

Accepted Manuscript

Molecular Dynamics as a tool for in silico screening of skin permeability

Paolo Rocco, Francesco Cilurzo, Paola Minghetti, Giulio Vistoli, Alessandro Pedretti



PII: S0928-0987(17)30354-8
DOI: doi: [10.1016/j.ejps.2017.06.020](https://doi.org/10.1016/j.ejps.2017.06.020)
Reference: PHASCI 4105

To appear in: *European Journal of Pharmaceutical Sciences*

Received date: 23 March 2017
Revised date: 2 June 2017
Accepted date: 12 June 2017

Please cite this article as: Paolo Rocco, Francesco Cilurzo, Paola Minghetti, Giulio Vistoli, Alessandro Pedretti, Molecular Dynamics as a tool for in silico screening of skin permeability, *European Journal of Pharmaceutical Sciences* (2017), doi: [10.1016/j.ejps.2017.06.020](https://doi.org/10.1016/j.ejps.2017.06.020)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Molecular Dynamics as a tool for in silico screening of skin permeability

Paolo Rocco^{*§}, Francesco Cilurzo[§], Paola Minghetti[§], Giulio Vistoli[~], Alessandro Pedretti[~]

[§]Department of Pharmaceutical Sciences, Università degli Studi di Milano, via G. Colombo, 71
I-20133 Milan, Italy.

[~]Department of Pharmaceutical Sciences, Università degli Studi di Milano, Via Mangiagalli, 25,
I-20133 Milan, Italy.

* **Corresponding Author.** Department of Pharmaceutical Sciences, Università degli Studi di
Milano, Via G. Colombo 71, I-20133 Milan, Italy. Phone: +39 (2) 503 24656.

E-mail: paolo.rocco@unimi.it.

Abstract

Prediction of skin permeability can have manifold applications ranging from drug delivery to toxicity prediction. Along with the semi-empirical or mechanistic models proposed in the last decades, molecular dynamics simulations have recently become a fruitful tool for investigating membrane permeability, in particular as they allow the involved mechanisms to be modelled at a molecular level. Despite their significant structural complexity, molecular dynamics simulations can also be utilized to study permeation through the lipid matrix that characterizes the stratum corneum. In this work, Steered Molecular Dynamics simulations are performed on a suitably developed stratum corneum lipid matrix model. Regardless of their actual tortuous path within

Download English Version:

<https://daneshyari.com/en/article/5547753>

Download Persian Version:

<https://daneshyari.com/article/5547753>

[Daneshyari.com](https://daneshyari.com)