Abstract No: MO-11

In silico ADMET analysis of compounds identified in the genus Impatiens in oral administration

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New drug discovery and development avenues have opened up due to the rapid advancement of computational methodologies and technologies. Impatiens is a genus of flowering plants in the family Balsaminaceae that has a long history of traditional usage in folk medicine and cultural traditions. Although prior studies have been conducted on the phytochemical compounds of Impatiens species, there is limited information available about their pharmacokinetics and oral toxicity. Thus, the purpose of this study is to analyze the ADMET (absorption, distribution, metabolism, excretion, and toxicity) properties of compounds identified in the genus Impatiens, *in silico*. Due to the time-consuming and costly nature of traditional experimental methods, *in silico* approaches are required to screen and prioritize potential candidates. Sixteen (16) compounds from the genus Impatiens were chosen to evaluate the ADMET and physicochemical properties using the *in silico* online tools, pkCSM, and Molinspiration. As a standard for comparison, Colchicine was used as the negative control as it is a known toxic compound. Molinspiration results showed that all the compounds, except for Esculin, followed Veber's rule. Conversely, all compounds including Esculin adhered the Lipinski's rule. Additionally, pkCSM results indicated Caffeic acid, Sinapinic acid, (R)-(-)-Linalool as promising candidates for oral drug administration because of their advantageous ADMET profiles and non-toxic properties. On the other hand, compounds such as Esculetin, Scopoletin, Esculin, and 2-methyl-1,4-naphthoquinone, were classified as toxic compounds since they had unfavorable ADMET profiles and exhibited Low LD50 values, hepatotoxic and mutagenic properties. R)-(-)-Linalool emerged as the phytochemical with the greatest potential for the development of oral drugs, meeting the crucial requirements outlined by Veber's and Lipinski's rules. Remarkably, it showcases outstanding attributes, including high intestinal absorption (93.163%), impressive Blood-brain barrier permeation (0.598 logBB), notable Caco2 permeability (1.493 log Papp in 10-6 cm/s), favorable water solubility (-2.612 log mol/L), significant fraction unbound (0.484 Fu), a high LD50 (2.024 mol/kg), and no inhibition of CYP450 enzymes. Additionally, it demonstrated non-mutagenic and non-hepatotoxic properties. Nonetheless, further *in vivo and in vitro* studies are required to promote R)-(-)-Linalool as a promising oral medication candidate. These experimental studies will assure the chemical compound's effectiveness, security, and possible applicability for therapeutic usage in humans.

Keywords: *In silico,* ADMET properties, Genus Impatiens, Physicochemical properties, pKCSM

Acknowledgment
This work was supported by Oxford Brookes University-United Kingdom and British College of Applied Studies, in Colombo.