

## عنوان مقاله:

Phenolic Compounds and Skin Permeability: An In Silico Investigation

## محل انتشار:

مجله بیوشیمی پزشکی، دوره 11، شماره 1 (سال: 1402)

تعداد صفحات اصل مقاله: 8

## نویسندگان:

Majdi Hammami

Emna Chaabani

Walid Yeddes

Wissem Aidi Wannas

Soumaya Bourgou

## خلاصه مقاله:

Background: The skin is the largest organ of the body and provides the main barrier between the internal and external environment. Assessment of skin permeability is of critical importance for understanding and predicting in vivo efficacy and bioavailability of bioactive phenolic compounds. Objectives: This study investigated the relationship between skin permeability and phenolic compounds using in silico methods. Methods: Screening of skin permeability was performed on ۴۷۵ randomly selected phenolic compounds. Molecules were expressed in SMILE format downloaded from Phenol-Explorer Database (version ۳.۶, ۲۰۱۶). Then, their skin permeability was determined by the linear model of the quantitative structure-activity relationship (QSAR). The obtained results were investigated for normal distribution and correlation with pharmacological properties. Results: Our investigation showed that ferulate hydroxycinnamic acid derivatives were the most important phenolic subclass with a permeability of  $-۱.۶۵$  cm/s. The relationship between permeability and lipophilicity, water solubility, synthetic accessibility, and bioavailability was evaluated. The statistical analysis revealed that the highest skin permeability was associated with three parameters: the topological polar surface area (TPSA), molecular weight, and lipophilicity (iLog P). Conclusion: The cutaneous permeability depended on several chemical parameters of the molecule used. The classification of phenolic compounds according to their structures proved a wide variability in this permeability.

## کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/1908826>

