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In silico prediction of absorption and distribution properties of molecules identified in Algerian fir (*Abies numidica* de Lannoy ex CARRIERE) needles

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Abstract

The computational approach is one of the newest and fastest developing techniques in pharmacokinetics, ADME (absorption, distribution, metabolism, excretion) evaluation, drug discovery and toxicity. The current study aimed to determine the physicochemical characteristics and to predict the Absorption and distribution properties of molecules identified in Algerian fir (*Abiesnumidica* de Lannoy ex CARRIERE) needles. Swiss ADME is the software used as *in silico* tool for the determination of the properties. The compounds luteolin and apigenin are moderately soluble with increasing of log P value, from 2.2824 to 2.5768; respectively. On the other hand, the molecules: rutin (-1.6871), hesperidin (-1.1566), chlorogenic acid (-0.6459), hyperoside (-0.5389), astragalin (-0.2445), luteolin-7-glucoside (-0.2445), apigetrin (0.0499), quercitrin (0.4887), protocatechic acid (0.796), and quercetin (1.9880) possess high solubility in aqueous media and recorded very low Log P values which demonstrates the hydrophilic nature of these compounds. The results of absorption and distribution of molecules indicated that all molecules exeptrutin presented a high intestinal absorption, while all molecules proved a weak ability to across the blood barriere in brain. Quercitin and quercitrin revealed a high distribution volume. Controlled access to these data could be particularly helpful in validating new *in silico* approaches.

Keywords : *Abies numídica* leaves, Physicochemical, Absorption, Distribution, *In silico*.