CURRENT RESEARCH TOPICS IN PHARMACY:

In silico Approaches for Drug Design and Discovery

January 25th, 2023 13.00 PM
ISTANBUL

FOR REGISTRATION:

First Session- *Moderator: Esra TATAR 13.00-14.30 PM*

Welcome- Prof. Mesut SANCAR

***In silico* pharmakokinetics prediction of major coumarins present in *Aegle marmelos* L – Assist. Prof. Sneha Agrawal**
Bharati Vidyapeeth's College of Pharmacy, Maharashtra, India

Pharmakokinetics evaluation with SimCYP program - Assoc.Prof.Enkelejda Goci
Aldent University, Tirana, Albania

A new approach in drug discovery: Network pharmacology - Dr. Yağmur Diker
Hacettepe University, Ankara, Turkey

Second Session- *Moderator: Esra TATAR 15.00-16.30 PM*

Computational identificaion of novel targets for drug candidate compounds - Assoc.Prof.Ceren Sucularlı
Hacettepe University, Ankara, Turkey

Designing novel mitochondrial fission inhibitors targeting Drp1-GTPase interaction using computational methods - Dr.Sefer Baday
Istanbul Technical University, Istanbul, Turkey

Artificial Intelligence: A member of drug discovery team – Assoc.Prof.Somaieh Soltani
Tabriz University of Medical Sciences, Tabriz, Iran

Discovery of novel Hepatitis C NS5B polymerase Inhibitors by in silico approaches - Dr. Berin Karaman Mayack
University of California Davis, Davis, USA

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PHARMAKOKINETIC EVALUATION WITH SIMCYP PROGRAM

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The anticonvulsant carbamazepine is a first-line drug in the treatment of most forms of epilepsy and also the drug of first choice in trigeminal neuralgia. It is a known substrate and inducer of cytochrome P450 (CYP) 3A4 and CYP2B6. Carbamazepine induces the metabolism of various drugs (including its own); on the other hand, its metabolism can be affected by various CYP inhibitors and inducers. The aim of this work was to develop a physiologically based pharmacokinetic (PBPK) model of carbamazepine dosing in pediatrics by using Simcyp Simulator platform. The model is based in vivo pharmacokinetic data and verified using an independent set of published clinical pharmacokinetic data in adult and pediatric population. The PK data observed and predicted were compared and evaluated, by visual predictive check [1-3].

The major enzyme in carbamazepine metabolism is CYP3A4 that, according to Simcyp, its activity increases with 2-fold. CL is more accurately predicted in multi-dose simulations compared to single-dose simulations. Moreover, pediatric predictions are very accurate, including the CL [1-3].

Overall, the adult multi-dose predictions are better than adult single-dose. Paediatric exposure is accurately predicted. Thus, the paediatric multi-dose carbamazepine exposure can be simulated by Simcyp. When the simulation results are combined with the pharmacodynamics of carbamazepine, dosing recommendations may be suggested [1-3].

Keywords: Carbamazepine; Simcyp, PBPK model, Pharmacokinetic

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REFERENCES

[1] Bäckman E, Dahlstr6m G, Eeg-Olofsson O, Bertler. The 24 hour variation of salivary carbamazepine and carbamazepine- 10,11-epoxide concentrations in children with epilepsy. Pediatr Neurol. 1987;3:327-330. [CrossRef]

[2] Eeg-Olofsson O, Nilsson HL, Tonnby B, Arvidsson J, Grahn PA, Gylje H, Larsson C, Norén L. Diurnal variation of carbamazepine and carbamazepine-10,11-epoxide in plasma and saliva in children with epilepsy: a comparison between conventional and slow-release formulations. J Child Neurol. 1990;5(2):159-165. [CrossRef]

[3] Thakker KM, Mangat S, Garnett WR, Levy RH, Kochak GM. Comparative bioavailability and steady state fluctuations of Tegretol commercial and carbamazepine OROS tablets in adult and pediatric epileptic patients. Biopharm Drug Dispos. 1992;13(8):559-569. [CrossRef]

http://dx.doi.org/10.29228/jrp.453