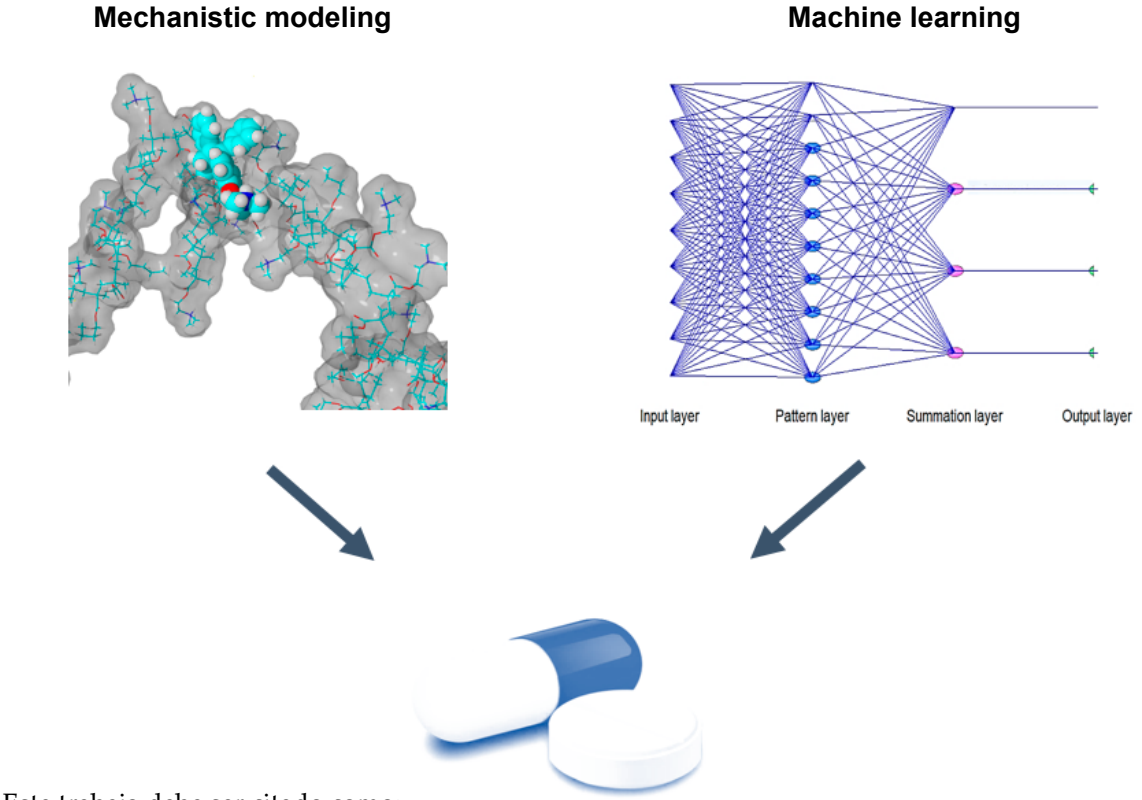
rescifar
REVISTA
ESPAÑOLA DE
CIENCIAS
FARMACÉUTICAS

Merits in computational pharmaceutics – selected case studies

Martin Kuentz

University of Applied Sciences and Arts
Northwestern Switzerland
HLS- Institute of Pharma Technology
martin.kuentz@fhnw.ch

The digital revolution is taking place in many fields, which includes the pharmaceutical sciences. Computational tools are these days increasingly used in pharmaceutics to define the formulation strategy or to guide the selection of excipients. Some of the computational approaches are entirely data-driven, while other computational calculations make use of mechanistic modeling. There is even an intermediate modeling strategy in which theoretical considerations help with the selection of molecular descriptors to setup a quantitative structure property relationship (QSPR). The presentation gives a brief introduction to the field before individual case studies of computational pharmaceutics are presented that cover data- and theory- driven approaches and there is also an example given of a theory-guided QSPR. Practical advantages of the different computational methods are discussed, while keeping the theoretical basics of the individual methods to a minimum. Finally, an outlook is provided of possible future research that would advance this thriving field of pharmaceutics.



Este trabajo debe ser citado como:

Martin Kuentz. Merits in computational pharmaceutics – selected case studies. Rev Esp Cien Farm. 2021;2(2):1.