenapoleone@tiscali.it