Propuesta de Trabajo Fin de Máster
Año académico 2021-2022
MÁSTER EN MÉTODOS COMPUTACIONALES EN CIENCIAS

Project Nº 08

Título:
In silico toxicology: an overview of computational methods for the genotoxicity prediction of a series of bioactive compounds.

Departamento/ Laboratorio:
Departamento de Tecnología y Química Farmacéuticas (sección modelización molecular), en colaboración con Departamento Farmacología y Toxicología (unidad de Toxicología). Facultad de Farmacia y Nutrición. Universidad de Navarra.

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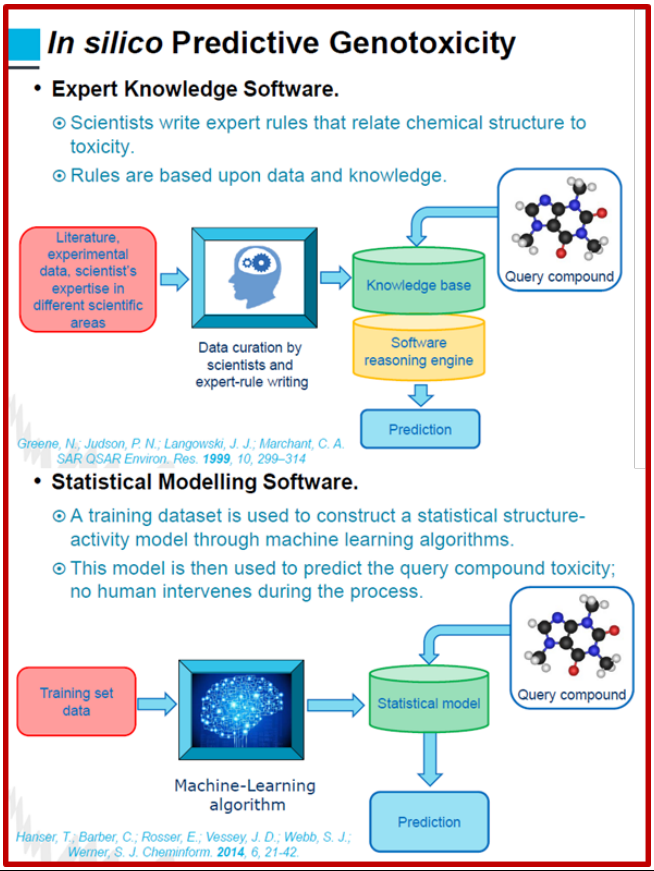
Resumen

It is necessary to determine the toxicity of chemicals (pharmaceuticals, cosmetics, food additives…) to identify their harmful effects on humans, animals, plants or the environment. Genotoxicity testing evaluates the damage caused to DNA that in turn might cause mutations or cancer. In fact, it is one of the critical steps in the design of any new substance to be launched into the market. Animal models have long been used for toxicity testing. However, tests on animals *(in vivo)* are limited by time, ethical and economic considerations. Therefore, computational methods to estimate the toxicity of chemicals are considered useful. *In silico* toxicology is a type of toxicity assessment that uses computational methods to analyze, simulate, visualize or predict the toxicity of chemicals. *In silico* toxicology aims to complement existing toxicity testing strategies to predict toxicity, prioritize chemicals, guide toxicity tests and minimize late-stage failures in the research and development of new molecules.



ASIGNATURAS OPTATIVAS RECOMENDADAS

1. **Métodos en química computacional**
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