Abstract

In Silico Test of Physicochemical Properties and Pharmacokinetic Profile (ADMET) of Betulinic Acid Derivatives as HIV Drug Candidate

Adinda Adelia Wulandari

This study aims to determine the physicochemical properties and pharmacokinetic profiles (ADMET) of betulinic acid derivative compounds as HIV drug candidates. This research was conducted in silico using the ChemDraw 17.0 and pkCSM online tool. Based on the physicochemical properties test results with the ChemDraw 17.0 programme, it is known that the five betulinic acid derivatives tested have non-ideal physicochemical properties based on Lipinski's law: Rule of Five (RO5). The five derivates have a molecular weight (WT) value of > 500 g/mol; LogP > 5; Hydrogen Bond Donors < 5; Hydrogen Bond Acceptor < 10; tPSA <140 Å; and the amount of rotatable bonds from compounds 3, 4, and 5 > 10. Based on the ADMET test with the pkCSM online tool, it is known that the five compounds have good intestinal absorption with an absorption value of 59% -100%, low skin permeability, and the five compounds tend to be p-glycoprotein II inhibitors. The five compounds are also predicted to not be distributed to the brain due to the low permeability blood brain barrier (BBB) value. The five test compounds also did not become cytochrome P450 inhibitors and had a total clearance value ranging from log -1.2 to 0.1 ml/minute/kg. However, it is known that only compound 2 is not hepatotoxic. Through this in silico test, it is hoped that it can become an initial reference in the development of betulinic acid derivative compounds for further testing as an HIV drug.

Keywords: betulinic acid derivatives, *in silico,* physicochemical properties, pharmacokinetic profile